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Wastewater Stabilization Ponds System: Parametric and Dynamic Global Sensitivity Analysis

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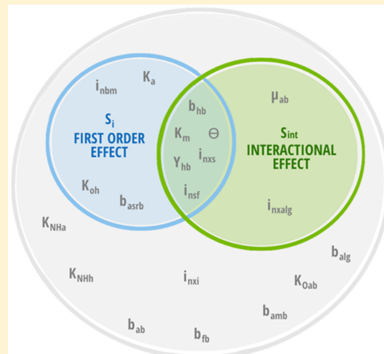
S *Supporting Information*

ABSTRACT: In this work, a global sensitivity analysis (GSA) is performed on a kinetic-dynamic model for a stabilization pond system, consisting of two aerobic ponds in series followed by a facultative one, to determine the most influential parameters of the model, as well as parameter ranking. GSA is implemented using Sobol's method, a variance-based technique which allows factor prioritization and factor fixing considering the whole range of parameter variation. The technique is implemented within the gPROMS platform, a differential algebraic equation oriented environment where stochastic simulations are performed. Time profiles for first order, total order, and interactional sensitivity indices are obtained for 72 differential state variables considering 20 parameters as uncertain. Numerical results provide useful information about the complex relationships between the variables of the wastewater treatment processes.



1. INTRODUCTION

In a previous work, a wastewater treatment network (WWTN) embedding rigorous models of different types of stabilization ponds was developed with synthesis and design purposes by Ochoa et al.[1] The model was formulated as a mixed integer nonlinear programming (MINLP) problem to establish both the optimal configuration system and pond dimensions necessary to fulfill environmental discharge regulations. In addition, different scenarios of inlet concentration of the organic load were explored to take into account process uncertainty leading to the conclusion that the model was highly influenced by the initial organic load.

In this paper, another type of uncertainty is considered, related to time-invariant model parameters such as kinetic parameters, whose uncertainty results from measurement errors or the impossibility of modeling accurately the physical behavior of a system. The values of the state variables can be greatly influenced by this type of uncertainty. For this reason, it is important to identify the parameters to which model state variables are most sensitive, which is achieved in general by a sensitivity analysis (SA). Techniques for sensitivity analysis can be classified into local and global. Local techniques provide a measure of the local effect of input variation on the model outputs by varying the model factors with respect to a nominal point usually carried out by computing partial derivatives of the output functions with respect to the input parameters one at a time,[2] whereas global sensitivity analysis (GSA) aims to quantify the relative importance of input parameters or factors in determining the value of an output variable considering their influence as a whole set. GSA methods should be used when the model is nonlinear, and various input variables are affected by uncertainties of different orders of magnitude, because they take into account the influence of the whole range of variation and the form of the probability density function in the input. GSA methods compute the effect of factor x_i while all others x_j, $j \neq i$, are varied as well. Time profiles of the influence of factors and input variables are obtained when dynamic models are analyzed, leading to a great insight on the sources of uncertainty during the time horizon.[3]

1.1. Literature Review. Most of the SA applications in the environmental modeling field are local and derivative-based due to the fact that these methods are computationally very efficient. However, local sensitivity analysis (LSA) methods can be misleading in the case of nonlinear models due to the requirements of linearity and additivity.[4] LSA does not allow identifying interacting or noninfluential factors. These limitations can be overcome by applying GSA, which can be classified into three types:

- Global screening methods: e.g., Morris screening method[5] and derivative-based global sensitivity measures (DGSM)[6]
- Regression/correlation-based methods: e.g., the standardized regression coefficients (SRCs) method[3]
- Variance-based methods: e.g., Sobol's method[7] and extended Fourier amplitude sensitivity testing (extended-FAST)[8,9]

Kiparissides et al.[10] compared the performance of two sensitivity methods, Sobol's method and the derivative-based global sensitivity measures (DGSM), based on the computational time. They applied both methods to a biological model of

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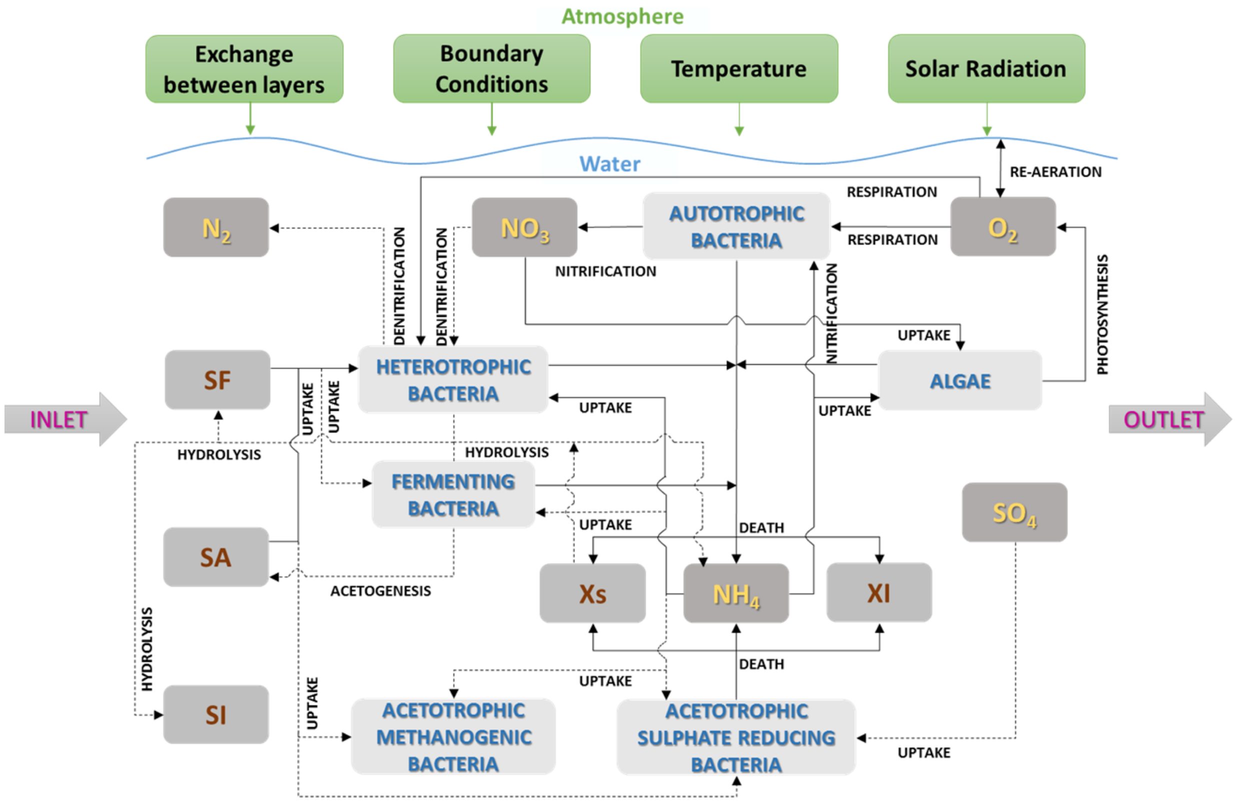

Figure 1. Scheme of the facultative pond model. Biomass variables: heterotrophic, autotrophic, fermenting, acetotrophic sulfate reducing and acetotrophic methanogenic bacteria; and algae. Nutrients: soluble nitrogen, ammonium and ammonia nitrogen, nitrate and nitrite nitrogen, dissolved oxygen, and sulfate sulfur. Organic load: fermentation products; fermentable, readily biodegradable soluble COD; inert soluble COD; inert particulate COD and slowly biodegradable particulate COD. → indicates aerobic processes; - - - → indicates anaerobic processes.

moderate complexity (5 differential variables and 16 parameters) at three specific times, and they found agreement between the obtained results, with Sobol's method being much more computationally expensive. They performed the same analysis over a more realistic model with 15 differential variables and 33 parameters. However, in this case the analysis was done over 5 groups of uncertain parameters instead of the individual parameters.

Especially in the field of wastewater modeling, Sin et al.[11] performed linear regression on Monte Carlo simulation output, also known as standardized regression coefficient, as a sensitivity analysis method in the benchmark simulation model no. 1 plant layout,[12] considering three different scenarios of uncertainty sources by taking into account 26, 7, and 33 uncertain factors, respectively. The sensitivity analysis results are conditional to the way the problem is framed; hence, results should be interpreted within the context. It was found that the method is able to decompose satisfactorily the variance performance criteria for sludge production, energy demand, and effluent nitrate and ammonium concentration. The SRC is an intuitive and simple method and relatively straightforward to perform. Nevertheless, it still requires the resulting system to be linear or at least linearizable.

Cosenza et al.[13] compared three global sensitivity analysis (GSA) methods to assess the most relevant processes occurring in wastewater treatment systems. In particular, the SRC, Morris screening, and extended-FAST methods are applied to a complex highly nonlinear integrated membrane bioreactor model considering 21 model outputs and 79 model factors. The use of multiple sensitivity analysis methods in a GSA study allows increasing the accuracy of the conclusions. Using the three methods simultaneously is extremely computational expensive, but it allowed identification of problems with Morris screening as the two other methods provided consistent results, even though the SRC method was applied outside its range of applicability.

Chen et al.[14] applied the extended Fourier amplitude sensitivity test to the activated sludge model 3[15] extended with the incorporation of the soluble microbial products (SMP) concept and simultaneous growth and storage phenomenon in membrane bioreactors, considering 29 model uncertain factors. The study quantified the uncertainty involved in predicting the biological process at different sludge retention times (10, 30, and 50 day), including sludge production, organic removal, SMP production, and nitrification efficiency. It was found that the interpretation of sensitivity analysis results depended much on the framing of the analysis, in this case the operating SRT.

Only temporal behavior of the sensitivity indices was studied by Estrada et al.,[16] Gambonis et al.,[17] and Massmann and Holzmann[18] on hydrologic complex models; by Di Maggio et al.[19] on a metabolic network model; and by Ochoa et al.[20] on bioreactor networks for a bioethanol production model. However, the spread of the GSA applications has been limited due to their high computational costs. A detailed review of GSA in environmental modeling can be found in Mammina et al.[4]

In this work, the implemented GSA strategy is variance-based[7] and allows the determination and classification of model parameters, according to their sensitivity indices through factor prioritization (FP) and factor fixing (FF) settings. The wastewater stabilization pond network model and the GSA

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methodology were implemented in an equation oriented environment with a differential algebraic equation solver in gPROMS.[21] Time profiles of first order effect sensitivity indices, total sensitivity indices, and those due to interactions with other model parameters have been calculated for 20 uncertain kinetic parameters in a model for a wastewater stabilization pond system. Numerical results show that the higher computational cost of global sensitivity analysis is thoroughly justified, because first order effects caused by the variation of one parameter alone can be captured, as well as the effects arising from interaction with other model parameters.

2. METHODOLOGY

2.1. Wastewater Stabilization Pond Model. The differential algebraic equation system represents three stabilization ponds in series for biological wastewater treatment. The system is composed by two aerobic ponds in series followed by a facultative one. A flowchart of the process involved in the biochemical model of the facultative pond is given in Figure 1 (which can also represent an aerobic pond if all anaerobic processes are neglected).

Differential equations include dynamic mass balances for the prevailing groups of bacteria: heterotrophic, autotrophic, fermenting, acetotrophic sulfate reducing and acetotrophic methanogenic bacteria, algae biomass, the different sources of organic matter, and main nutrients.

$$\frac{dV_i}{dt} = Q_i^{\,in} - Q_i^{\,out} + Q_i^{\,prec} - Q_i^{\,evap} \tag{1}$$

$$\frac{dC_{X,ij}}{dt} = \frac{Q_i^{\,in}C_{x,i}^{in} - Q_i^{\,out}C_{X,ij}}{V_{ij}} + F_{X,ij} - \frac{k_m A_i}{\Delta h_{ij}\cdot V_{ij}}(C_{X,ij} - C_{X,ij+1}) - \frac{C_{X,ij}}{h_{ij}}\frac{dh_{ij}}{dt} \; j = 1 \tag{2}$$

$$\frac{dC_{X,ij}}{dt} = F_{X,ij} + \frac{k_m A_i}{\Delta h_{ij} V_{ij}}(C_{X,ij-1} - C_{X,ij}) \; j = 2 \tag{3}$$

The subscripts i, j, and X refer to the pond, the layer, and the variables related to organic load, nutrients, and biomass in the Nomenclature list. Q_i^{in}, Q_i^{out}, Q_i^{prec}, and Q_i^{evap} stand for volumetric flow (m^3/d). $C_{X,ij}$ is the concentration of component X related to pond i at layer j (g_x/m^3); V_{ij} is the pond volume i of the layer j (m^3). A_i (m^2) and h_i (m) are the area and height of the pond i, respectively. Δh_i (m) is the distance between half height of the upper layer and half height of the lower layer, and k_m stands for the transfer mass coefficient between layers in the facultative pond. $F_{X,ij}$ is reaction rate of component X in layer j of pond i. The facultative type pond has two layers to account for the different conditions within it. Therefore, transfer between layers only occurs in this type of pond. The height of the lower layer is assumed to be constant.

Algebraic equations of the model describe pond interconnections, forcing functions (such as temperature; irradiance; inlet, precipitation, and evaporation flow rates; and inlet concentration of organic load and nutrients), and reaction rates of the processes. Kinetic expressions of the reaction rates and nominal values of stoichiometric coefficients were taken from Sah et al.[22] Process equations and generation and consumption terms of the mass balances can be found in Tables S1 and S2 of the Supporting Information.

2.2. Global Sensitivity Analysis Technique. In this work, global sensitivity indices are computed following Sobol's methodology. This method is based on variance decomposition, using Monte Carlo simulation.[23,24]

The main features of variance-based methods are the independence of the model structure, the capability to analyze the influence of each factor within its entire range and to quantify the interaction among factors.[3] Given a function $y = f(x, t)$, where y is a differential or algebraic state variable (e.g., heterotrophic bacteria concentration), x is a vector of k input parameters, and t is the independent variable in differential equations, e.g., time, when all uncertain parameters x_i vary under its probability density function, the uncertainty in $y(x, t)$ can be quantified by its unconditional variance $V(y, t)$. It can always be decomposed as the sum of the variance of a conditional expected value and the expected value of a conditional variance, such conditioning with respect to both x_i and all parameters except x_i (x_{-i}).[25]

$$V(y, t) = V(E(y|x_i, t)) + E(V(y|x_i, t)) \tag{4}$$

$$V(y, t) = V(E(y|x_{-i}, t)) + E(V(y|x_{-i}, t)) \tag{5}$$

Equations 4 and 5 are two ways of computing the same unconditional variance. V and E correspond to variance and expected value operators, respectively. In eq 4, $V(y, t)_i = V(E(y|x_i, t))$ computes the variance (over all possible realizations of parameter x_i) of the conditional expected value of the state variable y under all parameter variations, except x_i. It represents the expected reduction in the state variable variance that would be obtained if x_i could be known or fixed. $V(y, t)_i$ is the first order effect associated with parameter x_i. The residual effect, $E(y, t)_i = E(V(y|x_i, t))$, is the expected value (over all realizations of parameter x_i) of the conditional variance of the state variable y when all parameters except x_i change. It represents the average state variable variance if x_i could be known or fixed.

The same can be stated for eq 5, by replacing x_i for "all parameters except x_i" (x_{-i}). Thus, the term $V(y, t)_i^{tot} = V(E(y|x_{-i}, t))$, which is found by combining eqs 4 and 5 due to its computationally expensive calculation by definition, computes the average state variable variance if all parameters except x_i could be known or fixed. If eqs 4 and 5 are normalized, the first order sensitivity index, $S(y, t)_i$, and the total sensitivity index $S(y, t)_i^{tot}$ are defined as

$$S(y, t)_i = \frac{V(E(y|x_i, t))}{V(y, t)} = \frac{V(y, t)_i}{V(y, t)} \tag{6}$$

$$S(y, t)_i^{tot} = \frac{E(V(y|x_{-i}, t))}{V(y, t)} = \frac{V(y, t)_i^{tot}}{V(y, t)} \tag{7}$$

First order ($S(y, t)_i$) and total effect ($S(y,t)_i^{tot}$) indices measure the effect of the variation of the parameters on the model state variables. First order sensitivity indices provide the reduction on the unconditional variance of the state variable that can be obtained if x_i is fixed at its true value. On the other hand, total sensitivity indices take into account the interactions among parameters, providing information on the nonadditive part of the model.

The interactional sensitivity index is defined by the difference between the total sensitivity index and the first order sensitivity index.[16,19]

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$$S_{\mathrm{int},i} = S_i^{\mathrm{tot}} - S_i \tag{8}$$

For example, given a function $f(A, B, C)$, its sensitivity indices can be represented as shown in Figure 2.

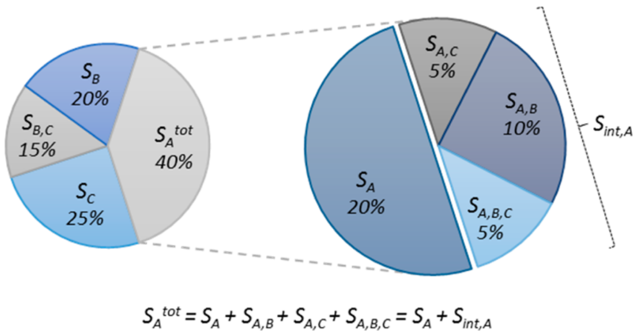

Figure 2. Graphical representation of the different types of indices.

Variance-based methods allow prioritization of factors, factors with high values of S_i, and factor fixing. Only when S_i^{tot} values are small can the factor be fixed anywhere within its range of variation. Indeed, if the S_i values are small but S_i^{tot} values are high, the factor is important through its interactional effects.

To calculate sensitivity indices, it is necessary to compute the unconditional and conditional variances of each state variable, involving the calculation of multiple integrals. However, the variances can be computed considering only Monte Carlo simulations of the model; a detailed demonstration of the method can be found in Sobol's work.[23] Saltelli et al.[26] compiled and also suggested estimators for first order and total effect sensitivity indices.

Allan variance, based on two samples, is used to compute the unconditional variance.

$$V(Y) = \frac{1}{2N}\sum_{N}^{j=1}(y_{A_j} - y_{B_j})^2 \tag{9}$$

Here, A, B, C_i, and D_i are matrices of dimension $(N \times k)$. N the sample size used for the Monte Carlo estimate, and k is the number of uncertain model parameters.

$$A = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1k} \\ x_{21} & x_{22} & \dots & x_{2k} \\ \dots & \dots & \dots & \dots \\ x_{N1} & x_{N2} & \dots & x_{Nk} \end{bmatrix} \tag{10}$$

$$B = \begin{bmatrix} x'_{11} & x'_{12} & \dots & x'_{1k} \\ x'_{21} & x'_{22} & \dots & x'_{2k} \\ \dots & \dots & \dots & \dots \\ x'_{N1} & x'_{N2} & \dots & x'_{Nk} \end{bmatrix} \tag{11}$$

$$C_i = \begin{bmatrix} x'_{11} & x'_{12} & \cdots & x_{1i} & \cdots & x'_{1k} \\ x'_{21} & x'_{22} & \cdots & x_{2i} & \cdots & x'_{2k} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ x'_{N1} & x'_{N2} & \cdots & x_{Ni} & \cdots & x'_{Nk} \end{bmatrix} \tag{12}$$

$$D_i = \begin{bmatrix} x_{11} & x_{12} & \cdots & x'_{1i} & \cdots & x_{1k} \\ x_{21} & x_{22} & \cdots & x'_{2i} & \cdots & x_{2k} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{N1} & x_{N2} & \cdots & x'_{Ni} & \cdots & x_{Nk} \end{bmatrix} \tag{13}$$

Each column of both A and B matrices is a sample from the distribution function of the uncertain parameter. Each row is an input sample, for which a model output y can be evaluated. A is considered the "sample" matrix, and B is the "resample" matrix. C_i is the matrix where all parameters except x_i are resampled, whereas D_i is the matrix where only x_i is resampled. y_A and y_B are vectors of N model outputs values obtained when model variables are evaluated with matrices A and B, whereas y_{Ci} and y_{Di} are matrices of kN model evaluations from C_i and D_i, respectively. Thus, the total number of model evaluations is $N(2k + 2)$.

The dimensionality of the sensitivity analysis problem is defined by the number of model parameters k, which together with the number of scenarios determine the number of model evaluations required for the Monte Carlo integrals to converge, limited only by the computational cost. The wastewater stabilization pond system model studied is composed of 61 parameters and 72 differential equations, leading to a problem of high dimensionality. In order to reduce the dimensionality of the problem, a two-step procedure including a factor screening by using a local method followed by a GSA step of the important factors identified during the first step is implemented as suggested by Mannina et al.[4]

To perform this calculation, local sensitivity indices are computed as the first partial derivative of model output variables with respect to the uncertain parameter, varying each parameter one at a time and using the finite difference method. Then, parameters are ranked on the basis of their sensitivity index values and their frequency of relevance over all differential variable output.

Table 1. Formulas To Compute S_i and S_i^{tot} for the Output Variables y at Each Instant of Time t

first order index	ref	total order index	ref
$S_i = \dfrac{\frac{1}{N}\sum_{j=1}^{N} y_{A_j} y^i_{C_j} - y_A^{\ 2}}{V(Y)}$	7	$S_i^{\mathrm{tot}} = \dfrac{V(Y) - \frac{1}{N}\sum_{j=1}^{N} y_{A_j} y^i_{D_j} + y_A^{\ 2}}{V(Y)}$	28
$S_i = \dfrac{\frac{1}{N}\sum_{j=1}^{N} y_{B_j}(y^i_{D_j} - y_{A_j})}{V(Y)}$	26	$S_i^{\mathrm{tot}} = \dfrac{\frac{1}{N}\sum_{j=1}^{N} y_{A_j}(y_{A_j} - y^i_{D_j})}{V(Y)}$	29
$S_i = \dfrac{V(Y) - \frac{1}{2N}\sum_{j=1}^{N}(y_{B_j} - y^i_{D_j})^2}{V(Y)}$	27	$S_i^{\mathrm{tot}} = \dfrac{\frac{1}{2N}\sum_{j=1}^{N}(y_{A_j} - y^i_{D_j})^2}{V(Y)}$	27

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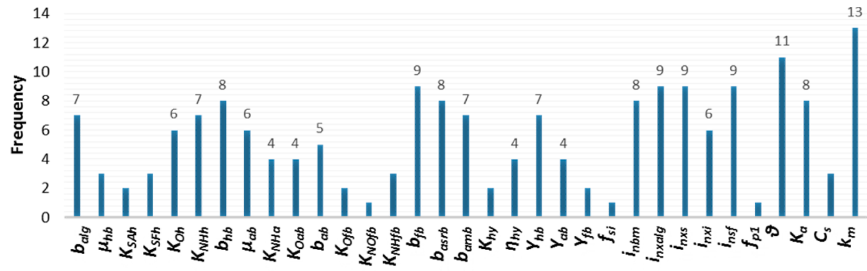

Figure 3. Local sensitivity analysis results: frequency of parameter influence over the differential variables (zero frequency parameters are not shown).

The problem still has associated a great dimensionality with it and cannot be solved in a straightforward way, as was done by the authors in a previous work when considering smaller models.[20] Therefore, the problem has to be divided. First, 20 runs of stochastic simulations of 100k uncertain parameters scenarios must be solved, each one within a gPROMS platform (10 runs are performed to calculate S_i and 10 runs to calculate S_i^{tot}). The random samples for each one of the 20 runs are derived from a single large random sample generated in Excel, which is subsequently fragmented into 20 subsets. The total number of sampled points is 40 000.

Then, results are exported to a Fortran 90 environment to calculate the global sensitivity indices at each instant of time for the different estimators (listed in Table 1). It is necessary to generate the random sample matrices in Excel and then import them to the gPROMS platform, because gPROMS always seeds the random number generator with the same value each time a stochastic simulation is started in order to allow reproducible results.[21] Previous versions of the software had the possibility to generate irreproducible type random numbers, using a seed value derived from the system clock.[30]

3. NUMERICAL RESULTS

In this work, dynamic global sensitivity analysis (DGSA) is performed on the model presented in Section 2.1. Model inputs are given by polynomial functions representing wastewater stream flow rate, organic load, nutrient content, temperature, irradiance, etc.

As explained in Section 2.2, for reduction of the size of the problem, a local sensitivity analysis is performed. Figure 3 shows the frequency plot for the parameters which generate local sensitivity indices with absolute values greater than 1. All model parameters are described in the Nomenclature list, and a subset of the 20 parameters that are most locally influential is identified and listed in Table 2.

As a first step, normal probability distributions have been associated with each parameter, as these types of distributions have been frequently related to parameters for ecological water models in the literature.[16,31−33] For the generation of the sample matrices, N = 1000 scenarios are considered. The time horizon is set to an operating time of 12 days. Sensitivity indices profiles are calculated for 72 differential variables, corresponding to component concentrations in each pond of the wastewater biological treatment system (aerobic−aerobic−facultative) and each layer of the facultative pond, considering 20 uncertain parameters. Numerical results show that two parameters can explain most of the differential state variable variance: the coefficient in the temperature limiting function (θ) and the mass transfer coefficient between layers in several variables of the facultative pond (k_m), whose influence is summarized in the radial plots of Figure 4. The presented results correspond to the first order estimator and total estimator proposed by Jansen.[27]

Table 2. Uncertain Parameters[a]

uncertain parameter	description	unit	nominal value
θ	coeff in the temp limiting function		1.070
k_m	mass transfer coeff between layers in facultative pond	m^2/d	0.022
i_{nxs}	fraction of nitrogen in slowly biodegradable particulate COD, C_{Xs}	g_N/g_{COD}	0.040
i_{nsf}	fraction of nitrogen in fermentable, readily biodegradable soluble COD, C_{sf}	g_N/g_{COD}	0.030
K_{NHh}	saturation/inhibition coeff of ammonium and ammonia nitrogen, C_{NH4}, for heterotrophic bacteria, C_{hb}	g_N/m^3	0.050
K_{NHa}	saturation/inhibition coeff of ammonium and ammonia nitrogen, C_{NH4}, for autotrophic bacteria, C_{ab}	g_N/m^3	0.200
b_{ab}	decay rate of autotrophic bacteria, C_{ab}	d^{-1}	0.015
b_{fb}	decay rate of fermenting bacteria, C_{fb}	d^{-1}	0.020
b_{asrb}	decay rate of acetotrophic sulfate reducing bacteria, C_{asrb}	d^{-1}	0.012
b_{amb}	decay rate of acetotrophic methanogenic bacteria, C_{amb}	d^{-1}	0.008
i_{nxalg}	fraction of nitrogen in algae	g_N/g_{CODalg}	0.063
b_{hb}	decay rate of heterotrophic bacteria, C_{hb}	d^{-1}	0.400
i_{nbm}	fraction of nitrogen in bacteria	g_N/g_{CODbm}	0.070
K_a	rate of reaeration	d^{-1}	0.230*
b_{alg}	decay rate of algae, C_{alg}	d^{-1}	0.100
Y_{hb}	yield factor for heterotrophic bacteria, C_{hb}	g_{CODbm}/g_{CODsf}	0.630
K_{Oh}	saturation/inhibition coeff of oxygen, C_{O2}, for heterotrophic bacteria, C_{hb}	g_{O2}/m^3	0.200
μ_{ab}	max growth rate of autotrophic bacteria, C_{ab}	d^{-1}	2.000
i_{nxi}	fraction of nitrogen in slowly biodegradable particulate COD, C_{XI}	g_N/g_{CODxi}	0.030
K_{Oab}	saturation/inhibition coeff of oxygen, C_{O2}, for autotrophic bacteria, C_{ab}	g_{O2}/m^3	0.500

[a]Range of variation 12.5%, except K_a (*) which is 27.5% (to account for important variations in the literature).

In order to validate results, the same global analysis is performed including 5 random parameters, which had been considered noninfluential by the local analysis. Unconditional variances for all variables of both global analyses are calculated and compared to the values without considering the neglected parameters. Almost 90% of the obtained values vary less than 15%. This slight variation corroborates the previous classification.

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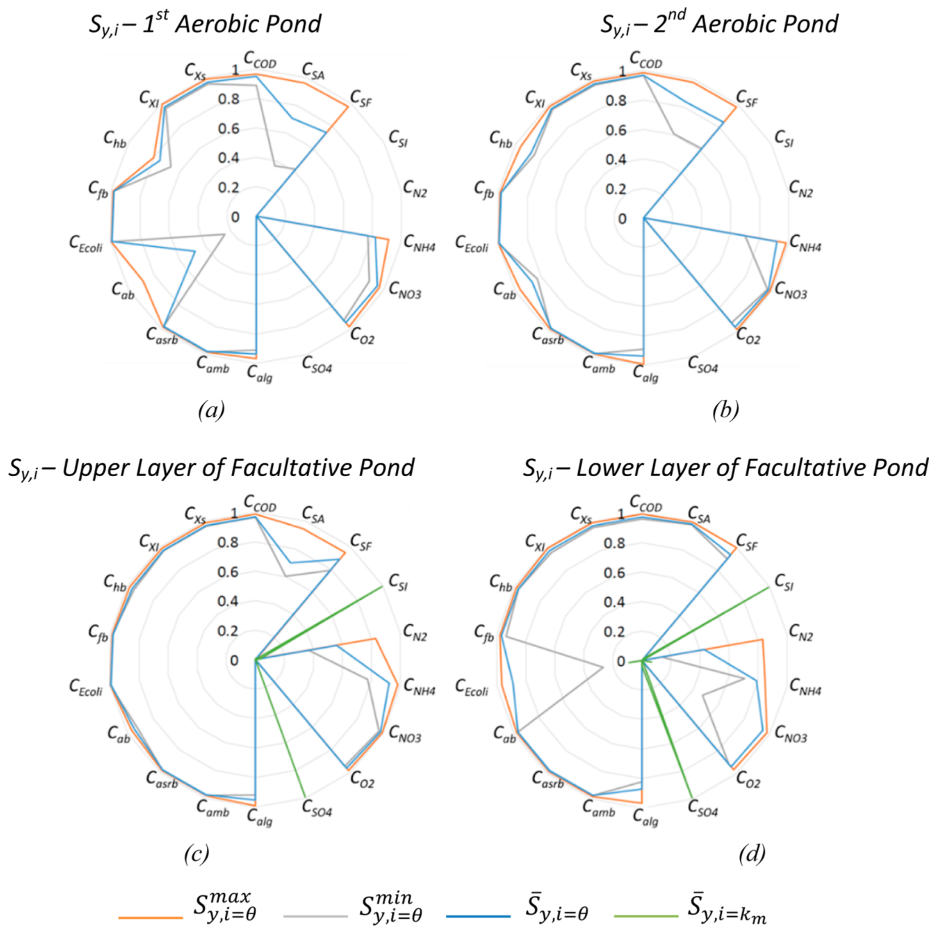

Figure 4. Maximum ($S_{y,i}^{\max}$), minimum ($S_{y,i}^{\min}$), and time average ($\bar{S}_{y,i}$) for the first order sensitivity indices for the coefficient in the temperature limiting function (θ) for the first aerobic pond 1 (a) and for the second aerobic pond 2 (b) state variables. For the upper (c) and lower (d) layers of the facultative pond, the time average sensitivity indices $\bar{S}_{y,i}$ for the mass transfer coefficient between layers (k_m) are also shown.

3.1. Factor Prioritization and Factor Fixing Settings. To obtain accurate predictions with complex mathematical models that involved environmental variables, good modeling practice includes calibration of the model to site-specific experimental data. To select the indicated input factors to be estimated from the large number of the wastewater treatment system (WWTS) model parameters, previous to the calibration, it is necessary to determine which ones produce the largest expected reduction in the variance of the model outputs.[24] On the basis of the first order sensitivity index values, the factor prioritization allows performing a ranking of the most influential parameters of the model which will be included in the parameter estimation problem.

Factor prioritization for the numerical results of the DGSA of this work indicates that, despite the model complexity, only two parameters (θ and k_m) explain a large percentage of the output model uncertainty. The ranges of expected reduction in the output variance if θ is fixed to its true value are 100%−67%, 100%−61%, and 100%−13% for the aerobic pond 1, aerobic pond 2, and facultative pond, respectively. Figure 4a−d shows maximum, minimum, and time average value of first order sensitivity indices for all differential variables with respect to the two most influential uncertain parameters (θ and k_m). Figure 4a,b presents maximum, minimum, and time average values of the first order indices for the temperature coefficient ($S_{y,i=\theta}$) in aerobic ponds. It can be seen that, for organic matter concentration (C_{COD}) for the first aerobic pond, θ explains almost all output variance through the time horizon reaching S_i maximum, minimum, and time average values of 0.966, 0.889, and 0.949, respectively. S_i for θ for autotrophic bacteria concentration (C_{ab}) reaches a maximum value of 0.885, a minimum of 0.247, and a time average value of 0.478 in the same pond (Figure 4a).

Furthermore, Figure 4a−d shows that first order effects are mainly dominated by temperature coefficient θ for 15 of the 18 studied differential variables of each pond. This parameter is also influential through interactional effects with the remaining parameters (see Supporting Information, Table S4). For other ecological systems, the adjustment temperature parameters also show a great influence. This is actually an expected and intuitive result because of the great influence of temperature on growth and related processes carried out by the communities of modeled microorganisms.[16] Therefore, focusing efforts on a more accurate determination of this parameter can lead to important reductions in the unconditional variance of the differential state variables describing the WWTS. In most state variables (Figures 5a,c, 6a, 7a,c, 8a,c, and 9a), first order effects of θ are greater at the beginning and decrease over time reaching a minimum value at the end of the simulation. As the influence of θ decreases, there is a slight increase in the first effects of other parameters as well as in interactions between parameters.

Figure 4a,b also shows that first order sensitivity indices of θ for C_{N2}, C_{SO4}, and C_{SI} are null in the aerobic ponds. This is

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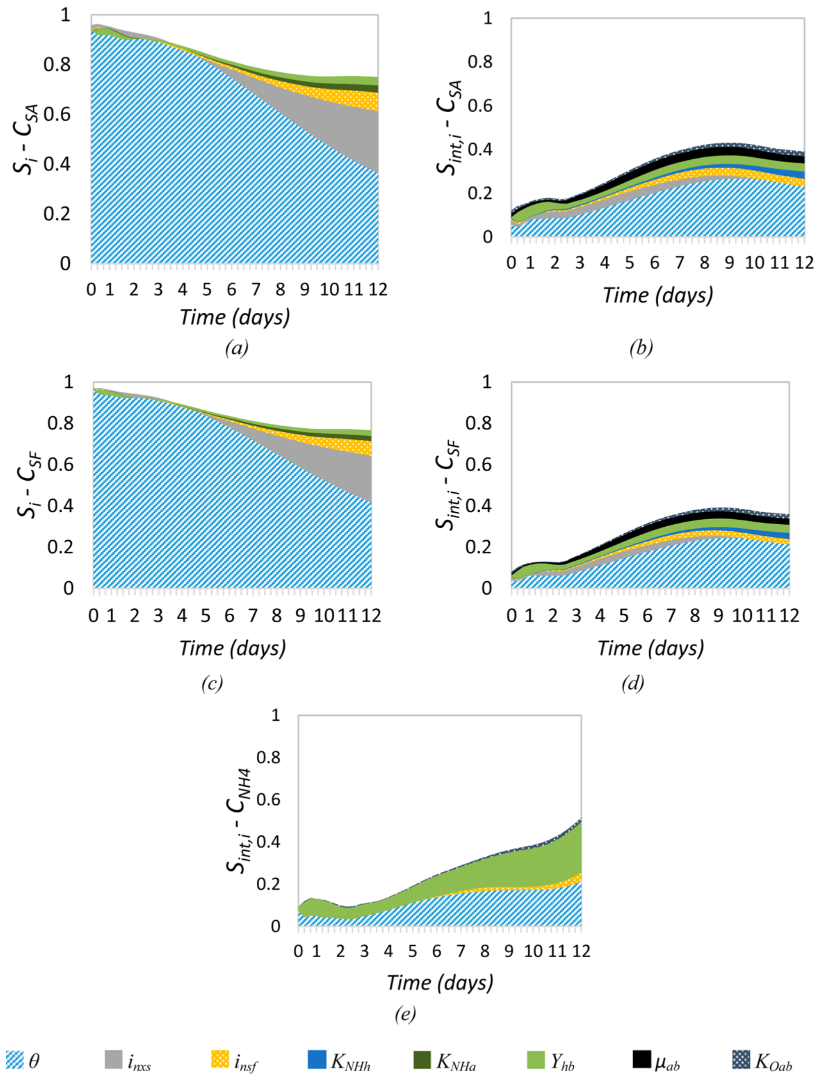

Figure 5. Aerobic pond 1: First order and interactional sensitivity indices profiles for fermentation products (C_{SA}) (a, b) and fermentable, readily biodegradable soluble COD (C_{SF}) (c, d) concentrations, and interactional sensitivity index profile for ammonium and ammonia nitrogen concentration (C_{NH4}) (e).

because the two former compounds are only produced by anaerobic microorganisms and the latter is only involved in the hydrolysis process, which takes place within an anaerobic environment. A relevant parameter for C_{SO4} and C_{SI} is the mass transfer coefficient between layers (k_m), in the facultative pond (Figure 4c,d), reaching reductions in the output expected variance up to 100% if k_m would be fixed to its true value. Another important result is setting the list of model parameters that can be fixed anywhere in their range of variation, without effects on the model output variance (factor fixing).[24,28] Null or small total sensitivity index values indicate that parameters K_{NHh}, K_{NHa}, K_{Oab}, b_{ab}, b_{fb}, b_{amb}, b_{alg}, and i_{nxi} are irrelevant and can be fixed to their actual nominal values.

For a more detailed discussion of results, cumulative plots are presented for first order and interaction sensitivity indices time profiles of the main differential variables describing the wastewater treatment system, where interactional effects are stronger and whose variance is composed by other parameters rather than θ and k_m (Figures 5–9). A detailed description is given for each pond.

A complete report of first order and interaction indices (maximum, minimum, and time average value) for the entire wastewater stabilization pond system is presented in Tables S3 and S4 of the Supporting Information.

3.2. Aerobic Pond 1. The first pond receives the wastewater stream with the highest organic load concentration. This fact has an impact on the sensitivity indices profiles, leading to higher interactional effects among the parameters within the pond. Figures 5 and 6 show time profiles for the main indices in this pond.

As already mentioned, first order effects are dominated by the temperature coefficient θ throughout the entire operating time (Figures 5a,c and 6a,c). It also dominates the interactional effects, as can be appreciated in Figures 5b,d,e and 6b,d.

Regarding fermentation products (C_{SA}) and fermentable, readily biodegradable soluble COD (C_{SF}) concentration, similar sensitivity indices profiles are obtained (Figure 5a–d), because similar kinetics describe the processes in which these components are involved. Another relevant parameter (apart from θ) is the fraction of nitrogen in slowly biodegradable particulate COD, i_{nxs}, which represents up to 25% of the total variances for both state variables with greater influence at the end of the time horizon. It is followed in importance by the fraction of nitrogen in fermentable, readily biodegradable

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Ind. Eng. Chem. Res. 2016, 55, 11403–11416

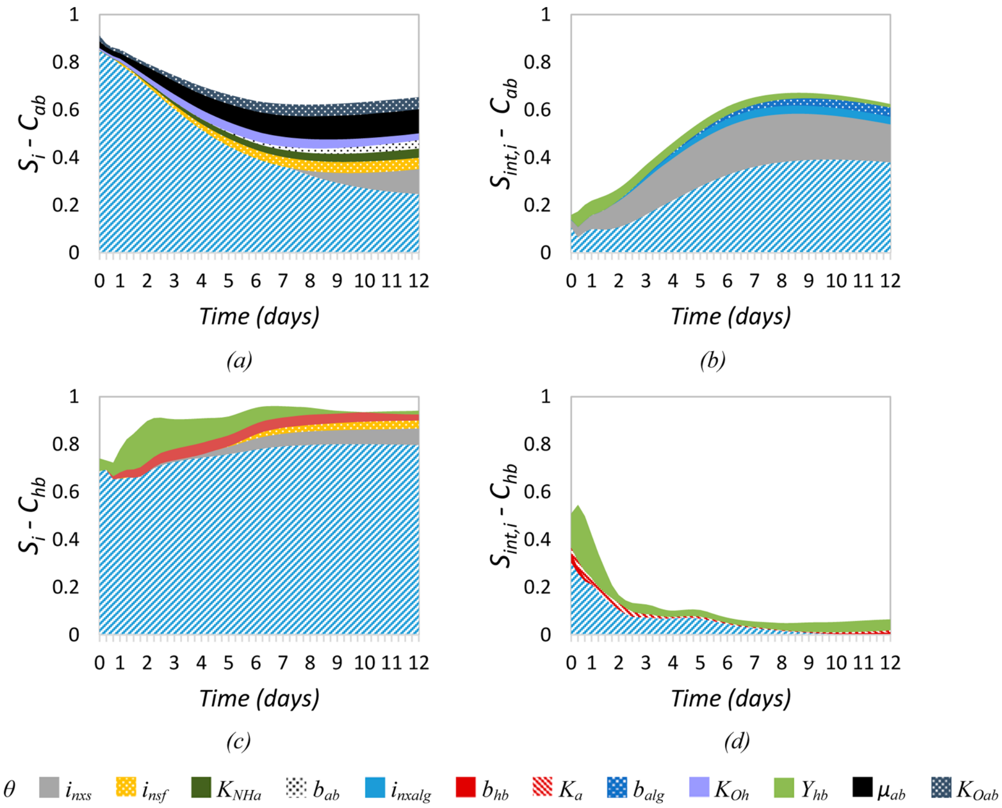

Figure 6. Aerobic pond 1: First order and interactional sensitivity indices profiles for autotrophic (C_{ab}) (a, b) and heterotrophic bacteria (C_{hb}) (c, d) concentrations.

soluble COD, i_{nsf}, which means up to 7.5% of the variables variances. The yield factor for heterotrophic bacteria, Y_{hb}, and the saturation/inhibition coefficient of ammonium and ammonia nitrogen for autotrophic bacteria, K_{NHa}, have little contribution to total variance output, up to 3.5%.

Interactional effects are again dominated by θ, reaching $S_{int,i}^{max}$ values of 0.25 (Figure 5b,d). There is also some influence of the yield factor for heterotrophic bacteria, Y_{hb}, and the maximum growth rate of autotrophic bacteria, μ_{ab}, during the complete operating time. Parameters which have slight influence through interactions are i_{nxs}, i_{nsf}, K_{NHa} (saturation/inhibition coefficient of ammonium and ammonia nitrogen for autotrophic bacteria), and K_{Oab} (saturation/inhibition coefficient of oxygen for autotrophic bacteria), with $\overline{S}_{int,i}$ values ranging from 0.011 to 0.022.

Figure 5e shows the interactional sensitivity indices profile for ammonium and ammonia nitrogen concentration (C_{NH4}). In this case, interactional effects are dominated almost equally by Y_{hb} and θ, with maximum $S_{int,i}$ values of 0.24 and 0.21, respectively. Parameters μ_{ab} and K_{Oab} also contribute, but to a lesser extent.

Regarding biomass related variables, sensitivity indices profiles are shown in Figure 6 for autotrophic (C_{ab}) and heterotrophic bacteria (C_{hb}) concentrations. In the case of C_{ab}, its variance is composed of the contribution of several parameters. θ contributes up to 88.5% at the beginning of the process, with a time average value of 48%. It is followed by i_{nxs} and μ_{ab} meaning up to 10% each one of the output variance at the end of the process. K_{Oab}, K_{Oh}, and i_{nsf} contribute with a time average value around 3.5% each. Finally, there is a little contribution of K_{NHa} and b_{ab}. There are strong interactional effects contributing to autotrophic bacteria concentration variance, reaching a maximum value of $\sum S_{int,i}$ of 0.7, as can be seen in Figure 6b. They are mainly described by θ and i_{nxs} during the entire time horizon. There are also small contributions to interactional effects of Y_{hb}, b_{alg}, and i_{nxalg}.

In the case of heterotrophic bacteria concentration (C_{hb}), θ dominates first order effects, with an average time value of 75.5%, and Y_{hb} contributes up to 17.2% especially at the beginning of the process. They are followed in importance by b_{hb} and i_{nxs}, with $\overline{S}_i$ of 0.04 and 0.036, respectively, and there is a small contribution of i_{nsf}.

C_{hb} also presents strong interactional effects ($\sum S_{int,i}$ up to 0.6) at the beginning of the operation horizon (Figure 6d). These effects are described by θ and Y_{hb}, which reach a $S_{int,i}^{max}$ of 0.303 and 0.235, respectively, whereas their $\overline{S}_{int,i}$ is 0.064 for the former and 0.05 for the latter one. Finally, there is a little contribution of b_{hb} and K_a to the interactional effects.

3.3. Aerobic Pond 2.

The second pond of the treatment system is also aerobic, with a lower level of organic matter because it receives treated wastewater from the first aerobic pond output.

First order and interactional sensitivity indices profiles for C_{SA} and C_{SF} are similar to those obtained for the first aerobic pond. However, variance contribution from θ is larger, and fewer parameters contribute to these state variables variances. First order effects for both variables are dominated by θ, with $\overline{S}_i$ around 0.85; i_{nxs} reaches a value of 0.102 at the end of the time horizon. Also, i_{nsf} and Y_{hb} contribute to the output variances up to 2.7% (Figure 7a,c). The interactional effects are lower for this pond than the first one, reaching a $\sum S_{int,i}$ of 0.4. Again, θ is the most relevant parameter through interactions, with $\overline{S}_{int}$ of 0.12. A similar contribution is obtained for i_{nxs}, μ_{ab}, Y_{hb}, and i_{nsf} with $S_{int,i}^{max}$ around 0.035, as can be seen in Figure 7b,d.

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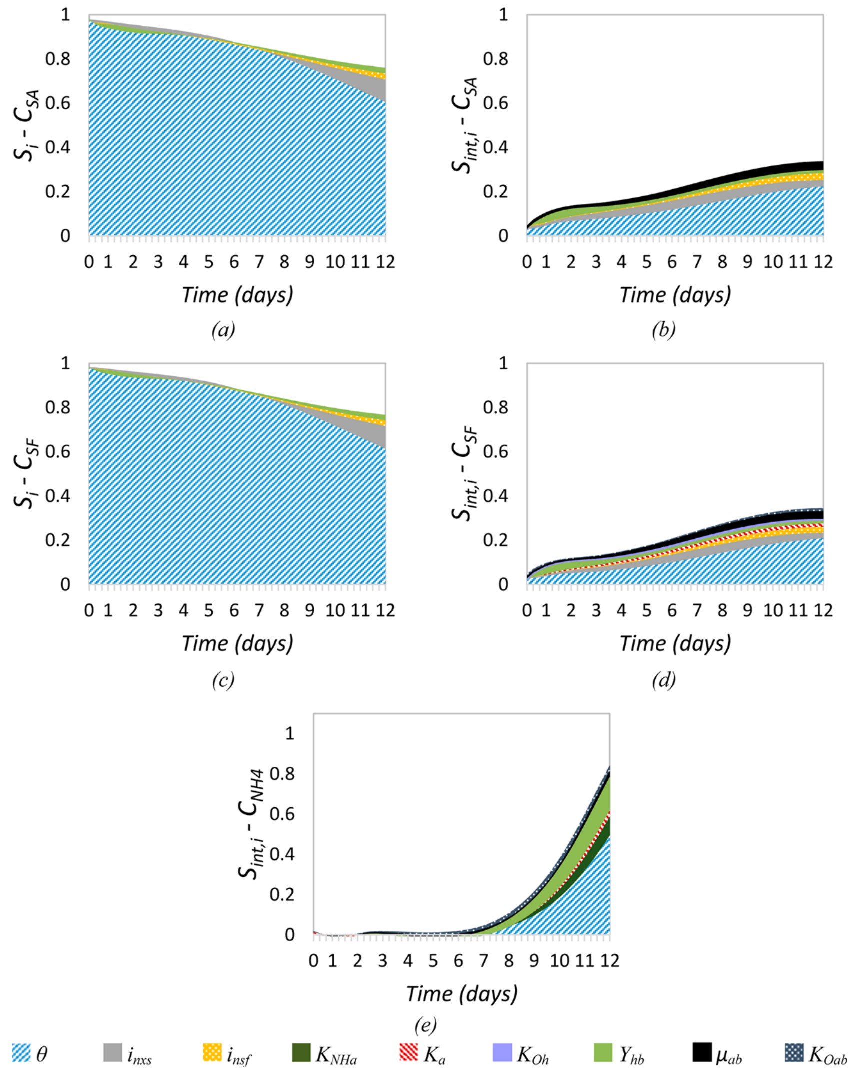

Figure 7. Aerobic pond 2: First order and interactional sensitivity indices profiles for fermentation products (C_{SA}) (a and b) and fermentable, readily biodegradable soluble COD (C_{SF}) concentrations (c and d); interactional sensitivity index profile for ammonium and ammonia nitrogen concentration (C_{NH4}) (e).

In the case of C_{NH4} sensitivity interactional indices profiles, the growing influence at the end of the process is repeated, as shown in Figures 5e and 7e. Even when $\sum S_{int,i}$ reaches a value of 0.8, the effects are concentrated in a short period of time, with $S_{int,i}^{max}$ of θ of 0.5, followed in relevance by Y_{hb} ($S_{int,i}^{max}$ = 0.17) and K_{NHa} ($S_{int,i}^{max}$ = 0.095). Also, a small contribution of K_a, μ_{ab}, and K_{Oab} can be noted.

Heterotrophic (C_{hb}) and autotrophic bacteria concentration (C_{ab}) sensitivity indices profiles are not shown for this pond, because they are mostly dominated by θ, as it can be appreciated in the radial plot of first order indices in Figure 4b and in Tables S3 and S4 of the Supporting Information.

3.4. Upper Layer of Facultative Pond. The facultative pond receives the organic matter, which could not be degraded in aerobic ponds and is modeled considering two layers in order to distinguish the different processes that take place within the pond. The upper layer is an aerobic environment, whereas the lower layer is an anaerobic one.

Figure 8a presents the first order sensitivity indices profile for the fermentation products concentration (C_{SA}). In this case, the parameter θ is the most relevant one, with a $\overline{S_i}$ of 0.7. There is also a considerable contribution to this state variable variance of Y_{hb} up to 12.3%, especially during the third day of operation. i_{nxs} and K_{NHa} contribute to the variance up to 5% each one, and there is a low contribution from K_a, K_{Oh}, and μ_{ab} with S_i^{max} values around 0.027.

Being an aerobic environment, similarities between the interaction sensitivity indices profiles are found for fermentation products (C_{SA}), fermentable, readily biodegradable soluble COD (C_{SF}), and ammonium and ammonia nitrogen concentration (C_{NH4}) concentrations (Figure 8b,e,f) with the profiles obtained for the second aerobic pond.

Regarding soluble nitrogen (C_{N2}) concentration, first order effects are dominated by θ and Y_{hb}, with $\overline{S_i}$ values of 0.56 and 0.35, respectively. They are followed in relevance by k_m and K_{Oh} that reach S_i values up to 0.046 and 0.025, respectively, as can be seen in Figure 8c. Interaction effects for these variables are mainly composed by the contribution of Y_{hb} and b_{hb}, with $\overline{S}_{int,i}$ values around 0.036. There is also a low contribution of θ and k_m at the beginning of the process.

3.5. Lower Layer of Facultative Pond. The lower layer of the facultative pond is an anaerobic environment; therefore, there are some processes that only occur within this layer of the

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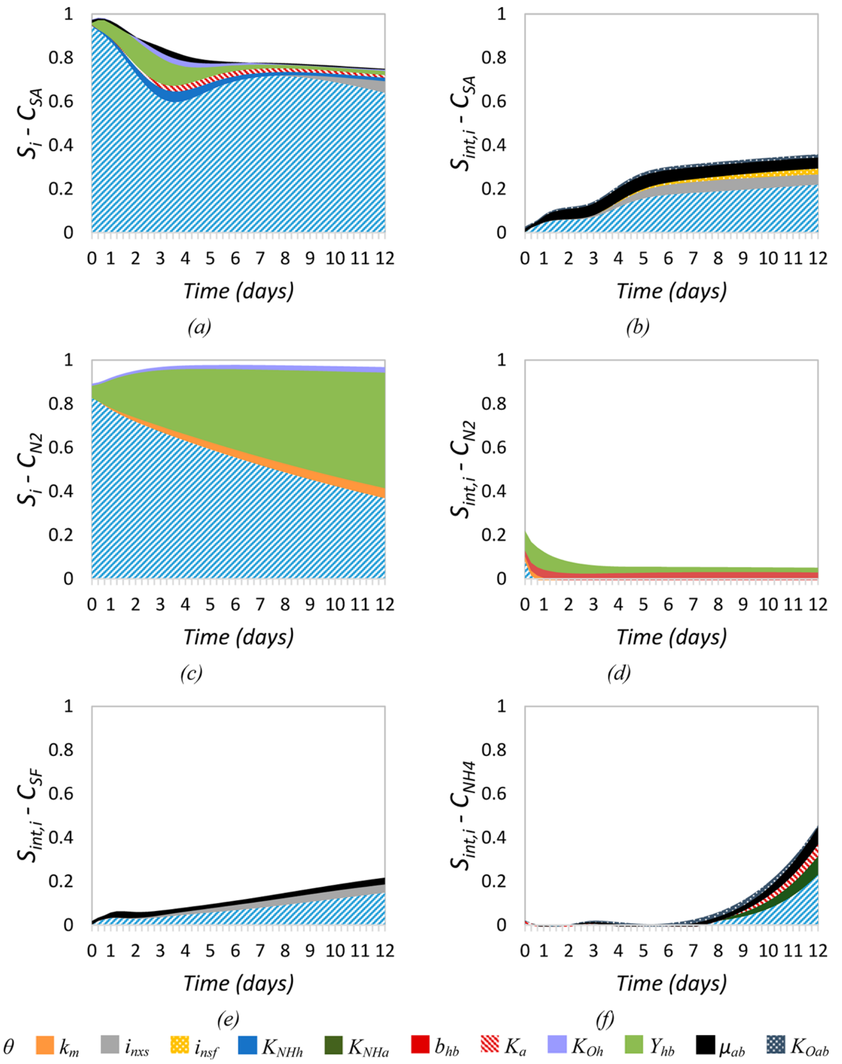

Figure 8. Upper layer of facultative pond: First order and interactional sensitivity indices profiles for fermentation products (C_{SA}) (a and b) and nitrogen (C_{N2}) (c and d) concentrations, and interactional sensitivity index profiles for fermentable, readily biodegradable soluble COD (C_{SF}) (e) and ammonium and ammonia nitrogen concentration (C_{NH4}) (f).

pond, such as hydrolysis and the growth of strict anaerobic microorganisms.

Only numerical results for nutrient related variables are presented in Figure 9a−e in order to show interactional effects between parameters. For the remaining variables of the lower layer of the facultative pond, only θ and k_m (Figure 4d) have influence on model outputs variances, and the interactions between parameters are not relevant (Table S4). Figure 9a,b shows first order and interaction sensitivity indices profiles for soluble nitrogen (C_{N2}) concentration. At the beginning of the operational time, the first order effects are described mainly by θ, explaining almost 80% of C_{N2} variance and decreasing along the time to around 2%.

As the importance of θ decreases, there is an increase of the first order effect of the yield factor of heterotrophic bacteria (Y_{hb}) which are the microorganisms responsible to hydrolyze the organic matter. Also, K_{Oh} appears to have a small contribution. Interaction effects are not high ($\Sigma S_{int,i} < 0.25$), and involve the contribution of Y_{hb}, b_{hb}, and θ. Both profiles are similar to those obtained for the upper layer of the pond, but without contribution of k_m in the C_{N2} concentration in the lower pond.

Regarding nitrite nitrate N concentration (C_{NO3}), first order effects are dominated by the parameter θ, presenting a $\overline{S}_i$ value of 0.95 as can be appreciated in Figure 9c. Y_{hb} has a contribution to the state variable variance up to 20% only at the beginning of the time horizon. In addition, the mass transfer coefficient between layers (k_m) has a low contribution also at the beginning. This variable presents a strong interactional effect among the uncertain parameters, reaching a $\sum S_{int,i}$ of 0.8, but concentrated in the first operation day (Figure 9d). θ is again the most relevant parameter, with $S_{int,i}^{max}$ value of 0.49 and $\overline{S}_{int,i}$ value of 0.022. There is an important contribution of Y_{hb} ($S_{int,i}^{max}$ = 0.22) and low contribution of k_m and b_{hb}.

Finally, Figure 9e presents the first order sensitivity indices profile for the ammonium and ammonia nitrogen concentration (C_{NH4}); again, θ dominates first order effect contributing up to 85% to the total variance, but there is also an important contribution to C_{NH4} variance from k_m, i_{nxs}, and i_{nsf}, up to 14%, 13%, and 12%, respectively, and low contribution from i_{nxalg} and i_{nbm}.

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Ind. Eng. Chem. Res. 2016, 55, 11403−11416

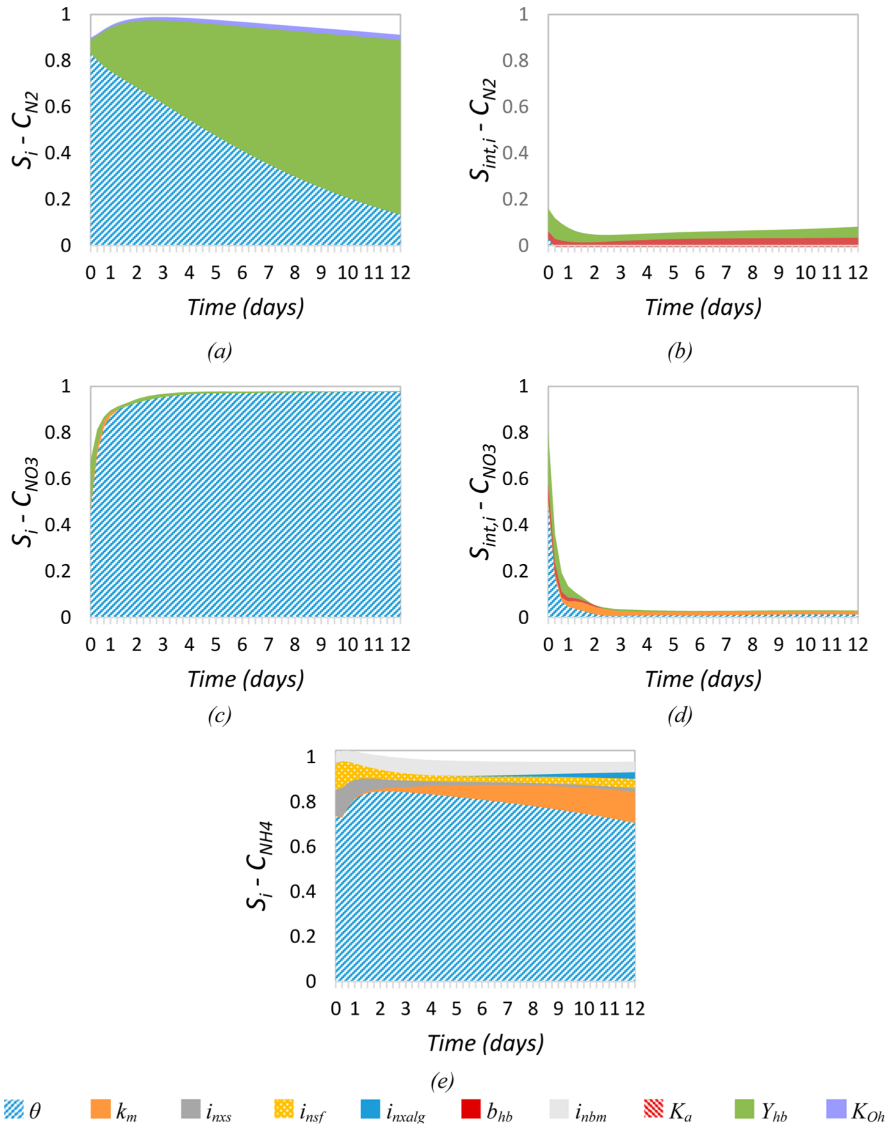

Figure 9. Lower layer facultative pond: First order and interactional sensitivity indices profiles for atmospheric nitrogen (C_{N2}) (a and b) and nitrite nitrate N (C_{NO3}) (c and d) concentrations; first order sensitivity index profile for ammonium and ammonia nitrogen concentration (C_{NH4}) (e).

4. CONCLUSIONS

In this work, a dynamic global sensitivity analysis on a wastewater biological treatment system has allowed determining which parameters are the most influential on main compound concentration variances, both through first order effects and interactions with other parameters along the entire operation time. A mechanistic model including 72 differential and 224 algebraic state variables has been implemented for a system of aerobic–aerobic–facultative ponds within an equation oriented environment.[21] Global sensitivity index profiles have been obtained by performing stochastic simulations in gPROMS and exporting state variable concentration profiles to calculate first order, total, and interaction sensitivity indices profiles in the Fortran 90 environment. A deep knowledge of model parameter contributions to the unconditional variance of the differential state variables provides useful information for parameter estimation. The temperature coefficient θ is the parameter that has the strongest first order influence during the time horizon, which indicates the need for its proper estimation. It is also important to estimate the most accurate values of other parameters like k_m and Y_{hb} in order to avoid their first order effects that explain 100% of the variance during some intervals within the time horizon of some variable output. Such information is crucial for identifying the set of these three parameters that need to be determined more precisely (factor prioritization), as stated in the Numerical Results section, and allows the identification of the set of parameters that has no contribution to the total output variance (factor fixing). Finally, it is important to note that, despite the complexity of the model, the interactional effects between parameters are not relevant and that only few parameters involve most of the uncertainty, which makes solving the problem of parameter estimation easier.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.iecr.6b02841.

Process equations; generation and consumption terms of mass balances; maximum, minimum and time average value of first order sensitivity indices for the 72 differential state variables; and maximum, minimum

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Ind. Eng. Chem. Res. 2016, 55, 11403–11416

and time average values of interactional sensitivity indices value for the 72 differential state variables (PDF)

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Notes

The authors declare no competing financial interest.

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■ NOMENCLATURE

Variables

Q_i^{in} = inlet volumetric flow, m^3/d
Q_i^{out} = outlet volumetric flow, m^3/d
Q_i^{prec} = precipitation volumetric flow, m^3/d
Q_i^{evap} = evaporation volumetric flow, m^3/d
$C_{X,ij}$ = concentration of component X related to pond i at layer j, g_x/m^3
$F_{X,ij}$ = reaction rate of component X related to pond i at layer j, g_x/m^3
V_{ij} = volume of layer j of the pond i, m^3
A_i = pond i area, m^2
h_i = pond i height, m
Δh_i = distance between half height of the upper layer and half height of the lower layer, m

Organic Load

$C_{COD,i,j}$ = COD, g_{COD}/m^3
$C_{SA,i,j}$ = fermentation products, g_{COD}/m^3
$C_{SF,i,j}$ = fermentable, readily biodegradable soluble COD, g_{COD}/m^3
$C_{SI,i,j}$ = inert soluble COD, g_{COD}/m^3
$C_{XI,i,j}$ = inert particulate COD, g_{COD}/m^3
$C_{Xs,i,j}$ = slowly biodegradable particulate COD, g_{COD}/m^3

Nutrients

$C_{N2,i,j}$ = soluble nitrogen, g_N/m^3
$C_{NH4,i,j}$ = ammonium and ammonia nitrogen, g_N/m^3
$C_{NO3,i,j}$ = nitrate and nitrite nitrogen, g_N/m^3
$C_{O2,i,j}$ = dissolved oxygen, g_{O2}/m^3
$C_{SO4,i,j}$ = sulfate sulfur, g_S/m^3

Biomass

$C_{alg,i,j}$ = algae, g_{COD}/m^3
$C_{amb,i,j}$ = acetotrophic methanogenic bacteria, g_{COD}/m^3
$C_{asrb,i,j}$ = acetotrophic sulfate reducing bacteria, g_{COD}/m^3
$C_{ab,i,j}$ = autotrophic bacteria, g_{COD}/m^3
$C_{Ecoli,i,j}$ = *E. coli*, MNP/m^3
$C_{fb,i,j}$ = fermenting bacteria, g_{COD}/m^3
$C_{hb,i,j}$ = heterotrophic bacteria, g_{COD}/m^3

Sensitivity Indices

$S_{y,i}$ = first order sensitivity index of parameter i for variable y
$S_{y,i}^{max}$ = maximum value of the first order sensitivity index of parameter i for variable y along the horizon of time
$S_{y,i}^{min}$ = minimum value of the first order sensitivity index of parameter i for variable y along the horizon of time
$\overline{S}_{y,i}$ = time average value of the first order sensitivity index of parameter i for variable y
$S_{int,i}$ = interactional sensitivity index of parameter i
$S_{int,i}^{max}$ = maximum value of the interactional sensitivity index of parameter i along the horizon of time
$S_{int,i}^{min}$ = minimum value of the interactional sensitivity index of parameter i along the horizon of time
$\overline{S}_{int,i}$ = time average value of the interactional sensitivity index of parameter i
S_i^{tot} = total order sensitivity index of parameter i

Parameters

μ_{alg} = maximum growth rate of algae, 2 d^{-1}
K_{NHalg} = saturation/inhibition coefficient of ammonium and ammonia nitrogen for algae, 0.01 g_N/m^3
K_{NOalg} = saturation/inhibition coefficient of nitrite nitrate N for algae, 0.01 g_N/m^3
b_{alg} = decay rate of algae, 0.100 d^{-1}*
μ_{hb} = maximum growth rate of heterotrophic bacteria, 6 d^{-1}
K_{SAh} = saturation/inhibition coefficient of fermentation products for heterotrophic bacteria, 4 g_{COD}/m^3
K_{SFh} = saturation/inhibition coefficient of fermentable, readily biodegradable soluble COD for heterotrophic bacteria, 3 g_{COD}/m^3
K_{Oh} = saturation/inhibition coefficient of oxygen for heterotrophic bacteria, 0.2 g_{O2}/m^3*
K_{NHh} = saturation/inhibition coefficient of ammonium and ammonia nitrogen for heterotrophic bacteria, 0.050 g_N/m^3 *
K_{NOh} = saturation/inhibition coefficient of nitrite nitrate N for heterotrophic bacteria, 0.5 g_N/m^3
η_{hb} = correction factor for anoxic growth of heterotrophic bacteria, 0.8
b_{hb} = decay rate of heterotrophic bacteria, 0.4 d^{-1}*
μ_{ab} = maximum growth rate of autotrophic bacteria, 2 d^{-1}*
K_{NHa} = saturation/inhibition coefficient of ammonium and ammonia nitrogen for autotrophic bacteria, 0.2 g_N/m^3*
K_{Oab} = saturation/inhibition coefficient of oxygen for autotrophic bacteria, 0.5 g_{O2}/m^3*
b_{ab} = decay rate of autotrophic bacteria, 0.015 d^{-1}*
μ_{fb} = maximum growth rate of fermenting bacteria, 6 d^{-1}
K_{SFfb} = saturation/inhibition coefficient of fermentable, readily biodegradable soluble COD for fermenting bacteria, 28 g_{COD}/m^3
K_{Ofb} = saturation/inhibition coefficient of oxygen for fermenting bacteria, 0.2 g_{O2}/m^3
K_{NOfb} = saturation/inhibition coefficient of nitrite nitrate N for fermenting bacteria, 0.5 g_N/m^3
K_{NHfb} = saturation/inhibition coefficient of ammonium and ammonia nitrogen for fermenting bacteria, 0.01 g_N/m^3
b_{fb} = decay rate of fermenting bacteria, 0.02 d^{-1}*
μ_{asrb} = maximum growth rate of acetotrophic sulfate reducing bacteria, 0.18 d^{-1}
K_{SAasrb} = saturation/inhibition coefficient of fermentation products for acetotrophic sulfate reducing bacteria, 24 g_{COD}/m^3
K_{SOasrb} = saturation/inhibition coefficient sulfate sulfur for acetotrophic sulfate reducing bacteria, 19 g_S/m^3
K_{Oasrb} = saturation/inhibition coefficient of oxygen for acetotrophic sulfate reducing bacteria, 0.0002 g_{O2}/m^3
K_{NOasrb} = saturation/inhibition coefficient of nitrite nitrate N for acetotrophic sulfate reducing bacteria, 0.0005 g_N/m^3
K_{NHasrb} = saturation/inhibition coefficient of ammonium and ammonia nitrogen for acetotrophic sulfate reducing bacteria, 0.01 g_N/m^3
b_{asrb} = decay rate of acetotrophic sulfate reducing bacteria, 0.012 d^{-1}

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Ind. Eng. Chem. Res. 2016, 55, 11403−11416

μ_{amb} = maximum growth rate of acetotrophic methanogenic bacteria, 0.085 d^{-1}
K_{SAamb} = saturation/inhibition coefficient of fermentation products for acetotrophic methanogenic bacteria, 56 g_{COD}/m^3
K_{Oamb} = saturation/inhibition coefficient of oxygen for acetotrophic methanogenic bacteria, 0.0002 g_{O2}/m^3
K_{NOamb} = saturation/inhibition coefficient of nitrite nitrate N for acetotrophic methanogenic bacteria, 0.0005 g_N/m^3
K_{NHamb} = saturation/inhibition coefficient of ammonium and ammonia nitrogen for acetotrophic methanogenic bacteria, 0.01 g_N/m^3
b_{amb} = decay rate of acetotrophic methanogenic bacteria, 0.008 d^{-1}*
K_x = saturation/inhibition coefficient for hydrolysis, 0.1 g_{CODsf}/g_{CODbm}
K_{hy} = hydrolysis rate, 3 d^{-1}
η_{hy} = correction factor for hydrolysis, 0.1
b_{Ecoli} = decay rate of *E. coli*, 0.25 d^{-1}
Y_{hb} = yield factor for heterotrophic bacteria, 0.630 g_{CODbm}/g_{CODsf} *
Y_{ab} = yield factor for autotrophic bacteria, 0.24 g_{CODbm}/g_N
Y_{amb} = yield factor for acetotrophic methanogenic bacteria, 0.032 g_{CODbm}/g_{CODsa}
Y_{fb} = yield factor for fermenting bacteria, 0.053 g_{CODbm}/g_{CODsf}
Y_{asrb} = yield factor for acetotrophic sulfate reducing bacteria, 0.05 g_{CODbm}/g_{CODsa}
f_{si} = fraction of inert soluble COD formed during hydrolysis, 0 g_{CODsi}/g_{CODxs}
i_{nbm} = fraction of nitrogen in bacteria, 0.070 g_N/g_{CODbm}*
i_{nxalg} = fraction of nitrogen in algae, 0.063 g_N/g_{CODalg}*
i_{nxs} = fraction of nitrogen in slowly biodegradable particulate COD, 0.04 g_N/g_{COD}*
i_{nxi} = fraction of nitrogen in slowly biodegradable particulate COD, 0.03 g_N/g_{CODxi}*
i_{nsi} = fraction of nitrogen in inert soluble COD, 0.01 g_N/g_{CODsi}
i_{nsf} = fraction of nitrogen in fermentable, readily biodegradable soluble COD, 0.030 g_N/g_{COD}*
f_p = fraction of slowly biodegradable particulate COD formed during decay processes, 0.1 g_{CODxi}/g_{CODbm}, g_{CODxi}/g_{CODalg}
θ = coefficient in the temperature limiting function, 1.07*
K_a = rate of reaeration, 0.230 d^{-1}*
C_s = saturation concentration of oxygen, 7.75 gO^2/m^3
K_1 = light attenuation coefficient for algae, 0.02 m^2/g_{CODalg}
K_2 = background light attenuation, 2.137 m^{-1}
L_o = optimal light intensity, 150 ly/d
k_m = mass transfer coefficient between layers in facultative pond, 0.022 m^2/d*
* = uncertain parameters for the GSA

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