

A SIMPLIFIED MATHEMATICAL MODEL FOR AN UPFLOW ANAEROBIC FIXED FILM REACTOR UNDER TRANSIENT LOADING

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For upflow anaerobic fixed film reactors with high hydraulic retention time, biofilm sloughing or attrition may result in rather large and active microbial aggregate fragments that are retained in the reactor. Detailed modelling and validation of this system has been previously published.

The present paper is focused on a simplified semi-empirical mathematical model developed for this system, based on Contois kinetics and the definition of some parameters related to the capability of the reactor for biomass retention and its substrate distribution at a given time. The model is represented by two ordinary differential equations corresponding to substrate and biomass evolution on time. These equations have been solved analytically using simplification assumptions, obtaining a simple equation depending on a one lumped parameter only. This solution has been applied for prediction of some variables representing the average reactor performance on periods of approximately a week, such as the average efficiency on substrate removal or total methane production during the period, under transient loading rates of a low degradable substrate -swine wastes-, with satisfactory results.

Introduction

The upflow anaerobic filter reactor basically is a contact process in which wastes pass over or through a mass of biological solids contained within the reactor by a fixed media [1]. Anaerobic filters were first described in 1968 [2, 3], and have grown to represent an advanced technology that has been used effectively for treating a wide range of industrial wastes.

In a wide range of wastes, such as livestock wastes, there is a continuous modification of influent properties due to changes on farm operation, and so it is difficult to maintain steady state operating conditions on reactor treating wastes. Models capable of prediction on non-steady state situations are needed to evaluate the impact of transient loading to reactors performance.

Anaerobic packed bed reactors performance is influenced by many characteristics and phenomena: type of support matrix, biofilm dynamics and its distribution inside the reactor, retention and distribution of sloughed biomass and other particulate organic matter, influent chemical and biological

properties and its loading pattern, plug flow model modification by gas production, hydraulic retention time, etc. Detailed and structured dynamic modelling of this system has a doubtless pedagogic interest, it may allow discover relations among variables, to establish response tendencies, to detect some limit situations and to explain how it works, but its usual complexity and the multiple parameters involved difficulties the calibration and the industrial applicability for design and for accurate prediction purposes.

For anaerobic fixed film reactors, activity is considered to be due to microbial biofilm development over the support matrix. This clearly requires the biofilm to be stationary and the net biomass grown fraction to be rapidly sloughed and washed-out, in order not to consider its activity. For low retention time reactors, loaded with soluble and high degradable substrates, structured models based on biofilm kinetics allow to explain, to simulate and to predict reactor performance accurately.

For high retention time reactors, or discontinuously loaded, biofilm sloughing may result in rather large microbial aggregate fragments that are retained in the

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reactor, following its own dynamics. FLOTATS and PUIGJANER [4] developed a structured model for this system, considering soluble substrate, based on the dynamics of a discrete bivariate distribution of bacterial aggregates and gas bubbles. This PMB model developed allowed to achieve a mathematical synthesis of empirical knowledge about the considered phenomena, and the numerical simulations, applied to an upflow anaerobic filter reactor with oriented support, showed the same pilot plant tendencies and it was a good tool for some limit situations calculation, but difficulties on calibration (there was 13 parameters) not allowed a full quantitative validation for design purposes. In this common situation, empirical models, based on observed correlation between plant performance and its main design and operating variables, are better for industrial use, although the involved parameters have no physical or biological sense often.

In early studies over anaerobic filters, YOUNG and McCARTY [3] realised that efficiency on COD removal showed an inversely relation with hydraulic retention time, θ ,

$$E = 1 - \frac{\varepsilon}{\theta}, \quad (1)$$

applying it for steady state conditions. TRULEAR and CHARACKLIS [5] applied the logistic equation

$$E = \frac{e^{kt}}{1 - (S_0/S_{\max})(1 - e^{-kt})}, \quad (2)$$

to fit experimental data of time evolution of glucose removal. This expression was applied to biofilm thickness and suspended biomass experimental data too.

Another expression used with satisfactory results is

$$E = 1 - \varepsilon'\theta^{-m}, \quad (3)$$

referenced by YOUNG [1]. YOUNG proved that this relationship could be used to describe both pilot and full-scale reactors treating a number of wastes and operating under a variety of field conditions. This author used it to predict the effluent concentration for a reactor fed with a variable organic loading rate, substituting θ by S_0 / L_s , and working with averaged data obtained within a periods of 7 days. Although the predictions were not accurate, Eq.(3) followed the same experimental data tendencies.

YOUNG [1] analysed data from several authors, using a more general empirical expression,

$$E = \varepsilon''\theta^a (S_0)^b (A_s)^c (\alpha)^d, \quad (4)$$

with the aim to compare results and to make a statistical screening and ranking of parameters

affecting anaerobic filters performance, using a multivariable linear correlation. This screening showed that hydraulic retention time was the most important factor affecting COD removal.

Empirical models are useful to fit experimental data, and also for main design variables detection, but, due to the difficulty to find a physical sense to the involved parameters, do not allow reactors performance explanation at all. Semi-empirical models are on the middle way between those structured and empirical. They are based on simple structured models with the use of parameters, lumped parameters, that incorporate the simultaneous effect of some variables of difficult quantification.

The most profusely used semi-empirical model is due to CHEN and HASHIMOTO [6], applied to anaerobic digestion of high strength wastes, basically livestock wastes, for completely mixed reactors. It is based on Contois kinetics [7], that can be considered as another semi-empirical expression.

BOLTE, referenced by THOMAS and NORDSTEDT [8], proposed the concept of "bacterial retention coefficient" or BRC, as a function of the type of reactor, recycle rate, surface to volume ratio and media type. The BRC represents the amount of active biomass which is retained in the reactor by modifying the washout term in the bacterial mass balance equation,

$$\frac{dX}{dt} = \left[\mu - k_d - (1 - BRC)\frac{1}{\theta} \right] X. \quad (5)$$

THOMAS and NORDSTEDT [8] used it for the development of a generic model for the simulation of various reactors types and substrates, which was able to satisfactorily simulate literature data from 42 studies of three different reactor types under steady state conditions. For dynamic simulations, the BRC concept was not used.

The objective of the present work is the development of a simple semi-empirical model, capable of performance prediction of a packed bed anaerobic reactor, fed with liquid fraction of swine wastes, under transient loading rates.

Development of the Semi-Empirical Model

For anaerobic digestion of livestock wastes, hydrolysis of particulate or colloidal organic matter can be considered the rate-limiting step of the whole anaerobic process [9]. The hydrolysis rate is usually described as a simple first order process respect of hydrolyzable materials. Several models use a more complicated expression, of the saturation type [10], where a given biomass X has a maximum hydrolysis capacity,

$$\rho_h = K_h \frac{S/X}{B + S/X} X. \quad (6)$$

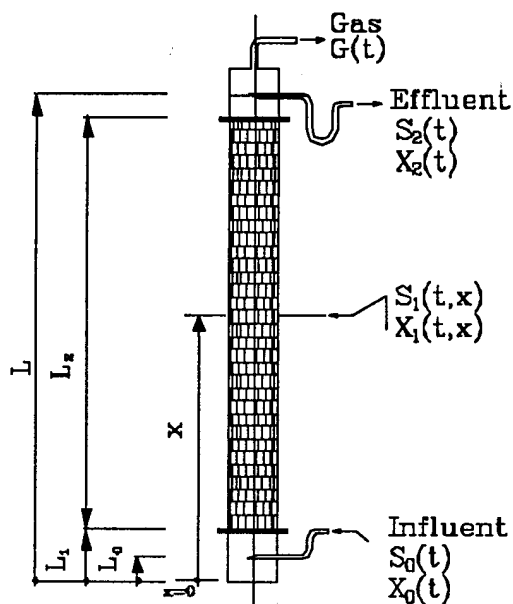


Fig.1 Schematics of the filter reactor, indicating symbols used in dimensions and flow compositions: S and X mean substrate and biomass concentrations respectively

Rearranging this expression, a similar Contois kinetics expression is obtained,

$$\rho_h = K_h \frac{S}{BX + S} X. \quad (7)$$

Using the Monod kinetics for fitting data obtained from a continuous culture of *Aerobacter aerogenes*, Contois realised [7] that the saturation constant was linear dependent with the reactor influent substrate concentration S_0 . Introducing the biomass concentration at steady state and redefining the maximum growth rate, Contois obtained a kinetic expression where the microorganisms growth rate depends on the steady state substrate and biomass concentrations,

$$\mu = \mu_m \frac{S}{BX + S}. \quad (8)$$

The Contois effect is generally interpreted as a diffusion limitation caused by "overcrowding" at very high substrate concentration [11]. Considering the good results obtained in literature about applicability of Contois kinetics for anaerobic digestion models of livestock wastes, and considering the hydrolysis of particulate COD as the rate limiting step of the process, Eq.(8) will be adopted.

Fig.1 shows the schematics of the reactor. Biomass and substrate concentration along the filter, X_1 and S_1 , are time and space dependent variables. In order to simplify, the model will consider time dependency only, and it will use the average values, as defined in Table 1.

The model is based on the two following simple differential equations, obtained from a mass balance on the reactor and the assumptions that influent biomass

Table 1 Definition of variables used for model construction and for experimental data analysis

Notation	Definition	Eqs.
S_0 : Average influent substrate concentration on a period (t_i, t_{i+1})	$\frac{\int_{t_i}^{t_{i+1}} Q(t) \cdot S_0(t) dt}{\int_{t_i}^{t_{i+1}} Q(t) dt}$	(9)
S_2 : Average effluent substrate concentration on a period (t_i, t_{i+1})	$\frac{\int_{t_i}^{t_{i+1}} Q(t) \cdot S_2(t) dt}{\int_{t_i}^{t_{i+1}} Q(t) dt}$	(10)
C_S : Substrate confinement coefficient on a period (t_i, t_{i+1})	$\frac{S_2(t_i) - S_1(t_i, L)}{S_1(t_i)}$	(11)
θ : Average retention time on a period (t_i, t_{i+1})	$\frac{(t_{i+1} - t_i)V}{\int_{t_i}^{t_{i+1}} Q(t) dt}$	(12)
$S_1(t)$: Average substrate concentration in the reactor at time t	$\frac{1}{L} \int_0^L S_1(t, x) dx$	(13)
$X_1(t)$: Average biomass concentration in the reactor at time t	$\frac{1}{L} \int_0^L X_1(t, x) dx$	(14)

concentration and the biomass decay rate in reactor are negligible ($X_0 \approx 0$, and $k_d \approx 0$),

$$\begin{aligned} \frac{dX_1(t)}{dt} &= -\frac{X_2(t)}{\theta} + \mu X_1(t), \\ \frac{dS_1(t)}{dt} &= \frac{S_0(t) - S_1(t)}{\theta} - \frac{\mu}{Y} X_1(t). \end{aligned} \quad (15)$$

Using the Contois kinetics and defining the following lumped parameters,

$$K = B \cdot Y, r = \frac{\mu_m - \mu}{K}, C_S = \frac{S_2(t)}{S_1(t)}, C_X = \frac{X_2(t)}{X_1(t)}, \quad (16)$$

the substrate balance equation can be expressed as a first order linear differential equation,

$$\frac{dS_1(t)}{dt} = -\left(r + \frac{C_S}{\theta}\right) S_1(t) + \frac{S_0(t)}{\theta}. \quad (17)$$

From these equations, some interesting relations can be derived for permanent or transient state.

Steady State Conditions

Under steady state conditions, the fluid flow and influent substrate concentrations are constants, the reactor substrate concentration has a constant distribution and it is no time dependent for a given retention time, with $S_2(t) = S_1(t, L)$. The average substrate concentration in the reactor will be

$$S_1 = \frac{K}{\mu_m \theta - C_X + K C_S} S_0. \quad (18)$$

Table 2 Definition of operating variables related to reactor response used for experimental data analysis and for the application of model

Notation	Definition	Application to Eq. (19)	Eqs.
E_m : Average efficiency on substrate removal, on a period (t_i, t_{i+1})	$1 - \frac{1}{(t_{i+1} - t_i)} \int_{t_i}^{t_{i+1}} \frac{S_2(t)}{S_0(t)} dt$	$1 - \frac{C_S}{r\theta + C_S} \left[1 - \frac{\theta}{(t_{i+1} - t_i) S_0} A_V \right]$	(20)
S_{1m} : Average reactor substrate concentration on a period (t_i, t_{i+1})	$\frac{1}{(t_{i+1} - t_i)} \int_{t_i}^{t_{i+1}} S_1(t) dt$	$\frac{1}{r\theta + C_S} \left[S_0 - \frac{\theta A_V}{(t_{i+1} - t_i)} \right]$	(21)
A_V : Volumetric substrate accumulation on a period (t_i, t_{i+1})	$\int_{t_i}^{t_{i+1}} \left(\frac{dS_1(t)}{dt} \right) dt$	$\left(S_1(t_i) - \frac{S_0}{r\theta + C_S} \right) \left(e^{-(r+C_S/\theta)(t_{i+1}-t_i)} - 1 \right)$	(22)
R_V : Volumetric substrate removal on a period (t_i, t_{i+1})	$\int_{t_i}^{t_{i+1}} r \cdot S_1(t) dt$	$\frac{r}{r\theta + C_S} \left[S_0(t_{i+1} - t_i) - \theta A_V \right]$	(23)
G : Accumulated gas production on a period (t_i, t_{i+1})	$V \cdot G_0 \cdot \int_{t_i}^{t_{i+1}} r \cdot S_1(t) dt$	$V \cdot G_0 \cdot R_V$	(24)

If the gas flow is high enough to homogenise the reactor substrate concentration, then $C_S=1$. FLOTATS and PUIGJANER [12] used this expression, in this situation, for fitting experimental data about evolution of soluble substrate concentration and gas production, obtained from an anaerobic filter treating the liquid fraction of swine wastes, with satisfactory results.

If there is a completely homogenisation of biomass and substrate concentrations, the parameters C_X and C_S equals 1, and the Chen-Hashimoto model [6] is obtained for completely stirred tank reactors, that has been profusely validated for high strength wastes. The parameter K is known as the Chen-Hashimoto constant, and they experienced that its value increased when the influent substrate concentration or transport limitations (no reactor agitation) increased, being a measure of inhibition.

Non Steady State Conditions

For solving Eq.(11), in a non steady state situation, it will be assumed that the values $r + C_S / \theta$ and S_0 / θ are constants for a period of time (t_i, t_{i+1}) where the equation will be solved. For this period, C_S , S_0 and θ will be evaluated as defined in Table 1. With this simplification assumption, the solution of Eq. (17) is

$$S_1(t) = \frac{S_0}{r\theta + C_S} + \left(S_1(t_i) - \frac{S_0}{r\theta + C_S} \right) \cdot \exp\left[-(r + C_S/\theta)(t - t_i)\right], \quad t \in (t_i, t_{i+1}), \quad (19)$$

where the first addend is the concentration $S_1(t)$ at steady state, if there is no transient reactor loading. Model is expressed by this equation and there is one parameter involved only, r . According the definition, Eq.(16), it depends on biomass growth rate μ and the inhibition constant K , increasing with generalised biomass activity. From Eq.(19), some operating response variables have been derived, and they are shown in Table 2.

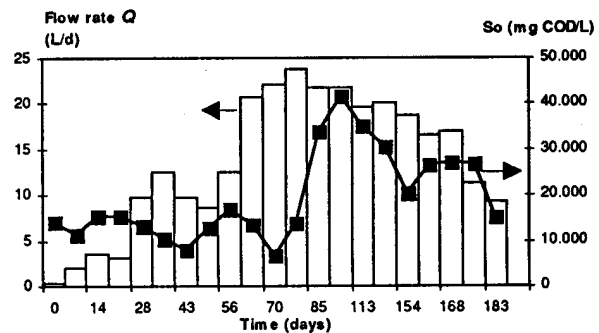


Fig.2 Time evolution of the weekly averaged values of the influent flow rate, Q , and the influent substrate concentration S_0 (mg COD/L)

Materials and Methods

Data for model checking were obtained from an anaerobic packed bed pilot plant reactor, installed in a piggery farm of La Garrotxa (Catalonia-Spain), fed with liquid fraction of swine wastes and operated at 35°C under real conditions during 191 days. This means that the continuous changes in farm practices are translated on changes in hydraulic and chemical properties of wastes and so, it is very difficult to operate under steady state conditions.

Reactor is a column of 0.25 m diameter, with dimensions, according to Fig.1, as follow: $L = 2.28$ m, $L_0 = 0.22$ m, $L_1 = 0.25$ m, $L_2 = 2$ m. The packed bed zone, of length L_2 , is filled by a PVC vertically oriented support with a porosity of 0.82. The reactor has 18 sample ports uniformly distributed along the column.

One or two times at week samples from the influent, the effluent and the 18 ports were taken in order to know the substrate concentration distribution inside the reactor. Influent flow rate and gas production were measured daily. During this period the average flow rate and the influent substrate concentration, measured as total COD, are indicated in Fig.2.

Average values, defined in Tables 1 and 2, were calculated for 21 periods of time, using the Simpson's rule. $X_1(t)$ concept has been applied for model

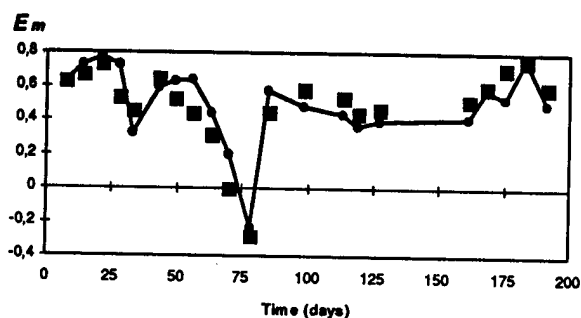


Fig. 3 Average efficiency on substrate removal E_m (■: experimental results; •: predicted by model, Eq.(20))

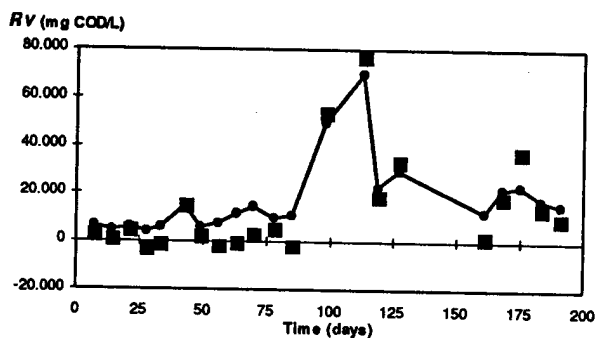


Fig. 5 Time evolution on the average volumetric substrate removal R_v (mg COD/L reactor) (■: experimental results; •: predicted by model, Eq.(23))

definition but it was not measured, and it is not used in the model base equation (Eq.(19)). G was calculated directly from measured gas production. R_v was calculated for each period using the relation: mass removal = mass input - mass output - mass accumulated.

Non-linear regression was used to fit the model to the calculated values of E_m , S_{1m} , R_v and G . For each of these operating variables, the corresponding predicted values were calculated using the derived equations detailed in Table 2.

Results and Discussion

The evolution of experimental and predicted values of the average reactor efficiency on substrate removal E_m is shown in Fig. 3. The fitting value of r has been $3 \cdot 10^{-3} \text{ h}^{-1}$ with a determination coefficient R^2 of 0.76. Negative values for the period over the 75th day are due to a low organic loading rate with high flow rate that produces a washout of retained particulate COD, increasing its effluent concentration over the influent concentration. Knowing the internal reactor COD concentration and distribution at the beginning of the period, the model can predict the washout very well. The fitting of the corresponding expression for steady state conditions has been attempted, but the R^2 value has been 0.2 only.

Experimental and predicted values for the average internal substrate concentration S_{1m} are shown in Fig. 4. The fitting value of r has been $5 \cdot 10^{-3} \text{ h}^{-1}$ with a

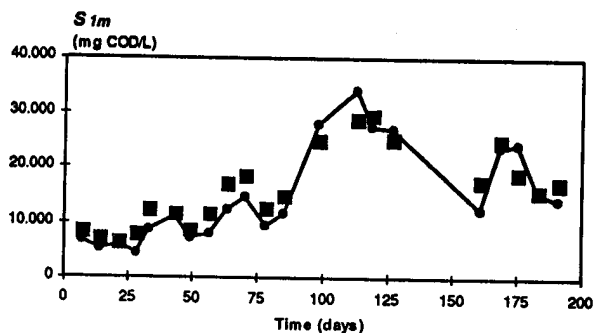


Fig. 4 Time evolution of the average reactor substrate concentration S_{1m} (mg COD/L) (■: experimental results; •: predicted by model, Eq. (21))

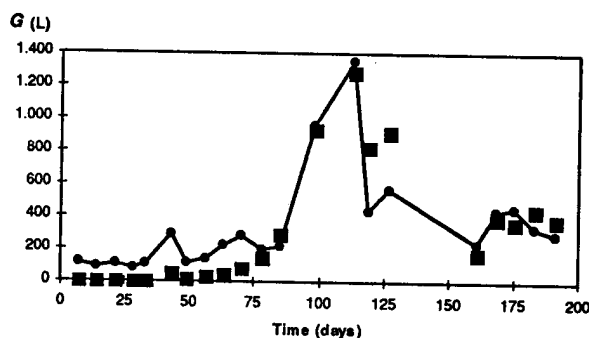


Fig. 6 Time evolution of the accumulated gas production during each period of time, G (L gas), (■: experimental results; •: predicted by model, Eq.(24))

determination coefficient R^2 of 0.78. For the steady state expression the r value has been the same, but the R^2 value has been 0.41. The fitting of the volumetric substrate accumulation A_v has presented a low determination coefficient and it is not shown.

Fig. 5 shows the evolution of the average volumetric substrate removal R_v . The fitting value of r has been $6 \cdot 10^{-3} \text{ h}^{-1}$ with a determination coefficient R^2 of 0.86. Non sense negative values for calculated R_v from experimental data are supposed to be due to the large delay between samples, that causes a low accuracy and negative values when real removal rate are near to zero. This low removal rate during the first days are translated to a low biogas production, as can be seen in Fig. 6. Here the G_0 value has been $0.2 \text{ m}^3 \text{ methane kg}^{-1} \text{ COD removed}$, with a fitting value r of $6 \cdot 10^{-3} \text{ h}^{-1}$ and a determination coefficient of 0.81.

In all plots it can be seen that system response is highly influenced by organic loading rate, product of the flow rate and the influent substrate concentration, rather than the hydraulic retention time. When the influent substrate concentration is constant, then the flow rate or the retention time controls the system, as observed by YOUNG [1].

As can be analysed from Eq.(19), the transient behaviour of the reactor during a given period of time is influenced, too, by the accumulated substrate concentration $S_1(t)$ at the beginning of the period. If it is high, r value will be low and will produce a low biomass activity and a low substrate removal rate. In this situation, a low influent substrate concentration

with high flow rate will produce a decrease of the observed efficiency of the filter.

Although the experimental data have been the same for the four fittings, the r value for the best fits has presented some differences, but they are of the same order of magnitude. This little differences are supposed to be logic, due to the large period of time between samples. The low values obtained support the slowly substrate degradation rate observed.

Conclusions

The model performs very well as a tool for predicting average values of reactor response under transient loading rate for a periods of time of approximately a week, knowing the internal reactor distribution of substrate concentration at beginning of the period. Its simplicity and the fact there are one parameter involved only, facilitates its calibration. Although its simplicity, as a semi-empirical model and by the use of lumped variables, it maintains a structure that allows explanation of reactor performance for the tested situations. More work must be done in order to validate the model for other slowly degradable substrates and other packed bed reactors.

SYMBOLS

A_s	Media specific surface area, $L^2 \cdot L^{-3}$
A_v	Volumetric substrate accumulation, $M \cdot L^{-3}$
a, b, c, d, m	Dimensionless parameters
B	Contois inhibition constant
BRC	Bacterial retention coefficient
C_s	Substrate confinement coefficient
C_x	Biomass confinement coefficient
E	Efficiency on substrate removal
E_m	Average efficiency on substrate removal
G	Accumulated methane gas production, L^3
G_0	Specific gas production, $L^3 \cdot M^{-1}$
k	Parameter used in Trulear and Characklis equation, T^{-1}
k_d	Specific biomass decay rate, T^{-1}
K	Chen-Hashimoto inhibition constant
K_h	Hydrolysis rate constant, T^{-1}
L_s	Organic loading rate, $M \cdot L^{-3} \cdot T^{-1}$
L	Reactor height, L
R_v	Volumetric substrate removal, $M \cdot L^{-3}$
r	Reaction rate coefficient, T^{-1}
S	Substrate concentration, $M \cdot L^{-3}$

S_{max}	Maximum effluent substrate concentration, $M \cdot L^{-3}$
S_{1m}	Average reactor-substrate concentration, $M \cdot L^{-3}$
t	Time, T
V	Reactor volume, L^3
X	Biomass concentration, $M \cdot L^{-3}$
x	Distance from de bottom of the column, L
Y	Yield constant

Greek Letters

α	Slope of the channels in modular support media
$\epsilon, \epsilon', \epsilon''$	Parameters used in <i>Eqs.(1), (3) and (4)</i>
μ_m	Maximum biomass growth rate, T^{-1}
μ	Specific biomass growth rate, T^{-1}
θ	Hydraulic retention time, T
ρ_h	Hydrolysis reaction rate, $M \cdot L^{-3} \cdot T^{-1}$

Subscripts

i	Corresponding to i^{th} period of time evaluated
0, 1, 2	Corresponding to the influent, inside and the effluent of the reactor, respectively

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