

A model to Predict the Behavior of UASB Reactors

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ABSTRACT: A model describing the main processes occurring in the UASB reactor was developed; in order to maintain simplicity and applicability of the model, only the fundamental aspects were considered. In the model, the reactor is divided in several well-stirred reactors coupled in series and it comprises substrate degradation, biomass growth and the reactions that take place within the granules. The important contribution of the paper is the development of a model taking into account the mass transfer through the film around the granules, the intra-particle diffusion, and the degradation reaction. The model enables the determination of the removal efficiency of the substrate and the increase of both the height of the sludge bed and the granule size with time. The simulated results of an experimental UASB reactor treating sugar-cane mill wastewater were found to be in good agreement with the performance of the reactor. The sensitivity analysis shows that the performance of the reactor is determined by several parameters. The most important parameters are: the bioconversion rate, the mass transfer coefficient in the film, the intra-particle diffusivity, the volumetric fraction of biomass in the reactor, and the number of CSTR considered. These parameters should therefore be carefully determined. The model could be a useful tool in the optimization and development of UASB reactors.

Key words: CSTR, Kinetic, Simulation, UASB, Wastewater

INTRODUCTION

Untreated wastewater coming from industries or cities causes a negative impact on the environment. The effect of discharging wastewater directly to a water reservoir was noticed, for instance, in 2004 and 2007 when countless amount of death fish appeared in the lake Cocibolca (Nicaragua). The death of these species was caused by the entry of untreated wastewater to the lake. To tackle this problem, and to protect the environment from pollution, the alternative of treating wastewater via an Upflow Anaerobic Sludge Blanket (UASB) reactor was recognized as a viable one, especially in developing countries like Nicaragua. The UASB reactor is simple to build; it works better in tropical climates, and its maintenance is not expensive compared to other reactors. In addition, the biogas produced in the UASB reactor may be used as fuel.

Noticeably, models handling most of the processes occurring in UASB reactors already exist, but they comprise too many parameters (e.g. Kalyuzhnyi *et al.*, 2006; Batstone *et al.*, 2002). The large number of mechanisms and parameters included in these kinds of models is almost impossible to assess in practice. Therefore, its applicability is reserved only for engineers

and scientists with large experience in anaerobic treatment of wastewater; i.e., universities and research centers. The use of these models is difficult for technical departments in municipalities. Other kinds of models are those focusing only on one or few processes occurring in a UASB reactor (e.g. Wu & Hickey, 1997; Narnoli & Merhotra, 1997; Sponza & Uluköy, 2008). Due to the simplicity of those models, some important processes may not even be accounted for, such as the advective and dispersive processes in UASB reactors.

The reasons discussed above motivated us to develop a model that includes the most important processes in a UASB reactor, but that is, at the same time, sufficiently simple and easy to operate. Therefore, the aim of this paper is to develop a model that properly predicts the degradation of the substrate and the behavior of the biomass in the reactor (i.e. sludge concentration, granule size, and distribution of the biomass in the reactor). The model is transient; therefore, it can handle the growth of biomass with time, the variable substrate concentration at the feed, and the variable flow rate through the reactor. An important contribution of the paper is the development

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of an analytical expression for describing the reaction within a granule. This expression takes into account the mass transfer through the liquid film around the granule, the intra-diffusion, the specific reaction rate within the granule, and the granule size.

Among the various parameters, the amount of biomass and the granule size are the two very important entities determining the performance of the UASB reactor, since they determine the substrate degradation rate. The granule size constitutes a critical point for the assessment of the optimal working conditions of the reactor. In presence of small granules, the substrate is consumed rapidly. However, too small granules may be dragged by the water flow. On the other hand, big granules imply that the substrate would be consumed mainly in the external layers of the granules. This causes starvation of the microorganisms in the interior of the granules, reducing the efficiency within the granule, and therefore the reactor will work in an unsatisfactory way.

Taking into consideration the above mentioned, some important issues for the formulation of the model are put forward. First, it is known that the axial dispersion model (ADM) and the model of the continuously stirred tank reactors (CSTRs) connected in series are commonly used to describe the processes of flow and mass transfer in UASB reactors. In the former, the reactor is viewed as a single tube with a dispersive plug flow, which includes both advection and reaction, in addition to axial dispersion. In the latter, the reactor is viewed as several CSTRs connected in series. In that case, the dispersive term is omitted because it is accounted for by the number of CSTRs. Hence, the parameter taking into account the mixing in the reactor is the Péclet number in the ADM and the number of reactor (N) in the CSTRs model (Levenspiel, 1999; Fogler, 2006). Comparison between them shows that both models are able to describe adequately the behavior of UASB reactors. However, the model of CSTRs in series offers computational advantages over the ADM (Abu-Reesh & Abu-Sharkh, 2003).

Secondly, the dispersion of a column reactor is commonly described by the Péclet number, which can be related with N as (Fogler, 2006; Abu-Reesh & Abu-Sharkh, 2003),

$$N = \frac{Pe}{2} + 1 \quad (1)$$

This expression indicates that a system composed of few CSTRs has a low Péclet number; i.e., large dispersion. On the other hand, a reactor with plug flow has a high Péclet number ($Pe \rightarrow \infty$) and therefore

would be represented by a large number of reactors ($N \rightarrow \infty$). Regarding the sludge distribution, researchers have reported that the concentration of solids along the height of the reactor could be the same after a long time of operation (Takahashi *et al.*, 2011; Gupta & Gupta, 2005; Huang *et al.*, 2003). However, as shown in Fig. 1, the studies of Kalyuzhnyi *et al.*, (2001) suggested that the fraction of biomass decreases with the height, reaching low values at locations close to the top of the reactor (Narnoli & Mehrotra, 1997) and generating a transition zone between the sludge bed and the blanket.

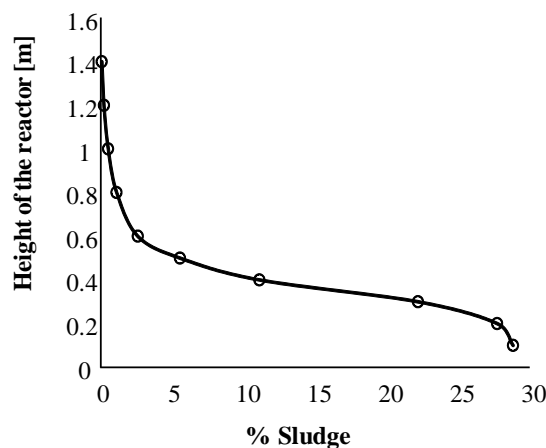


Fig. 1. Percentage of sludge along the height of the reactor (Kalyuzhnyi *et al.* 2001)

In addition, it should be stressed that the sludge is composed of both active and non-active biomass; the last one is formed by the decay of microorganisms. A part of the sludge may also be washed out (Kalyuzhnyi *et al.*, 2001; Gupta *et al.*, 2007; Yan *et al.*, 1989; Cavalcanti, 2003), affecting the efficiency of the reactor. This washout may be negligible if dense granules are already formed (Seghezzeo *et al.*, 2002). When the sludge bed has reached the top of the reactor, it is time to discharge the biomass. In UASB reactors, this occurs after a long period of operation (Seghezzeo *et al.*, 2002). It is important to keep in mind that a steady state is never reached, due to the continuous changes in the amount of biomass in the reactor. Regarding the size distribution of the granules in the sludge bed, the most important raising cause is the production of biogas (Narnoli & Mehrotra, 1997; Pereboom, 1994). Fig. 2 shows that granules larger than 0.1-0.2 mm would be kept at the bottom of the reactor if gas is not generated, even for upflow velocity of 1.0 m/h (Fig. 2 was created using the Stokes equation).

The model developed in this paper aims at accounting the most important processes in the UASB

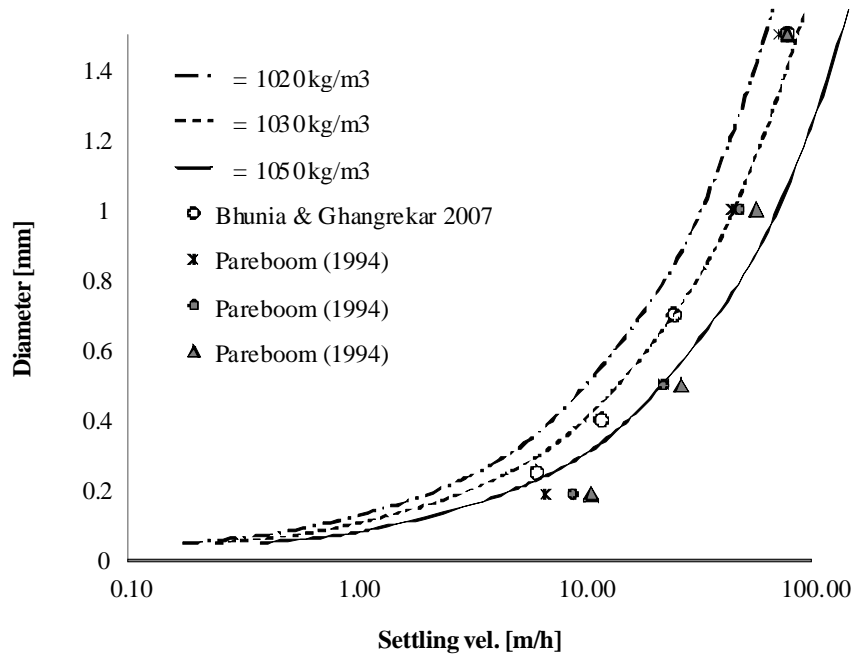


Fig. 2. Granule size vs. settling velocity

reactor while avoiding the use of a large number of parameters, as formulated and discussed in the following sections.

MATERIAL & METHODS

The main assumptions used in the model are;

1. In the sludge bed, the distribution of particle size is the same at any height in the bed. This allows the definition of an average radius common for the totality of the sludge bed.
2. No transition zone is considered in the sludge distribution.
3. Substrate degradation rate is controlled by the hydrolysis reaction, since it is the rate-limiting step in most of the cases (Dewil *et al.*, 2008). The substrate consists of only one biodegradable organic material.
4. The model is one-dimensional and transient; only variations along the height of the reactor are considered.
5. Granules are spherical in shape.

The reactions in the UASB reactor are considered in a simple and illustrative way by modeling the system as being composed of N small CSTRs (Fig. 3). In the sludge bed, a maximum volume fraction of sludge ($\varphi_{P_{max}}$) is defined; the sludge is made up of the active and non-active biomass. Initially the sludge is distributed in a certain number of reactors with a volume fraction of $\varphi_{P_{max}}$ and one reactor on the top of the

sludge bed with the remainder sludge. The others reactors have, then, no sludge. During operation of UASB reactor, the sludge bed expands as the amount of biomass increases. As illustrated in Fig. 3, however, the volume fraction (φ_P) of each CSTR can only reach at most, with the surplus being propagated into the next CSTR.

Based on this conceptual model, three sets of equations can conveniently be formulated to describe the mass balance of substrate, the active and the inactive biomass for each of the CSTRs. The equations for the i-reactor are, respectively,

$$\frac{dS_i}{dt} = \frac{Q}{V_i} * (S_{i-1} - S_i) - K_i * S_i \tag{2}$$

$$\frac{dX_i}{dt} = K_i * S_i * Y - K_d * X_i \tag{3}$$

$$\frac{dE_i}{dt} = K_d * X_i \tag{4}$$

In these equations, the terms on the left-hand side correspond to the accumulation of substrate, active biomass, and non-active biomass, respectively. In Equation (2), the first term on the right-hand side is the advective term and the second one is the reaction term. The reaction rate (K_i) in Equations (2) and (3) is determined by an expression later developed in the

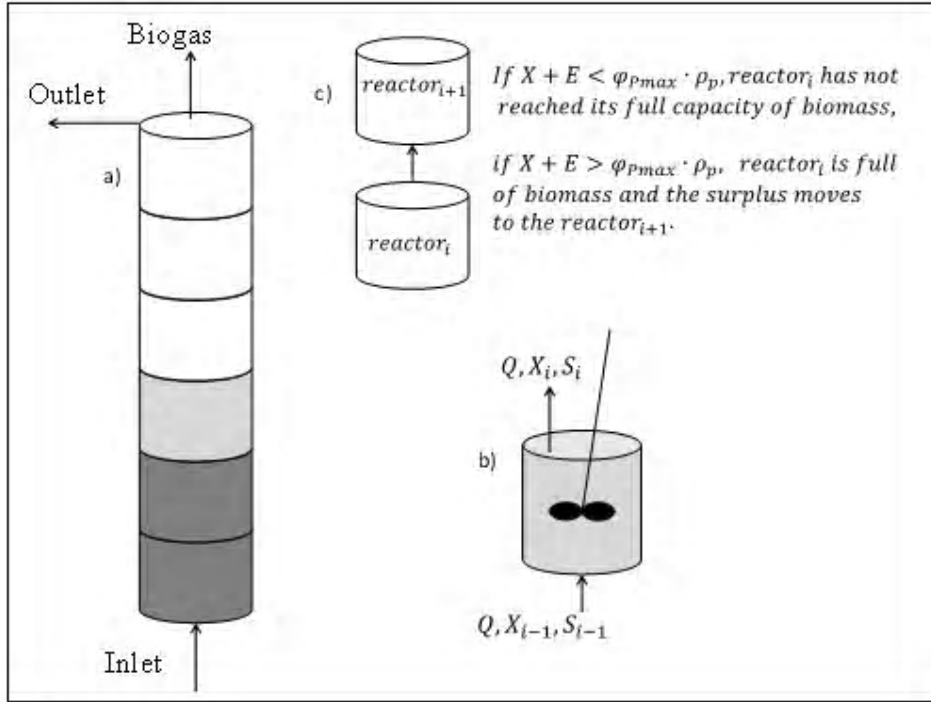


Fig. 3. a) UASB reactor seen as many CSTRs, b) i-reactor, c) Representation of i and i+1 reactors

paper. The advective terms are ignored in Equations (3) and (4), since the biomass is assumed to be kept in the reactor. The terms on the right-hand side of Equation (3) correspond to the biomass generation and decay rates respectively. Note that the effect of the washout may be included in the model in Equations (3) and (4), by changing the decay constant K_d to a new decay constant K'_d , which is a function of both the water flow-rate in the reactor and the granule structure (i.e. compaction).

To determine K_i in Equations (2) and (3), a quasi-steady state mass balance for the concentration of substrate in the granule is applied because the amount of substrate degraded in a time interval is much greater than the variation of substrate in the granule in the same time interval. This allows us to write,

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dS_p}{dr} \right) - \frac{k}{D_A} S_p = 0 \quad (5)$$

subjected to the following boundaries conditions:

$$D_A \frac{dS_p}{dr} \Big|_{r=R} = k_m (S - S_p|_{r=R}) \quad (6)$$

$$S_p|_{r=0} = \text{finite} \quad (7)$$

The solution of the ordinary differential equation (Equation 5) is then, as presented by Bird *et al.*, (2002),

$$S_p = \frac{C_1}{r} \cosh \left(\sqrt{\frac{k}{D_A}} \cdot r \right) + \frac{C_2}{r} \sinh \left(\sqrt{\frac{k}{D_A}} \cdot r \right) \quad (8)$$

The values of the constant C_1 and C_2 are determined by use of the boundaries conditions (Equation 6 and 7). The resulting expression describes the substrate concentration within the granule as a function of both the concentration at the granule surface and the concentration of the bulk liquid flow. It can be written as,

$$\frac{S_p}{S} = \frac{R^2}{r} \left[\frac{k_m \left(1 - \frac{S_p|_{r=R}}{S} \right) \sinh \left(\phi \frac{r}{R} \right)}{D_A (\phi \cosh \phi - \sinh \phi)} \right] \quad (9)$$

where $\phi = \sqrt{k/D_A} \cdot R$ is the Thiele Modulus (Levenspiel, 1999).

Thus, substrate concentration at the particle surface ($S_p|_{r=R}$) is given by,

$$(10)$$

$$\frac{S_p|_{r=R}}{S} = \frac{Rk_m \sinh \phi}{D_A (\phi \cosh \phi - \sinh \phi) + Rk_m \sinh \phi}$$

Substituting Equation (10) into (9) gives us a convenient expression describing the substrate concentration inside the granule,

$$S_p = S \frac{R^2}{r} \left[\frac{k_m \sinh\left(\phi \frac{r}{R}\right)}{D_A(\phi \cosh\phi - \sinh\phi) + Rk_m \sinh\phi} \right] \quad (11)$$

As a result, the mass flow rate (W_S) of the substrate into a single granule can be written, by applying Fick's law at the granule surface, as

$$W_S = -4\pi R^2 D_A \left. \frac{dS_p}{dr} \right|_{r=R} = \frac{4\pi R^2 k_m S [D_A(\phi \cosh\phi - \sinh\phi)]}{D_A(\phi \cosh\phi - \sinh\phi) + Rk_m \sinh\phi} \quad (12)$$

It follows that the kinetic rate (K) in Equations (2) and (3) may be determined using the number of granules per unit of volume of reactor (N_p) and the bulk concentration of substrate (S), giving rise to,

$$K = \frac{4\pi R^2 k_m N_p [D_A(\phi \cosh\phi - \sinh\phi)]}{D_A(\phi \cosh\phi - \sinh\phi) + Rk_m \sinh\phi} \quad (13)$$

where we have omitted the subscript "i" on K for the sake of simplicity in the notation. If N_p is further related to the volume fraction (φ_p) occupied by the granules (i.e. $E_i + X_i = \varphi_p \cdot \rho_p$), we can thus write,

$$K = 3k_m \frac{\varphi_p}{R} \frac{D_A(\phi \cosh\phi - \sinh\phi)}{D_A(\phi \cosh\phi - \sinh\phi) + Rk_m \sinh\phi} \quad (14)$$

This kinetic rate has different values in each of these small reactors, since different amounts of active biomass are found in the reactors. The calculations are initialized by determining the number of granules in the UASB reactor, which may be calculated by using the amount of biomass in the reactor and the initial average granule size. The kinetic rate, which is calculated from Equation (14), is posteriorly replaced in Equations (2) and (3). Since the amount of biomass is varying with time, the biomass is redistributed in the small reactors according to the maximum volume fraction. A new average radius is then determined. In what follows, three cases comprise the sets of simulations using data by Nacheva et al. (2009). The first set of simulations was performed to show the

capabilities of the model, while in the second set, the experimental data by Nacheva et al. (2009) were used to validate the model. Finally, an analysis of sensitivity was carried out in the last set.

RESULTS & DISCUSSION

Nacheva et al. (2009) studied the performance of a UASB reactor treating wastewater from a sugar cane mill. They divided their experimental work into four stages, each with different inlet substrate loading rates in the facility. The upflow velocities in the reactor were 0.02 m/h, 0.04 m/h, 0.08 m/h, and 0.12 m/h for stages 1, 2, 3, and 4 respectively. The operating time for each stage was 60 days. Since the flow rate of stage 1 was too low to demonstrate the capability of the model, the one of stage 2 was chosen. The operating time of the UASB reactor was extended to 2 years in order to observe clearly the process of microorganism growth and the expansion of the biomass bed with time. The growth of biomass with respect to the amount of degraded substrate was calculated according to Richardson and Peacock (1994) (i.e. Yield = 0.03). The reactor was loaded with 1.48 kg of active biomass and 1.0 kg of non-active biomass and the inlet substrate concentration was 4.3 kg/m³. The other data used in the simulation are given in Table 1. Fig. 4 shows the substrate concentration along the 16 small reactors. The profile of the substrate concentration is shown at 4 different times, with the last one corresponding to 2 years. Initially the biomass was located in the two reactors at the bottom; hence the substrate degradation took place only in those two reactors. At the end of the first time interval, i.e. after 180 days, the substrate degradation occurred in the three first reactors. After two years, the biomass reached reactor 6. Correspondingly, the methanogenic activity took place in the first six reactors, increasing the degradation

Table 1. Data used in the simulations

Entity	Value	Units
Height of the column	1.35	[m]
Yield	0.03	[-]
Number of CSTR, N	16	[-]
Maximum volume fraction of sludge, φ_{pmax}	25	[%]
Decay rate constant, K_d	2.6e-4	[1/h]
Reaction rate in granule, k	9.5	[1/h]
Diff. coeff. in particle, D_A	3.0e-7	[m ² /h]
* Mass transfer coeff., k_m	0.042	[m/h]
Density of sludge, ρ_p	1026	[kg/m]

* Taken from Gonzalez-Gil et al., (2001)

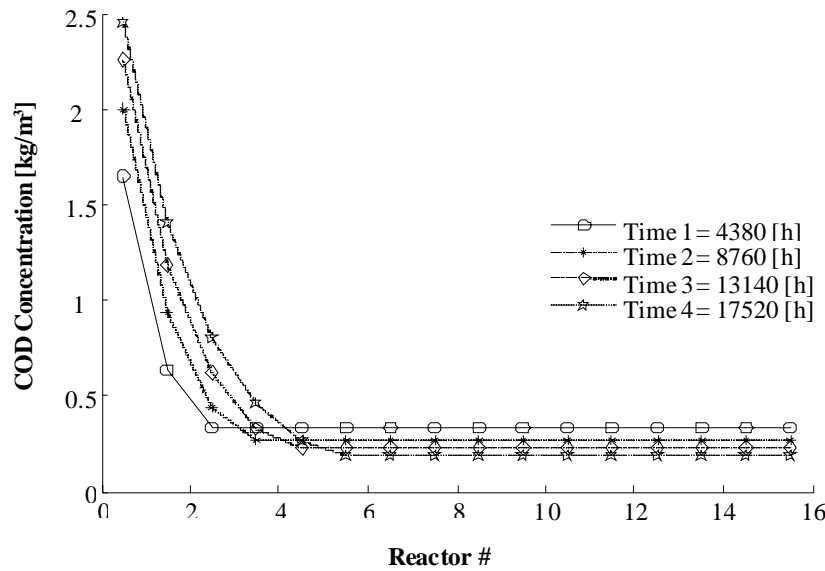


Fig. 4. Behavior of the substrate concentration along the height of the UASB reactor

of the substrate concentration until reaching a removal of 96%, and the sludge bed expanded to about one third of the UASB reactor.

The profile of the active biomass is shown in Fig. 5. It tends to propagate with time, due to the birth of new cells; but the decay of biomass reduces the active population in the UASB reactor. Despite the fact that active biomass is almost constant in the UASB reactor, its concentration decreases strongly in the reactors containing the sludge bed (Fig. 5). This occurs due to decay and to the limitation in the amount of biomass (active and non-active), which cannot exceed a predetermined value, $(\phi_{p,max})$. Correspondingly, the non-active biomass is continuously increasing.

In Fig. 6 the amount of active biomass in the UASB reactor is shown to decrease slightly in the first time interval, being however almost constant for the remaining time. This phenomenon is attributed mainly to decay, as Nacheva et al. (2009) have reported during their experiments. In addition, Fig. 6 shows that the total amount of biomass in the UASB reactor increases linearly with time. The average radius of the granules was initially set at 0.25 mm. Since the amount of total biomass is continuously increasing with time, a similar relationship is expected for the average granule size, which is determined by the total amount of biomass and the number of granules. Fig. 7 shows the variation of the average radius with time, assuming that the number of granules in the UASB reactor is kept unchanged. It reached a value of 0.38 mm after two years. To validate the model, a comparison between the experimental results obtained by Nacheva et al. (2009) and the simulated ones was done. Following

the experimental work, the simulations were divided in four stages with an operation time of 60 days in each stage, using the same sets of data as the ones given by Nacheva et al. (2009). The calculated results at the end of a stage (e.g., the amount of biomass and the granule size) were employed as input values for the next stage. The upflow velocity varied for every stage as reported by Nacheva et al. (2009). These values as well as some results from the simulations are shown in Table 2.

Using the data for the first stage, the volumetric substrate conversion rate was adjusted as 9.5 1/h, being constant for the others stages. This value is high compared to the values obtained by Huang & Chou (2005). The discrepancy could be explained by the different kinds of substrates used (i.e. sucrose, phenol, acetate, and sugar cane mill wastewater). Another possible cause could be the granule size, which affects the conversion rate (Wu *et al.*, 1995). For large granules, only the zone close to the granule surface is active, while for small granules, the totality of the granule may participate in the substrate degradation.

Fig. 8 shows the experimental from the simulations. It demonstrates that the behavior of the substrate removal from the model response is similar to that reported by Nacheva et al. (2009). The major substrate removal appears in stage 1. It subsequently shows lower values for every stage, due to the reduction of the hydraulic retention time (HRT) which decreases by a factor of 2 from one stage to the other. Nacheva et al. (2009) reported significant washout in stage 4, which was accounted for in the simulation.

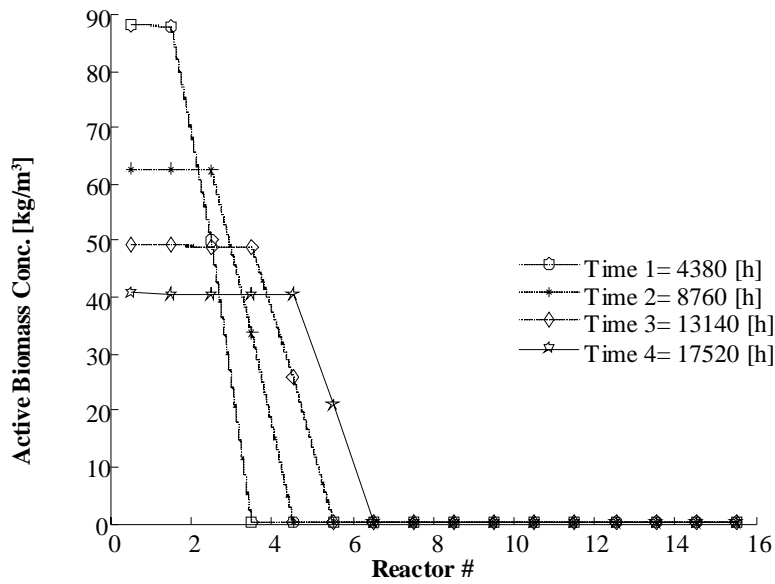


Fig. 5. Behavior of the active biomass along the height of the UASB reactor

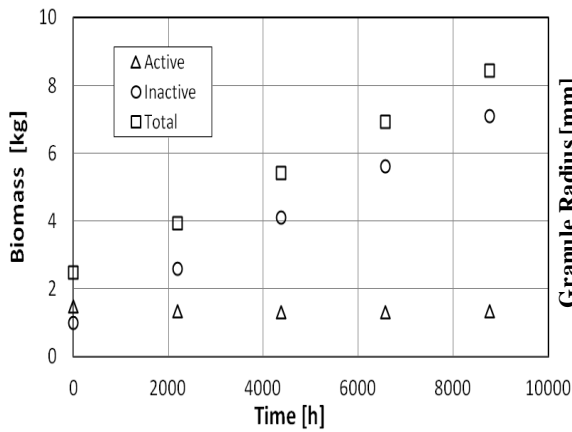


Fig. 6. Amount of active, inactive, and total biomass in the UASB reactor

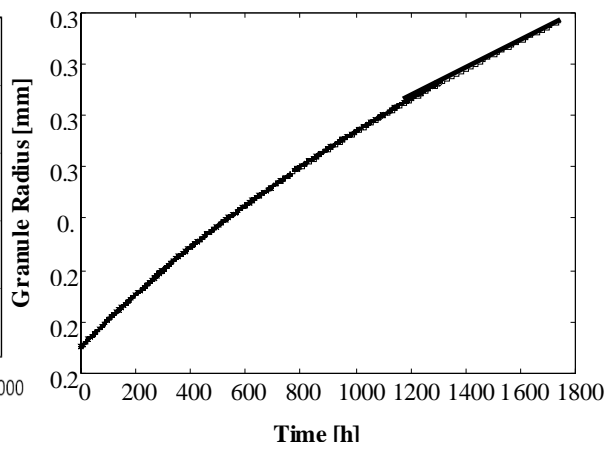


Fig. 7. Granule size as a function of time

Table 2. Experimental and simulated results

Entity	Stage 1	Stage 2	Stage 3	Stage 4
Upflow velocity, [m ³ /m ² h] ^a	0.02	0.04	0.08	0.12
Time interval, [days] ^a	0 - 60	60 - 120	120 - 180	180 - 240
Simulated granule radius ^b , [m]	0.22	0.27	0.29	0.30
Experimental removal of COD, [%] ^a	96	92	84	66
Simulated removal of COD, [%]	96	89	82	67

^aNacheva et al.¹²; ^bAt the end of the stage

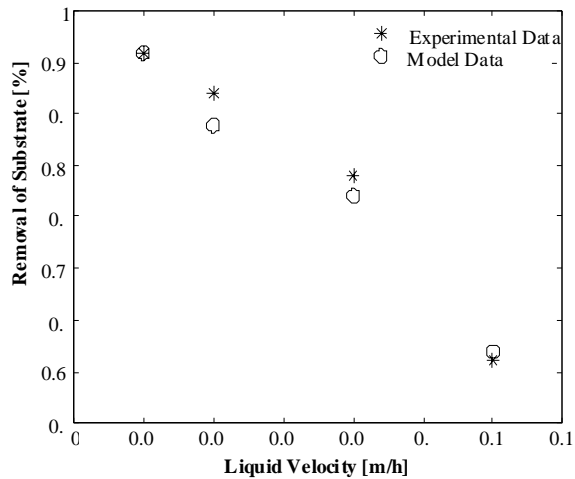


Fig. 8. Comparison between both the experimental

The sensitivity analysis was done by taking the data of stage 2 from Nacheva et al. (2009) as the basis, but extending the working time of the UASB reactor to 12 months. The model performance was studied by varying the number of CSTRs (N), the mass transfer coefficient (k_m), the volumetric conversion rate (k), the diffusion coefficient (D_A), and the maximum concentration of biomass in CSTR. The results show that the removal of substrate increases with the number of small reactors used to describe the UASB reactor, as shown in Fig. 9. Larger dispersion causes a reduction of substrate removal.

The mass transfer coefficient is important for the substrate removal when it exhibits low values. However, Fig. 10 shows that at high values of k_m , the removal of the substrate becomes constant because the substrate degradation is governed by the diffusion within the granule. Similar behavior occurs with the diffusion coefficient, as shown in Fig. 11. In the simulations, it

was established that the maximum volume fraction for the biomass in the reactors is 25%. According to literature, this value may be as high as 35% (Huang et al., 2003; Kalyuzhnyi et al., 2001). In the sensitivity analysis, the maximum volume fraction of biomass varies between 15% and 40% in the simulations. The results shown in Fig. 12 indicate that if the maximum volume fraction of biomass increases, the biomass is distributed in a smaller number of reactors, resulting in a significant reduction of the substrate removal.

The substrate conversion rate also influences significantly the removal of the substrate, as shown in Fig. 13. Large substrate removal is obtained when high values of k are used. This suggests that the parameter should be determined with a high degree of confidence, since different values of k can be obtained from the same sample, depending on the particle size. In practice, Wu et al. (1995) reported that the value of k increased with small granules size.

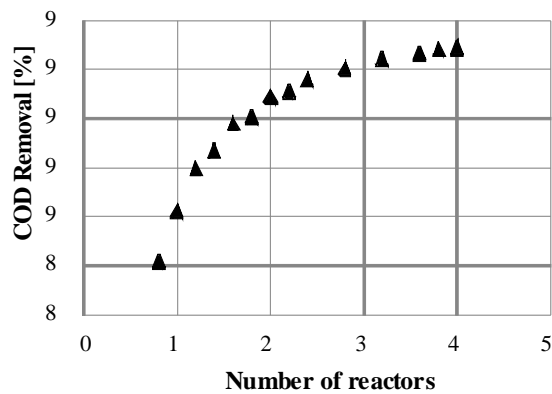


Fig. 9. Substrate removal with different values of N

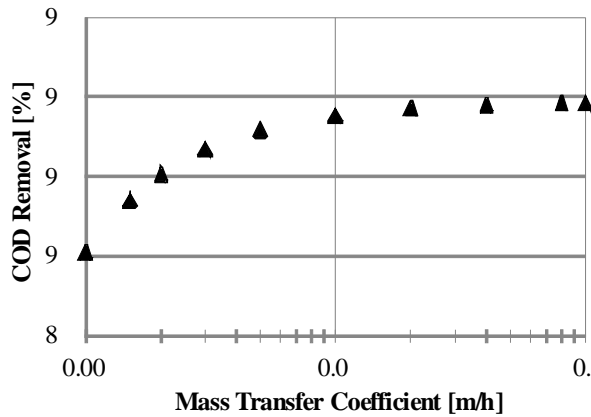


Fig. 10. Substrate removal with different values of k_m

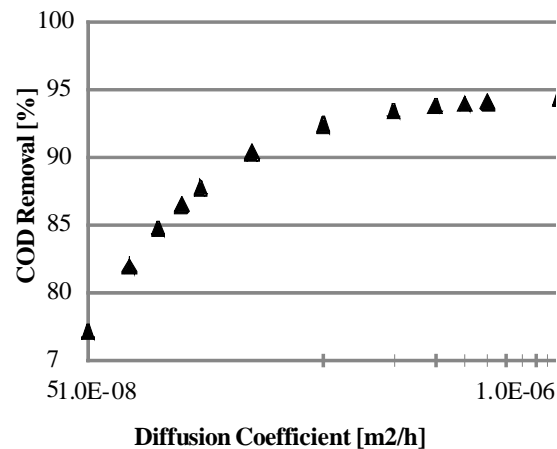


Fig. 11. Substrate removal with different values of D_A

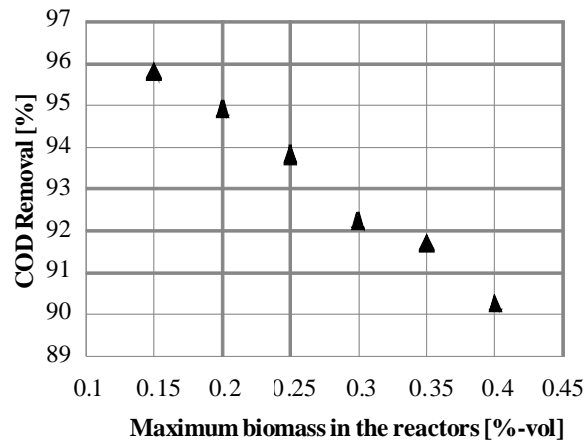


Fig. 12. Substrate removal with different maximum values of biomass per CSTR

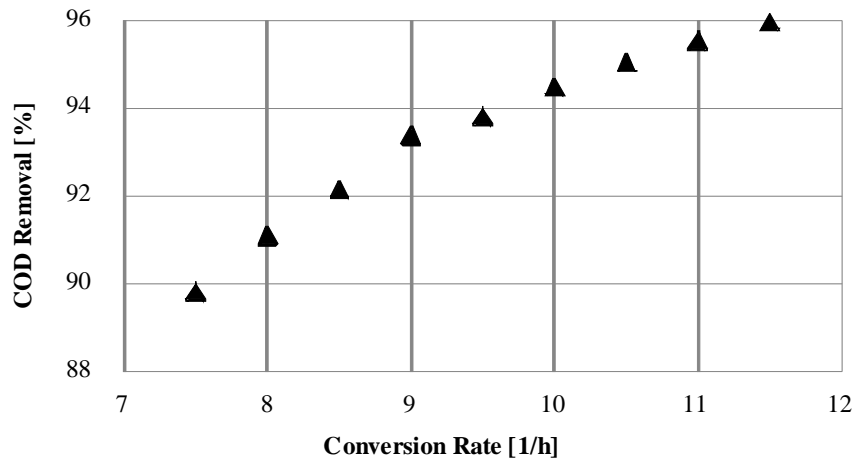


Fig. 13. Substrate removal with different conversion rates

CONCLUSION

The developed model describes the behavior of the substrate, the growth of the biomass, and the size of the granules in the reactor. It includes few parameters compared to the existing models, while still showing how the height of the sludge bed is increasing with time. The main contribution of the paper is, however, the development of an analytical expression describing the reaction within the granule, which takes into account mass transfer through the liquid film around the granule, the intra-diffusion and the specific reaction within the granule.

The model was successfully applied to simulate the behavior of a UASB reactor treating sugar cane wastewater. Both the experimental data and the response of the model show similar performance of the UASB reactor. The major concentration of substrate is degraded at the lower part of the UASB reactor where the major concentration of biomass is present. A better removal of COD occurred at the lowest upflow velocity, due to the longest time of contact between the substrate and the microorganisms. Based on the sensitivity analysis, it may be concluded that five studied parameters (i.e. k , k_m , D_A , N and the volumetric fraction of biomass in the small reactors) are important in determining the performance of the UASB reactor. Consequently, these parameters should be carefully determined. The model can be used to improve and control existing UASB reactors.

ACKNOWLEDGEMENTS

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NOTATION

D_A	Diffusion coefficient within the granule, m^2/h
D_L	Dispersion coefficient, m^2/h
E	Concentration of non-active biomass, kg/m^3
K	Kinetic rate constant, $1/h$
k	Substrate conversion rate within the granule, $1/h$
k_m	Mass transfer coefficient, m/h
K_d	Decay constant, $1/h$
N	Number of small reactors
N_P	Number of granules per reactor volume, $granules/m^3$
Pe	Péclet number
Q	Flow rate, m^3/h
r	Radial distance from the center of the granule, m
R	Radius of the particle, m
S	Substrate concentration in the reactor, kg/m^3
S_P	Substrate concentration inside the particle, kg/m^3
t	Time, h
u	Water velocity, m/h
V	Volume of the reactor, m^3
W_S	Mass flow at the granule surface, kg/h
X	Biomass concentration, kg/m^3
Y	Yield
ϕ	Thiele modulus
φ_P	Volumetric fraction occupied by the granules
ρ_P	Density of granules, kg/m^3

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