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Dynamic Modeling of Granular Sludge in UASB Reactors

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Abstract

In this paper, a mathematical model has been derived to predict the granulation time of anaerobic sludge in UASB reactors. In the proposed model, some physical, chemical and biological parameters affecting the granulation phenomena have been considered. To validate the model, 12 pilot-scale experiments in 4 UASB reactors are carried out and the results are discussed here. The reactors are started up at different environmental conditions and the granulation time in each experiment is determined. The results show that the model is able to explain different mechanisms involved in the granulation process.

Keywords: *Modeling, UASB Reactor, Granulation, Anaerobic Sludge*

Introduction

Bacterial aggregation in the form of granules is an essential process in UASB reactors. This aggregation occurs mainly during the start-up period of these reactors when suitable process parameters are maintained [1]. The nature of the microorganism connection into aggregates is not clear and a number of slightly different theories have been published. Theories of granulation include the influence of: a) surface activity, b) relative substrate kinetics, c) interactions and spatial requirements of obligate syntrophic groups and d) impact of a number of environmental factors such as pH, temperature, and intermediate concentrations [2].

In general, it is believed that many physical, chemical and biological factors are involved in granulation phenomena in UASB reactors such as: sludge loading rate, quantity or concentration of seed/biomass, initial microbial population, type of wastewater and operating conditions. Factors affecting the microbial aggregation have been studied in numerous reports in order to understand the granulation mechanism [3,4]. However, the granulation process has not been possible to characterize due to a large number of factors involved and also the difficulty in continuous measurement of dynamic granular growth [5]. This could be one of the reasons behind the very different values reported for granulation time even under similar operating conditions. Furthermore, there are still controversy about the impact of diffusion and mass-transfer resistance on substrate utilizetion rate in anaerobic systems [6].

The time taken for the formation of granules, i.e., granulation time, is a variable and depends on a number of parameters in-

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fluencing the process of granulation [7]. Generally, the microbial aggregation property seems to be inducible [1]. Therefore, a good mathematical model of granulation could serve as a valuable tool in understanding the behavior of the reactor and so, in providing the proper condition for granulation of sludge and shortening the start-up period of these reactors. Besides, these kinds of models could be generally used as a tool in automation of UASB reactors.

In this paper, a dynamic mathematical model has been derived for the granulation phenomena in UASB reactors. The model explains the growth in size of granules versus time.

Modeling Basis

In the literature, various definitions are proposed for the granulation phenomena. These are used to establish a basis for granulation modeling. According to one definition, granulation is referred to as a combination of different groups of bacteria in which their composition and populations are related to the type of wastewater, reaction rates and the produced intermediate products [8]. In fact, each granule particle is an indication of the whole sludge in the reactor in which all the degradation reactions from the synthesis to the methanisation stages occur.

In the second definition, a granule is a mass of bacteria stuck together on their surfaces by immobilization mechanism. Granules may be considered as a network of filaments (polysaccharides), held intact by fibrous strands interwoven with the component granule bacteria, resulting in an aggregated biomass of high activity [7]. It is a microbial selection process through dynamic selection pressures that is imposed on the sludge [5]. These pressures select the bacteria that form well-settling aggregates in contrast to those dispersed or loosely aggregated. Therefore, the major components of a granule are bacteria and the presences of mineral agents are considered as granulating aids [9,10].

In another representation, granules are called masses of bacteria that have enough resistance to suffer the hydraulic tensions produced in the reactor against breaking and washout off the reactor. Therefore, they can stay inside the reactor although their size may be smaller than a millimeter. In order to derive a mathematical model for the granulation of anaerobic sludge here, we consider the whole sludge as a mass of bacteria.

Mathematical Model

According to the above definitions, it is possible to establish a relation between synthesis of bacteria, creation of granules and sludge escape from the reactor. It is assumed here that all the bacteria produced are being converted into granules and the shattered granules are exiting from the reactor. In the start-up period, granule formation is predominant and at the end of the start-up stage or steady-state conditions, the rates of granule breaking and growing are equal. Therefore, the following model can be considered to describe the granulation phenomena:

$$\text{produced bacteria} \xrightarrow{k_1} \text{granules} \xrightarrow{k_2} \text{departed sludge (bacteria)}$$

This can be represented by the following equation:

$$d(\text{mass of granules})/dt = k_1\ (\text{bacteria production rate}) - k_2\ (\text{mass of granules}) \quad (1)$$

$$dM/dt = k_1\, dX/dt - k_2\, M \quad (2)$$

where

M = Mass of granules in the reactor
dX/dt = Bacteria production rate
k_1 = Coefficient of production
k_2 = Coefficient of declining

According to equation 2, it can be concluded that if $dM/dt>0$ then granulation occurs but if $dM/dt<0$, it does not. The term dX/dt can be expressed in terms of X (biomass concentration) by the following equation:

$$dX/dt = \mu X - k_d X \quad (3)$$

Where μ is specific growth rate (d^{-1}) and k_d is the bacteria decay coefficient (d^{-1}).
Assuming that all the bacteria in the reactor are in the form of granules (the non-granulated ones are washed out from the reactor), thus replacing X by M, we have:

$$dX/dt = \mu M - k_d M \quad (4)$$

Having:

$$\mu M = - Y.\ dS/dt \quad (5)$$

$$dS/dt = \frac{S_0 - S}{\tau_0} = \frac{S_0 - S}{\tau_0} \times \frac{S_0}{S_0} = -R \cdot VLR \quad (6)$$

Therefore:

$$dX/dt = Y.\ R.\ VLR - k_d M \quad (7)$$

where Y is bacteria yield coefficient, R is process efficiency, τ_0 is hydraulic retention time and VLR is volumetric loading rate.
The coefficients of equation 1 (k_1 and k_2) are functions of different physical, chemical and microbiological factors:

$$k_1 = g(pH, T, i) \quad (8)$$

$$k_2 = m_d f(U, D/UL, VLR, N, P, S, pH, etc) \quad (9)$$

Parameter k_2 is in fact indicating the fraction of bacteria that are not converted to granules and escape from the reactor. Parameter m_d is related to the breakage of bacteria. It is also assumed that each factor affecting the destruction of bacteria is operating individually. Therefore, equation 8 can be rewritten as the multiplication of several factors:

$$k_2 = m_d.\ f_1(U).\ f_2(D/UL).\ f_3(VLR) \quad (10)$$

Considering that k_1 and k_2 are known, equation 2 can be written in the following form:

$$dM/dt = k_1.\ Y.\ R.\ VLR - (k_2 + k_1 k_d)M \quad (11)$$

On the other hand:

$$VLR = S_0/\tau_0 \quad (12)$$

At T= 37.5 ºC and pH= 7-7.5 : $k_1=1$

Then, we have:

$$\mu \cdot X = Y \cdot R \cdot VLR \quad (13)$$

$$\mu \cdot X = Y \cdot R \cdot S_0 / \tau_0 \quad (14)$$

$$\tau_0 = Y \cdot R \cdot S_0 / \mu \cdot X \quad (15)$$

On the other hand:

$$\mu = \mu_m \cdot S/(K_s + S) \quad (16)$$

So;

$$\tau_0 = (YK_s / \mu_m X)R/(1-R) + (Y/\mu_m X)RS_0 \quad (17)$$

By substituting τ_0 in equation 4:

$$\begin{aligned} dM/dt &= (\mu_m M \cdot R \cdot S_0 /((R/1-R)\cdot k_s) + R \cdot S_0) \\ &\quad - (k_d + k_2)\cdot M \\ &= (\mu_m \cdot M \cdot S'/(k'_s + S')) - k'_d \cdot M \end{aligned} \quad (18)$$

$$\ln M / C = (\mu_m \cdot S'/(k'_s + S'))\cdot t - k'_d \cdot t \quad (19)$$

where:

$$S' = R \cdot S_0$$

$$k'_s = R/(1-R) \cdot k_s$$

$$k'_d = k_2 + k_d$$

Assuming that all granules are spherical and equal in size, then equation 15 can be rewritten as:

$$\ln D / D_0 = \left(\left(\mu_m . S' / \left(k'_s + S'\right)\right) - k'_d\right) \cdot t / 3 \quad (20)$$

In the above equations:

μ_m = Maximum specific growth rate

C = Sludge seed mass

R = COD removal efficiency

k_d = Bacteria's decay coefficient

k_2+k_d = Granule's decay coefficient

D_0 = Sludge seed diameter

D = Granule diameter at time t

S = Substrate concentration in reactors

S_0 = Influent COD concentration

Equation 20 indicates that granulation phenomena is a bacterial behavior and granules can be considered as fermentation products. This equation is very similar to that obtained by Yan and Tay in 1997 [5].

Materials and Methods

The effects of different parameters on the granulation phenomena have been investigated using 4 pilot-scale UASB reactors in which 12 experiments are carried out. The evaluated parameters are: influent upflow velocities, pH, sulfate concentration and feed to microorganism ratio (F/M). The results have been used for the evaluation of proposed models derived in the previous sections.

Wastewater and Sludge Characteristics

The feed comprises diluted molasses and the sludge seed is prepared from the digested sludge taken from an anaerobic digester of a municipal wastewater treatment plant. Before transferring the sludge to the reactors, the sludge was cultivated with the wastewater in batch conditions. It took a three-month rest period before the sludge was poured into the reactors to about 50 percent of the total reactor volume. The characteristics of the sludges of each reactor are indicated in Table 2. Sodium hydroxide was used for pH adjustment during the experiments.

Experimental Set-up

Four identical UASB reactors with a capacity of 37.5 l and a diameter of 20 cm were prepared and equipped with proper control systems and recirculation flow (Figure 1).
Four different experimental procedures were implemented in order to investigate the effect of different parameters on the granulation time:

Case 1: The Effect of F/M

The pH values in all reactors were 7. The experimental conditions are shown in Table 1.

Table 1. Experimental conditions of the reactors in case 1

Reactor No.	1	2	3	4
Upflow velocity, m/h	1.5	1.5	0.8	0.4
COD, mg/l	1000	1500	1500	3500
F/M	0.5	1	1	1.5

Case 2: The Effect of Sulfate at a Constant COD

The influent sulfate concentrations were different for each reactor. But, the influent COD was constant and equal to 1000 mg/l leading to different COD/sulfate ratios in the reactors. The upflow velocity was equal to 1 m/h in all the reactors. The operational conditions are specified in Table 2.

Table 2. Experimental conditions of the reactors in case 2

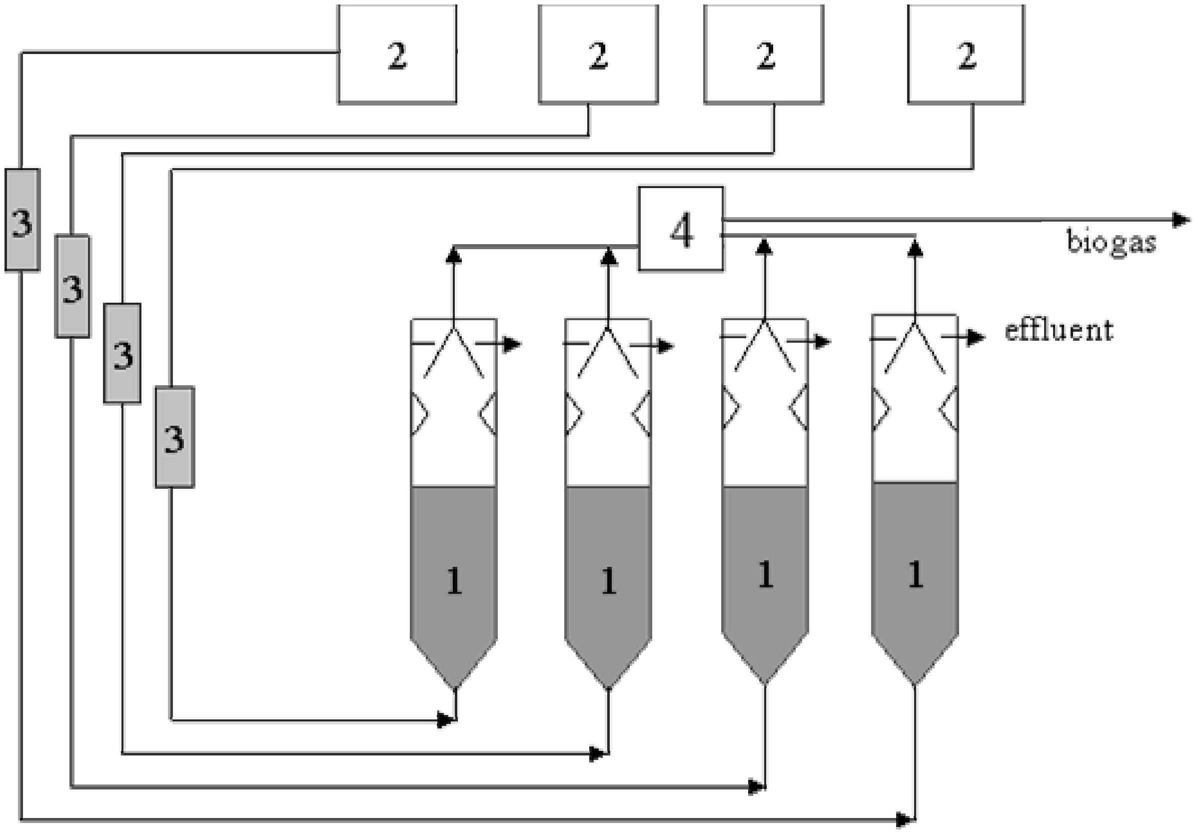
Reactor No.	1	2	3	4
Sulfate, mg/l	100	500	1000	1500
COD, mg/l	1000	1000	1000	1000
pH	7	7	7	7

Case 3: The Effect of pH

In this set of experiments, pH was different in the reactors while values of other parameters were the same, as shown in Table 3. Upflow velocity was kept at 1 m/h for all the reactors.

Table 3. Experimental conditions of the reactors in case 3

Reactor No.	1	2	3
Sulfate, mg/l	500	500	500
COD, mg/l	1000	1000	1000
pH	6.5	7	7.8



1. UASB reactors
2. Feed tanks
3. Heat exchangers
4. Gas collector
5. Sampling valves

Figure 1. Schematic diagram of UASB reactors

Case 4: The Effect of COD and Sulfate with a Constant COD/Sulfate Ratio

In these experiments, the upflow velocity was again equal to 1 m/h and the COD/sulfate ratio was equal to 2 in the reactors but CODs and sulfates were different, as indicated in Table 4.

Table 4. Experimental conditions of the reactors in case 4

Reactor No.	1	2	3
Sulfate, mg/l	500	1000	1500
COD, mg/l	1000	2000	3000
pH	7	7	7

Results

In this section, the results of different factors affecting the granulation time of the sludge obtained from the experiments explained above are summarized. The mathematical model of granulation (equation 20) has been calibrated with the experimental data obtained in this study. Values of some of the coefficients of the model are adopted from the literature; others are calibrated by fine-tuning the model to match the experimental data collected. In each case, the coefficient of decay of granules, i.e., k'_d, are calculated using the mathematical model and are reported in Tables 5-8. The kinetic parameters of the model are taken from reference [10] and indicted in Table 9. The variations of k'_d against the manipulated parameters are plotted in Figure 2 for the experimental cases.

Table 5. Experimental results of case 1

Reactor No.	1	2	3	4
Granulation occurrence	Yes	Yes	Yes	Yes
Granulation time, days	56	41	48	64
COD removal (R), %	88	90	87	93
k'_d	0.06	0.06	0.1	0.14
H_2S, mg/l	—	—	—	—

Table 6. Experimental results of case 2

Reactor No.	1	2	3	4
Granulation occurence	Yes	Yes	Yes	No
Granulation time, days	45	33	45	-
COD removal (R), %	85	90	84	78
k'_d	0.08	0.03	0.095	0.135
H_2S, mg/l	30	80	127	160

Table 7. Experimental results of case 3

Reactor No.	1	2	3
Granulation occurrence	No	Yes	Yes
Granulation time, days	-	33	52
COD removal (R), %	83	90	87
k'_d	-	0.03	0.076
H_2S, mg/l	124	80	22

Table 8. Experimental results of case 4

Reactor No.	1	2	3
Granulation occurrence	Yes	Yes	No
Granulation time, days	52	68	-
COD removal (R), %	87	87	89
k'_d	0.03	0.1	-
H_2S, mg/l	22	168	260

Table 9. Constants used in the calculations

Parameters	Values	Units
μ_m	$(4.7 \pm 0.8) * 10^{-5}$	s^{-1}
k_s	$(38 \pm 3) * 10^{-3}$	kg COD/m^3

Discussion

Table 5 shows that by increasing the influent COD from 1000 mg/l to 3500 mg/l, the granulation time increases. Also, k'_d obtained from the mathematical model increases from 0.06 to 0.14 implying that less granulation of sludge is occurring. This indicates consistency between the model and the experimental data in this case. Also, it can be concluded that granulation is faster in low-strength wastewater during the start-up of UASB reactors. It should be noted that in this case, the F/M ratio is actually changed from 0.5 to 1.5 and the minimum granulation time has been obtained at the lowest F/M ratio.

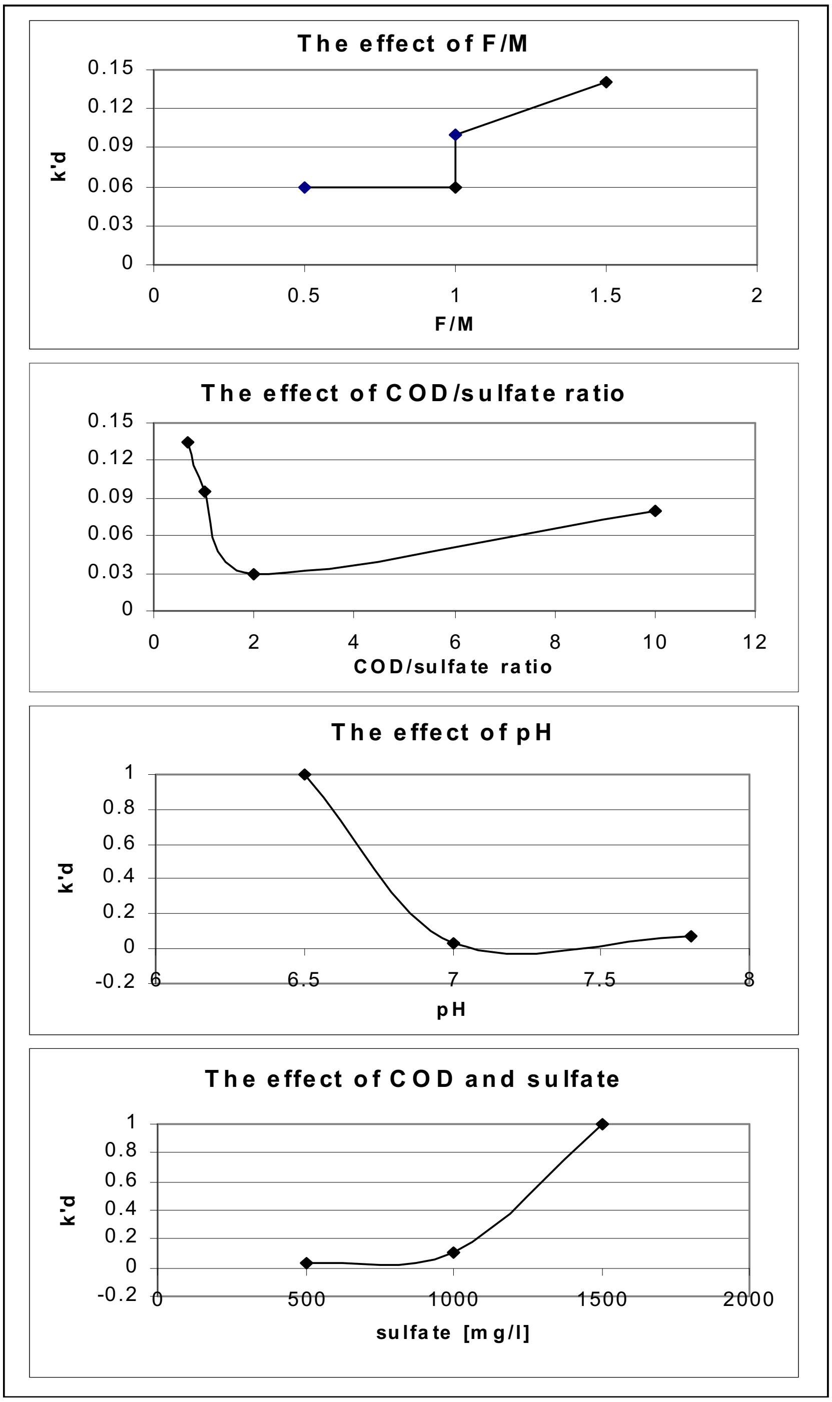


Figure 2. k'_d values obtained from the model and using the four cases of experimental data

Figure 2 shows that k'_d decreases from 0.08 to 0.03 for reactor 2 where sulfate concentration is changed from 100 to 500 mg/l or in other words, COD/sulfate ratio is changed from 10 to 2. Thereafter, an increase of k'_d can be observed by increasing the sulfate concentration or COD/sulfate ratios greater than 2. It can be concluded that here a value of sulfate concentration around 500 mg/l could be appropriate for the granulation in this case. Also, Table 6 indicates that the granulation time determined by the experiments is the lowest and this implies the consistency between the model and the experimental results.

Figure 2 also indicates that by decreasing the pH values, the values of k'_d increase from 0.03 to 0.1, implying a reduction in granulation of the sludge. Also, at pH values greater than 7.8 no granulation occurs. This is indeed revealed by the experimental data as shown in Table 7 in which the granulation time has increased by increasing the pH values. This reconfirms that an optimum pH value could be around 7, as stated in the literature.

In case 4 of the experiments, where the COD/sulfate ratio is constant, the values of k'_d increases by increasing the sulfate concentration from 500 to 1500 mg/l. This implies the destruction of granules at sulfate concentrations higher than 1000 mg/l, as can be clearly observed from Figure 2. Also, the granulation time determined by the experiment increases by increasing the sulfate concentration and no granulation occurs at a sulfate concentration of 1500 mg/l.

Conclusions

The following conclusions can be derived from the results of this research:

1. In an ideal situation (in the absence of inhibitors or granule destruction agents), estimation of granulation time using the concentration of influent wastewater is possible by the model proposed here.
2. Using the dynamic model of granulation, the proper environmental condition to achieve a minimum granulation time can be obtained.
3. It can be said that the granulation phenomena may be achieved faster in lower-strength wastewater or more precisely at lower F/M ratios during start-up of UASB reactors.
4. At the applied environmental conditions, an F/M ratio of 0.5, a COD/sulfate ratio of 2, a pH value of 7 and a sulphate concentration of 500 mg/l are appropriate for achieving the minimum granulation time of the sludge during start-up of UASB reactors for the applied wastewater.

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