Simulation of a periodic anaerobic baffled reactor (PABR): steady state and dynamic response

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Abstract The Periodic Anaerobic Baffled Reactor (PABR) is a novel high-rate configuration for wastewater treatment. The reactor resembles an ABR with the compartments arranged in a circular manner. The feeding and effluent points are periodically set in different compartments by proper manipulation of valves that determine the flow pattern. This way of feeding makes the reactor response oscillating and gives the PABR a great flexibility in the operation mode. A 15 litre PABR was operated on a gelatin based medium under steady and variable organic loading rate. The experimental conditions were simulated using a mathematical model whose primary feature was that each compartment was considered as a two-section tank, each section with a different biomass concentration in them. The degree of biomass accumulation was determined indirectly by the operating conditions and the reactor dynamics and was not set a-priori.

Keywords Gelatin; high-rate system; modeling; periodic anaerobic baffled reactor

Introduction

Anaerobic digestion has become a very popular microbial process for wastewater treatment, mainly because of the development of high-rate reactors that allow slow-growing anaerobic microorganisms to remain inside the reactors under short hydraulic retention times. The Anaerobic Baffled Reactor is a high-rate system that has been tested on a variety of wastewaters under a wide range of organic loading rates with success (Barber and Stuckey, 1999). Based on the ABR design concept, the PABR (Periodic Anaerobic Baffled Reactor) is an innovative reactor, initially developed by Skiadas and Lyberatos (1998). The PABR interior space is separated into compartments, each consisting of one downflow and one upflow part. The compartments are arranged in a circular manner in the annular region between two concentric cylinders (Figure 1a). In the PABR, the influent and effluent ports are not fixed as in the ABR, but they can be switched in a periodic mode within a certain time interval (switching period), so that each compartment becomes the first, taking in the influent, in the series within a fraction of the period (switching sub-period) (Figure 1b).

The frequency of the influent and effluent points switching is an operational parameter which can be manipulated to optimize the PABR performance. Depending on the switching frequency, the PABR can operate as an ABR (zero frequency) or as a UASBR (infinite frequency) or at an intermediate mode. Skiadas et al. (2000) studied the effect of the switching frequency on a glucose fed PABR at various dilution rates. At high dilution rates, the PABR performs better at a high switching frequency and vice versa. At intermediate dilution rates, there is a specific value of the switching frequency at which the PABR yields its optimal performance. The periodic behavior of the PABR, as simulations indicate, may be beneficial over the ABR in the case of severe overloading (Skiadas et al., 1998, 2000).

In the present paper, the behavior of a lab-scale PABR is presented under steady and changing conditions, while fed on a gelatin based medium. The PABR was operated at normal organic loading rates (between 3.125 and 6.25 g COD/l/d) at various conditions: 100% step change in the feed concentration or the hydraulic retention time and at steady state. In order to predict the experimental results, an improved modeling frame was developed...
incorporating a kinetic model for the anaerobic degradation of gelatin. The principles and basic equations of the model are described next.

**Materials and methods**

**Reactor configuration**

A 4-compartment, 15 litre PABR constructed out of stainless steel was used. The reactor was equipped with sample ports in every compartment, placed 10 cm from the surface of the mixed liquor and two biogas vents on the top of the reactor. The PABR was maintained at 35°C. The flow was directed via outer pipes by electronic valves (manipulated using a PC) that were programmed to vary the role of each compartment (influent, effluent or intermediate) counterclockwise over time, meaning that for a pre-selected switching period, $T$, the order of the compartments from the influent to the effluent would be (Figure 1b): A-B-C-D if 0 $< t < T/4$, D-A-B-C if $T/4 < t < T/2$, C-D-A-B if $T/2 < t < 3T/4$ and B-C-D-A if $3T/4 < t < T$.

**PABR modeling**

Modeling the anaerobic digestion process in a high rate reactor which retains most of the biomass should focus on the factors that determine solids accumulation. Skiadas et al. (2000) simulated a PABR fed on glucose considering a constant portion of the biosolids removed via the effluent. In order to relax this assumption, it was thought useful to adopt some concepts from previous works in the simulation of UASBR-like systems. As in Skiadas et al. (2000), the PABR was considered as a series of UASB reactors (in a similar way that an ABR is approximated by a series of UASBRs). Each compartment is then divided into two parts: the lower part where the biomass concentration is high and the upper part where biomass concentration is lower and can be considered uniformly distributed due to the adequate mixing caused by the biogas production.

The biomass transfer taking place between the two parts can be depicted as two main streams (Figure 1c) as it has been considered in UASBR modeling (Buijs et al., 1982). The upwards transfer rate of each microorganism group $j$ ($\Phi_{d \rightarrow u}$) is mainly caused by a liquid upward stream, $F_{g \rightarrow u}$, which is proportional to the biogas production rate of the lower part, $Q_{g d}$, (i.e. $F_{j \rightarrow u} = k_w \cdot Q_{g d}$) while the contribution of the flowrate to this direction is considered negligible compared to the adverse effect of the settling velocity:

$$\Phi_{j \rightarrow u} = k_w \cdot Q_{g d} \cdot x_{jd} \Rightarrow \Phi_{j \rightarrow u} = k_{xj} \cdot Q_{Sd} \cdot x_{jd} \quad (1)$$

where $k_w$ is the volume of the liquid transferred by the produced biogas, $k_{xj}$ reflects the ease of transferring the biosolids upwards, and $x_{jd}$ is the microorganism $j$ concentration in the lower part.

![Figure 1](https://iwaponline.com/wst/article-pdf/45/10/81/425019/81.pdf)
The downward biosolids transfer rate, \( \Phi \), is caused partly by the gravity effect on the sludge particles. It is also stimulated by a downward stream, \( F_{u \rightarrow d} \), induced to compensate for the upward stream, \( F_{d \rightarrow u} \). Since these two streams are equal (\( F_{u \rightarrow d} = F_{d \rightarrow u} \)), the downward stream can be directly correlated to the biogas production rate in the lower part:

\[
\Phi_{j u \rightarrow d} = (v_S - v_L) \cdot A_R \cdot X_j^u + k_{x_j u \rightarrow d} \cdot Q_g^d \cdot X_j^u
\]

(2)

where \( v_S \) is the settling velocity of biosolids, corrected by the linear fluid velocity \( v_L \). \( A_R \) is the cross section of each compartment, \( k_{x_j u \rightarrow d} \) quantifies the ease at which biosolids move downwards, and \( x_j^u \) is the microorganism concentration in the upper part.

The volumes of the two parts comprising such systems have been considered constant in previous studies (Buijs et al., 1982). In this work, the boundaries of both parts were allowed to move freely so as to meet the requirement that the biomass concentration in the lower part is constant. This approach is closer to reality, since the concentration of the accumulated biosolids is high enough and practically invariable (Bolle et al., 1986). Therefore, the mass balance equation on the lower part of the compartment, is:

\[
\frac{dV^d}{dt} = F - F_{d \rightarrow u} + F_{u \rightarrow d}
\]

(3)

where \( V^d \) is the volume of the lower part, \( F \) is the flowrate (= \( v_L \cdot A_R \)) and \( F_{d \rightarrow u} \) is the upward stream flowrate, which is a variable and depends on the relative movement of the boundaries of the two parts.

**Solid and liquid phase simulation.** The mass balances for each \( i \) of the \( n \) compounds that are dissolved in the liquid phase and each group of microorganisms, \( j \) (= 1, ..., \( m \)), of the lower (d) and upper (u) part of each compartment are:

\[
d(V^d \cdot S_i^d)/dt = F \cdot \left( \alpha(t) \cdot S_i^F + \beta(t) \cdot S_i^{u-1} \right) + F_{u \rightarrow d} \cdot S_i^u - F_{d \rightarrow u} \cdot S_i^d + V^d \cdot r_{S_i^d} \]

(4)

\[
d(V^u \cdot S_i^u)/dt = F_{d \rightarrow u} \cdot S_i^d - F \cdot S_i^u - F^u_{u \rightarrow d} \cdot S_i^u + V^u \cdot r_{S_i^u} \]

(5)

\[
d(V^d \cdot X_j^d)/dt = \beta(t) \cdot F \cdot X_j^{u-1} - \Phi_j^{d \rightarrow u} + \Phi_j^{u \rightarrow d} + V^d \cdot r_{X_j^d} \]

(6)

\[
d(V^u \cdot X_j^u)/dt = -F \cdot X_j^u + \Phi_j^{d \rightarrow u} - \Phi_j^{u \rightarrow d} + V^u \cdot r_{X_j^u} \]

(7)

where \( S \) and \( X \) are the concentrations of the compounds and microorganisms group respectively, \( \alpha(t) \), \( \beta(t) \) are switch functions that take values depending on whether the inlet flow is the feed flow (\( \alpha = 1 \) and \( \beta = 0 \)) or the effluent of the previous compartment (\( \alpha = 0 \) and \( \beta = 1 \)), \( S_i^F \) is the concentration of the compound \( i \) in the feed, while \( r_{S_i^d} \) and \( r_{X_j^d} \) are the net production rate of the compound \( i \) and the net growth rate of the microorganism \( j \) group.

The sum of the \( j \) equations (6) derives the rate of change for the lower part volume of each compartment (assuming that the biomass concentration in the lower part \( x_T^d \) is constant):

\[
X_T^d \cdot \frac{dV^d}{dt} = \beta(t) \cdot F \cdot \sum_{j=1}^{m} X_j^{u-1} - \sum_{j=1}^{m} \Phi_j^{d \rightarrow u} + \sum_{j=1}^{m} \Phi_j^{u \rightarrow d} + V^d \cdot \sum_{j=1}^{m} X_j^d
\]

(8)
Gas phase simulation. The simulation of the reactor gas phase was based on the assumptions of Costello et al. (1991a). It was also assumed that the changes in the gas phase composition take place so fast, that it could be assumed that the gas phase is in a quasi-steady state. The mass balance of the gas constituent $k (= 1, \ldots, l)$, in the quasi-steady state, is:

$$-Q_G \cdot P_k + R \cdot T \cdot \sum_{\text{compartments}} \left( V^d \cdot r^d_{G_k} + V^u \cdot r^u_{G_k} \right) = 0 \quad (9)$$

where $P_k$ is the gas partial pressure, $Q_G$ the total biogas production rate, $V_G$ the gas phase volume, $R$ the gas constant, $T$ the temperature and $r^d_{G_k}$ the gas production rate in the lower and upper part of the compartment. Depending on the kinetics of the substrate which is degraded in the reactor, so the expressions for the net growth rates of microorganisms $r_X$, and the production rates of the liquid compounds $r_S$ can be expressed.

Gelatin kinetic model. The kinetic model of gelatin degradation, was limited to the action of four bacterial groups (acidogens, acetogens, acetoclastic and hydrogen utilizing methanogens). Initially, gelatin hydrolysis to its constituent amino acids was considered and, in the sequel, the amino acids fermentation to propionic and acetic acid by the acidogenic bacteria (given that the higher volatile fatty acids were not detected). Gelatin, when hydrolyzed, is a mixture of amino acids with a typical composition of that referred to Merck index (1996). The calculated stoichiometric coefficients according to the fermentation reactions were: $C_{pr, am} = 0.270 \text{ mg propionate/mg aminoacids}$, $C_{ac, am} = 0.556 \text{ mg acetate/mg aminoacids}$, $C_{NH3, am} = 0.192 \text{ mg ammonium/mg amino acids}$, $C_{CO2, am} = 0.204 \text{ mg CO2/mg amino acids}$, $C_{H2, am} = 0.0033 \text{ mg H2/mg amino acids}$. Gelatin hydrolysis kinetics were assumed to follow Michaelis-Menten and the kinetic parameters were determined via linear regression on data found in the work of Breure et al. (1986): $v_{\text{max}} = 10,700 \text{ d}^{-1}$, $K_m = 246.78 \text{ mg gelatin/L}$. The specific consumption rates of the intermediate products of gelatin degradation were assumed to be (Costello et al., 1991a; Angelidaki et al., 1993):

Amino acids: $r_{am} = \frac{k_{am} \cdot S_{am} \cdot X_{am}}{K_{sa} + S_{am}}$  
Propionic acid: $r_{pr} = \frac{k_{pr} \cdot S_{pr} \cdot X_{pr}}{K_{sp} \left( 1 + \frac{S_{pr}}{K_{pr}} \right) + S_{pr}} \cdot F(pH)$  
Acetic acid: $r_{ac} = \frac{k_{ac} \cdot S_{ac} \cdot X_{ac}}{K_{sa} + S_{ac}}$  
Hydrogen: $r_{H2} = \frac{k_{H2} \cdot S_{H2} \cdot X_{H2}}{K_{P_{H2}} + S_{H2}} \cdot F(pH)$

where $F(pH)$ is a normalized pH function that accounted for pH inhibition (Angelidaki et al., 1993). The pH was determined through the balance of ions as they result from the partial ionization of the weak acids and bases. The kinetic parameter values that were used are shown in Table 1.

Experimental procedure – analytical methods
The PABR feed contained gelatin (8.38 g/l), casein hydrolysate and yeast extract (1.43 g/l), NaHCO$_3$ (5 g/l) and trace metals. The COD of the feed was 12.5 g/l. The HRT of the reactor was 4 days and the switching period was 2 days. Under these conditions, the PABR was operated until the dissolved COD concentration in the beginning and the end of each period deviated within 10%. This state was called the steady periodic state (SPS) and the response of the reactor was monitored thoroughly. The dynamic behavior of the PABR was studied when the HRT was decreased from 4 to 2 days. During the transition, the effluent was collected in vessels and the VSS were measured. The dissolved COD, VSS and NH$_3$ concentration were measured according to Standard Methods (APHA, 1989). The VFA
concentration was measured in a GC (FID), the pH by a portable pH-meter. The biogas production rate was measured by displacement of a dilute sulfuric acid solution.

Results and discussion

The profiles of the VFA and COD concentration of the upper part of each compartment as well as the biogas production rate are shown in Figure 2. The COD accumulated during the feeding period in every compartment. The COD decreases immediately after the feed stops and it gets smaller than anywhere else in the reactor at the time the compartment becomes the last in series. The counterclockwise manner of switching resulted in the feeding entering the compartment which was formerly the last in series, i.e. the effluent compartment. As a result, the compartment with the less COD concentration when accepted the high COD concentration of the feed, became temporarily “overloaded” and responded with a peak in the biogas production. The mean biomass concentration (as g VS/l) in the PABR was 12.84 ± 2.25 g VS/l and the model prediction was 10 g/l. The pH was 7.65 and NH₃ concentration was 1,860 mg/l (mean values), while the model predictions were 7.51 and 1,632 mg/l, respectively. The biomass concentration in the lower part of the compartment and the solids settling velocity were determined to be 32 g/l and 10 m/h, so that the total biomass concentration and solids removal could be predicted. Those were the only two adjusted parameters to secure adequate model fitting.

An increase in the organic loading rate was achieved by reducing the HRT. The PABR responded quickly to the disturbance and none of the measured parameters tended to accumulate. In Figure 3, the results concerning one compartment are shown, since the behavior of the other was similar. The ammonia concentration and pH did not show any change: 1,807 mg/l and 7.56 (model prediction: 1,541 mg/l and 7.49 respectively). The biogas production rate doubled, responding directly to the increase in the OLR. The VS concentration in the effluent seemed to increase, although there was an intense variance in the measurements.

The developed model predicted the measured parameters oscillation during the SPS and the transition examined quite satisfactorily. It should be noted that no adjustment of the kinetic parameters was attempted to improve the dynamic response. The correlation

<table>
<thead>
<tr>
<th>Micro/sms group</th>
<th>( k ) (mg S/mg X/d)</th>
<th>( K_s ) (mg S/l)</th>
<th>( K_I ) (mg I/l)</th>
<th>( B ) (d⁻¹)</th>
<th>( Y_{X/S} ) (g X/g S)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acidogens</td>
<td>48¹</td>
<td>19.92¹</td>
<td>–</td>
<td>0.025¹</td>
<td>0.039766¹</td>
</tr>
<tr>
<td>Acetogens</td>
<td>52.536²</td>
<td>39.22²</td>
<td>3²</td>
<td>0.0096³</td>
<td>0.06757³</td>
</tr>
<tr>
<td>Methanogens (acetoclastic)</td>
<td>9.84²</td>
<td>32.4²</td>
<td>61.6⁴</td>
<td>0.0192³</td>
<td>0.04166³</td>
</tr>
<tr>
<td>Methanogens (H₂)</td>
<td>3.12³</td>
<td>0.001 (atm)³</td>
<td>–</td>
<td>0.09³</td>
<td>1.25³</td>
</tr>
</tbody>
</table>

of the biomass retainment inside the reactor to the operating conditions was one of the goals of PABR modeling. The simulation of the transitory state of PABR shows that the biomass concentration in the effluent increased immediately when the HRT is decreased, due to the intense biogas production which raises more biomass from the lower to the upper part.

Conclusions

The PABR is a novel reactor which degraded a protein rich feeding medium (based on gelatin) efficiently during steady periodic operation and overloading. In this work, a model was developed for the PABR simulation, which has succeeded in predicting the peaks and lows in the oscillating response of the reactor. The modeling approach used considered that there are two distinct regions based on the different biomass concentration inside the reactor. In this way, the compartments were separated into two sections, the size of which is intrinsically determined by the system dynamics resulting from every change in the operating conditions. This model concept is being used to simulate PABR response at various operating conditions and on different substrates (glucose) also with success.

References


