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MODELLING OF THE PERIODIC ANAEROBIC BAFFLED REACTOR (PABR) BASED ON THE RETAINING FACTOR CONCEPT

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Abstract—The fact that the active biomass is continuously removed from the continuously stirred anaerobic digesters, leading to long retention times, has been overcome in a number of high rate systems based on immobilisation of the active biomass, such as the **U**pflow **A**naerobic **S**ludge **B**lanket **R**eactor (UASBR) and the **A**naerobic **B**affled **R**eactor (ABR). A kinetic model of glucose consumption, which was developed based on a batch kinetic experiment, was used for the development of a dynamic model for the prediction of the behaviour of the recently developed flexible reactor called the **P**eriodic **A**naerobic **B**affled **R**eactor (PABR) [(1998) *Wat. Sci. Technol.* **38**(8–9), 401–408]. The PABR may be operated as a UASBR, an ABR or at an intermediate mode. The key assumption of the model is that the hydraulic behaviour of a PABR is equivalent with the behaviour of CSTRs in series as concerning the dissolved matter, whereas the biomass is allowed to be retained in the PABR through a retention factor accounting for precipitation. The model adequately predicted the experimental behaviour of a glucose fed PABR. The model was subsequently used to examine the behaviour of the PABR as a function of operating conditions, both for constant and varying loading rates. It was shown that for different cases, the reactor should best be operated as a UASBR or as an ABR. © 2000 Elsevier Science Ltd. All rights reserved

Key words—modelling, periodic anaerobic baffled reactor, PABR, anaerobic digestion, biomass retention factor, kinetics

INTRODUCTION

The main problem of the continuously stirred tank reactor (CSTR) during the anaerobic treatment of wastewaters, i.e. the fact that the active biomass is continuously removed from the system leading to long retention times, has been overcome in a number of systems based on immobilisation of the active biomass. Such a typical reactor (Lettinga, 1980) is the Upflow Anaerobic Sludge Blanket Reactor (UASBR). In the UASBR the microorganisms are kept in the reactor due to the production of the highly flocculated, well settled, compact sludge granules which develop. Granular UASBR is the system of choice for low to medium-high strength wastewaters containing low or easily hydrolysable solids.

The Anaerobic Baffled Reactor (ABR), initially developed by McCarty and coworkers (Bachmann *et al.*, 1982, 1985), consists of a cascade of baffled compartments where the wastewater flows upward through a bed of anaerobic sludge after being transported to the bottom of the compartment. The ABR does not require the sludge to granulate in order to perform effectively, although granulation does occur over time (Barber and Stuckey, 1999). Experiments with lab-scale reactors have shown that the ABR is very stable under shock loads due to its compartmentalised structure (Nachaiyasit and Stuckey, 1997a, b). In addition, the ABR has many potential advantages, i.e. no requirement of biomass with unusual settling properties and low capital and operating costs coupled with mechanical simplicity (Barber and Stuckey, 1999). From a reactor design point of view a UASBR resembles a well-mixed reactor, whereas an ABR resembles a plug-flow reactor (Grobicki and Stuckey, 1991, 1992).

The Periodic Anaerobic Baffled Reactor (PABR) was initially developed by Skiadas and Lyberatos (1998) and consists of two concentric cylinders. The area between the cylinders is compartmentalised so

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that the reactor resembles an ABR with the compartments arranged in a circular manner in the annular region (Fig. 1(a)). The wastewater enters the digester at the downflow section of the feeding (first) compartment, comes up at the upflow section of the same compartment and passes on to the next (second) compartment through the outer tubing. The flow pattern is repeated at the third and fourth compartments. Wastewater eventually leaves the system after passing through the upflow part of the effluent compartment, which is the fourth one in counterclockwise order. The role of the four compartments is periodically changed by proper switching (on or off) the 12 valves of the outer tubing, in a clockwise manner. For instance, when A is the feeding compartment (Fig. 1(b)), D will be the effluent one and valves 1, 3, 6, 9, 11 are switched on, while valves 2, 4, 5, 7, 8, 10, 12 are switched off. Likewise, whenever the feeding compartment is the B, C or D, the effluent one will be the A, B or C, respectively. In the extreme of zero switching frequency (no switching) the reactor behaves as an ABR. In the other extreme (infinite frequency) the compartments become identical so that the reactor should behave like a UASBR. By setting the switching frequency, a great flexibility is obtained, taking advantage of the optimal reactor configuration (UASBR, ABR or "something in between") depending on the loading conditions.

The fact that the PABR has residence time distribution equivalent to four well mixed reactors in series (Skiadas and Lyberatos, 1998) allows simulation of the PABR, using kinetic models that were developed for the anaerobic digestion in continuously stirred tank anaerobic digesters. Simulation employing the model of Smith *et al.* (1988) (acidogenesis of glucose and methanogenesis are taken into account considering unionised volatile fatty acids (VFAs) concentration as a key parameter and methanogenesis as the rate limiting step) showed that: (a) for large values of organic loading, the PABR is expected to perform better when operated at a high frequency of switching feed point, namely

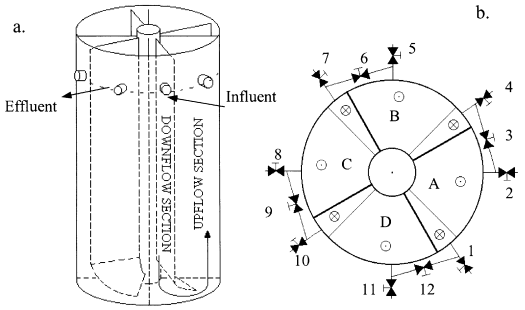

Fig. 1. (a) Front view of a four compartment PABR. (b) Top view of a four compartment PABR. 1, 2, ..., 12 valves. ⊙ Upflow, ⊗ Downflow.

it behaves as a UASBR; and (b) for smaller values of the organic loading the PABR should be operated at smaller frequencies approaching that of an ABR (Skiadas and Lyberatos, 1998). In addition, when a PABR is operated without switching of the feeding point (namely as an ABR), it fails when a relatively high step increase in the hydraulic retention time (HRT) is imposed. The PABR, when operated with periodic switching of the feeding point, is able to approach a *stable periodic state* (SPS) when exposed to the same step change (Skiadas and Lyberatos, 1998). The above simulation predicted that for a four day HRT and 16 g/l influent Chemical Oxygen Demand (COD) concentration, the PABR performance in SPS was optimum when operated at the UASBR mode (high switching frequency) with 12 g/l effluent COD concentration and 2.4 g/l biomass concentration. In contrast, experiments with a 15 l PABR, fed with a glucose-based synthetic wastewater of the same influent COD concentration and at the same HRT, resulted in about 1 g/l effluent COD concentration with a biomass concentration varying between 31 and 57 g/l (Skiadas, 1998). The difference between the model prediction and the experimental results is attributed to the high biomass retention in the compartments of the PABR, that a simple CSTR model neglects. The objective of this work is the development of an appropriate new model that will adequately describe the anaerobic digestion of glucose in the PABR.

MATERIALS AND METHODS

In order to determine the microbial growth constants under mesophilic conditions (35°C), a batch kinetic experiment was carried out in a continuously stirred batch anaerobic digester. The digester was inoculated with 1900 ml of inoculum preadapted to a glucose-based synthetic medium (Skiadas and Lyberatos, 1998). The adaptation took place in a 15 l anaerobic digester fed in a draw and fill manner (once a day an amount of supernatant anaerobic liquor was replaced by the same amount of synthetic medium). Thus, the biomass was allowed to accumulate in a period of 100 days up to a concentration of 14 g/l (Skiadas, 1998). The batch digester was fed with 100 ml glucose medium containing 30 g/l $C_6H_{12}O_6{\cdot}H_2O$, 4 g/l hydrolysed casein, 4 g/l yeast extract, 5 g/l $NaHCO_3$ and trace minerals. Measurements included concentration of dissolved carbohydrates, lactic acid, VFAs, volatile suspended solids (VSS), dissolved COD, biogas production and composition and pH.

In order to verify the predictions of the simulations, a four compartment PABR was constructed out of stainless steel with a total useful volume of 15 l. The PABR was inoculated with 15 l of the glucose preadapted inoculum which was used for the above kinetic experiment, and it was started up at 0.2 g COD/l d organic loading rate (OLR) and a switching period of 1 day. During a time of 100 days the OLR was increased gradually to 4.55 g COD/l d at a four day HRT and the biomass concentration reached the value of 31 g/l due to its accumulation in the compartments of the PABR. The digester behaviour was examined under three different SPSs at switching periods of 1, 1.5 and 2 days, respectively. Once the diges-

ter approached a SPS, dissolved COD and VFAs concentration were measured in each compartment during a time of one switching period. Biogas composition and production rate were measured as well. The digester was maintained under mesophilic (35°C) conditions.

Determinations of dissolved COD and VSS were carried out as described in Standard Methods. Glucose concentration was measured colorimetrically according to Josefsson (1983). Lactic acid concentration was measured using the diagnostic kits and reagents of "Sigma Chemical Company, Sigma Diagnostics—USA". VFAs were measured by a Flame Ionisation Gas Chromatograph. The biogas production rate was measured by displacement of a dilute sulphuric acid solution. The biogas composition was calculated from the volume of the remaining methane gas after the proper injection of specific volume biogas samples into a system of communicating vessels containing a sodium hydroxide solution (Skiadas, 1998).

RESULTS AND DISCUSSION

Batch experiment

The present kinetic study showed (Fig. 2) that the anaerobic decomposition of glucose to methane and carbon dioxide passes through the production of lactic, acetic and propionic acid. The concentrations of other VFAs such as butyrate were negligible, compared to those of acetate and propionate (data not shown). In addition, despite the complete consumption of glucose during the first hour of the batch experiment, the total carbon of the consumed glucose is greater than the total carbon of the produced VFAs, lactate and biogas. Furthermore, the measured dissolved COD value (1600 mg O_2/l) is greater than the sum of the COD values of the VFAs and lactate (500 mg O_2/l), but the difference (1100 mg O_2/l) is smaller than the COD of the consumed glucose in 1 h. These observations indicate that accumulation of some undetermined intermediate products (as the end product of bacterial metabolism), as well as accumulation of intracellular intermediate products of bacterial metabolism, is taking place during batch anaerobic digestion of glucose. Hence, an important improvement to a model for the anaerobic digestion of glucose would be the assumption of this intermediate accumulation.

Kinetic model development

It has been reported (Pullammanappallil, 1993) that the response of continuously stirred tank anaerobic digesters to an increase of OLR cannot be predicted precisely enough by mathematical models developed so far and describing the anaerobic digestion of carbohydrates in suspended growth. Such models predict that the VFAs accumulation takes place earlier than it is observed. This happens

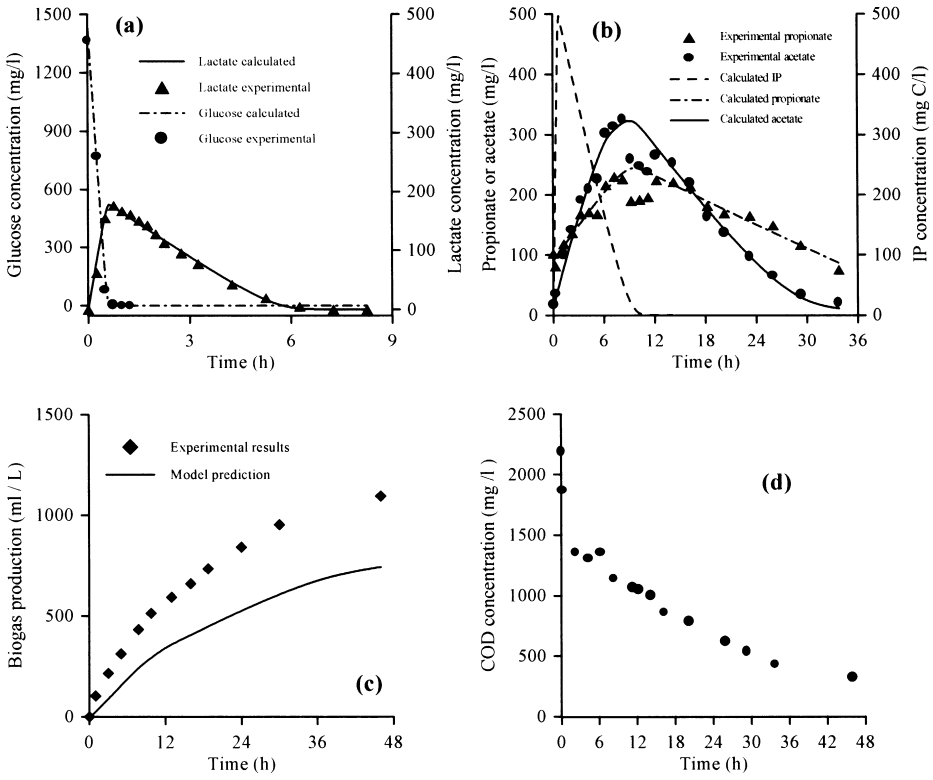

Fig. 2. Batch experimental results as well as model predicted values of glucose, lactate (a), propionate, acetate, IP (b) concentration, biogas production (c) and COD concentration (d) vs time.

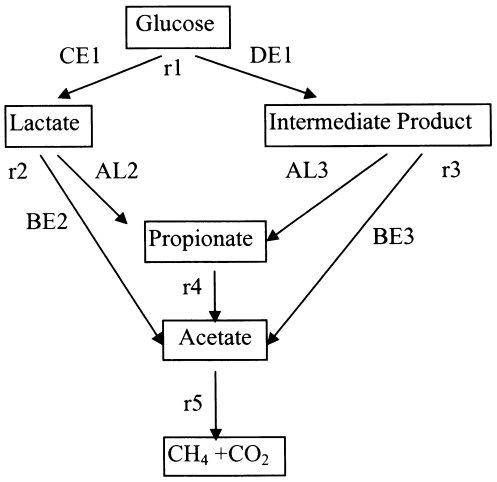

Fig. 3. Anaerobic bioconversion of glucose to biogas.

because these models do not take in consideration: (a) the accumulation of the intracellular intermediate products of bacterial metabolism (Pullammanappallil, 1993); and (b) the consumption of carbohydrates by bacteria producing substances other than VFAs (such as lactate) and the subsequent conversion of these substrates to VFAs by different groups of bacteria (Costello *et al.*, 1991).

The kinetic model developed in this work is schematically shown in Fig. 3. The conversion of glucose to biogas is completed according to the stoichiometric reactions shown in Table 1. It is assumed that the anaerobic biodegradation of glucose is completed in five steps: in the first step the acidogenic bacteria consume glucose (rate $r1$) and produce lactic acid, as well as an unknown intermediate (final and/or intracellular) product, from now on referred to as IP. Subsequently, different groups of acidogenic bacteria convert lactate and IP (rate $r2$ and $r3$, respectively) to a mixture of acetate and propionate. The propionate is converted by the acetogenic bacteria to acetate (rate $r4$) and finally the methanogens produce CH_4 and CO_2 (rate $r5$) using acetate as substrate. Also, it is assumed that all the above five consumption rates follow simple Monod kinetics:

$$ri = \frac{m_{\max\, i}\,[C_i]}{Ksi + [C_i]}X \tag{1}$$

where $m_{\max\, i}$ is the maximum specific consumption rate of the component i, [=]mg C_i/g biomass h, Ksi is the saturation constant of the component i, [=] mg/l, i = 1, 2, 3, 4 and 5 for the glucose, lactate, IP, propionate and acetate, respectively, $[C_i]$ is the component i concentration, [=]mg/l for components 1, 2, 4, 5 and mg carbon/l for component 3, X is the total biomass concentration, [=] g/l, and ri is the consumption rate of component i for products formation and cell synthesis.

The fact that only part of the total biomass is responsible for the degradation of a specific component is included in the $m_{\max\, i}$ constants expression (Gavala *et al.*, 1999):

$$m_{\max\, i} = \frac{\mu_{\max\, i} f_i}{Y_{x/i}} \tag{2}$$

where $\mu_{\max\, i}$ is the maximum specific growth rate of the bacteria consuming the component i, $Y_{x/i}$ is the substrate i biomass yield coefficient and f_i is the fraction of the bacteria consuming component i.

Table 1. The substrate consumption and the biomass synthesis stoichiometric reactions used in the model for the anaerobic degradation of glucose, as well as the resultant stoichiometric biomass yield coefficients assuming that one mole of produced ATP provides sufficient energy for the formation of 10 g of biomass (Bauchop and Elsden, 1960)

First and third step. Glucose consumption and production of lactate either VFAs through IP or lactate	
$C_6H_{12}O_6 \rightarrow 2CH_3CHOHCOOH + 2ATP$	$Y^1_{X\,\mathrm{Lac}} = 1.1111 \times 10^{-4}$ gr biomass/mg produced Lac
$C_6H_{12}O_6 + 2H_2O \rightarrow 2CH_3COOH + 2CO_2 + 4H_2 + 4ATP$	$Y^3_{X\,\mathrm{Ac}} = 3.3333 \times 10^{-4}$ gr biomass/mg produced Ac
$C_6H_{12}O_6 + 2H_2 \rightarrow 2CH_3CH_2COOH + 2H_2O + 2ATP$	$Y^3_{X\,\mathrm{Pr}} = 1.3514 \times 10^{-4}$ gr biomass/mg produced Pr
$5C_6H_{12}O_6 + 6NH_3 \rightarrow 6C_5H_9O_3N + 12H_2O$	$Y^3_{\mathrm{CO_2Ac}} = 4.2117 \times 10^{-4}$ 1 CO_2/mg produced Ac
Second step. Lactate consumption	
$CH_3CHOHCOOH + H_2 \rightarrow CH_3CH_2COOH + H_2O + 0.5ATP$	$Y^2_{X\,\mathrm{Pr}} = 0.6577 \times 10^{-4}$ gr biomass/mg produced Pr
$CH_3CHOHCOOH + H_2O \rightarrow CH_3COOH + CO_2 + 2H_2 + 1ATP$	$Y^2_{X\,\mathrm{Ac}} = 1.6667 \times 10^{-4}$ gr biomass/mg produced Ac
$5CH_3CHOHCOOH + 3NH_3 \rightarrow 3C_5H_9O_3N + 6H_2O$	$Y^2_{\mathrm{CO_2Lac}} = 2.4909 \times 10^{-4}$ 1 CO_2/mg consumed Lac
Fourth step. Propionate consumption (acetogenesis)	
$CH_3CH_2COOH + 2H_2O \rightarrow CH_3COOH + CO_2 + 3H_2 + 1ATP$	$Y^4_{\mathrm{Ac\,Pr}} = 0.7275$ mg produced Ac/mg consumed Pr
$3CH_3CH_2COOH + CO_2 + 2NH_3 \rightarrow 2C_5H_9O_3N + 2H_2O + H_2$	$Y^4_{X\,\mathrm{Pr}} = 1.2126 \times 10^{-4}$ gr biomass/mg consumed Pr, $Y^4_{\mathrm{CO_2Pr}} = 2.9471 \times 10^{-4}$ 1 CO_2/mg consumed Pr
Fifth step. Acetate consumption (acetoclastic methanogenesis)	
$CH_3COOH \rightarrow CH_4 + CO_2 + 0.25ATP$	$Y^5_{X\,\mathrm{Ac}} = 3.9772 \times 10^{-5}$ gr biomass/mg consumed Ac
$5CH_3COOH + 2NH_3 \rightarrow 2C_5H_9O_3N + 4H_2O$	$Y^5_{\mathrm{CH_4Ac}} = 4.0199 \times 10^{-4}$ 1 CH_4/mg consumed Ac, $Y^5_{\mathrm{CO_2Ac}} = 4.0199 \times 10^{-4}$ 1 CO_2/mg consumed Ac

According to this kinetic model, the mass balances for the anaerobic biodegradation of glucose to biogas in a batch continuous stirred digester take the form:

$$\frac{\mathrm{d[Gl]}}{\mathrm{d}t} = -r1 \tag{3}$$

$$\frac{\mathrm{d[Lac]}}{\mathrm{d}t} = CE1 \cdot r1 - r2 \tag{4}$$

$$\frac{\mathrm{d[IP]}}{\mathrm{d}t} = DE1 \cdot r1 - r3 \tag{5}$$

$$\frac{\mathrm{d[Pr]}}{\mathrm{d}t} = AL2 \cdot r2 + AL3 \cdot r3 - r4 \tag{6}$$

$$\frac{\mathrm{d[Ac]}}{\mathrm{d}t} = BE2 \cdot r2 + BE3 \cdot r3 + Y^{4}_{\mathrm{Ac\ Pr}} \cdot r4 - r5 \tag{7}$$

$$\begin{aligned}\frac{\mathrm{d}X}{\mathrm{d}t} = {} & CE1 \cdot r1 \cdot Y^{1}_{X\ \mathrm{Lac}} + AL3 \cdot r3 \cdot Y^{3}_{X\ \mathrm{Pr}} \\ & + AL2 \cdot r2 \cdot Y^{2}_{X\ \mathrm{Pr}} + BE2 \cdot r2 \cdot Y^{2}_{X\ \mathrm{Ac}} \\ & + BE3 \cdot r3 \cdot Y^{3}_{X\ \mathrm{Ac}} + r4 \cdot Y^{4}_{X\ \mathrm{Pr}} + r5 \\ & \cdot Y^{5}_{X\ \mathrm{Ac}}\end{aligned} \tag{8}$$

where [Gl], [Lac], [IP], [Pr] and [Ac] are the glucose, lactate, IP, propionate and acetate concentrations, respectively.

The factor f_i in equation (2) corresponds to a group of bacteria, the component i consuming bacteria, as a fraction of the total biomass. Such a group consists of bacteria which are using the same substrate i for their growth, but do not necessarily lead to the same metabolic end-product. The latter is reflected by the products between the consumption rates (ri) and the parameters $CE1$, $DE1$, $AL2$, $AL3$, $BE2$ and $BE3$ in the above differential equations, where $CE1$ is the produced lactic acid per unit of consumed glucose, [=] mg lactate/mg glucose, $DE1$ is the produced IP per unit of consumed glucose, [=] mg carbon of IP/mg glucose, $AL2$ is the produced propionic acid per unit of consumed lactic acid, [=] mg propionate/mg lactate, $BE2$ is the produced acetic acid per unit of consumed lactic acid, [=] mg acetate/mg lactate, $AL3$ is the produced propionic acid per unit of consumed IP, [=] mg propionate/mg carbon of IP, and $BE3$ is the produced acetic acid per unit of consumed IP, [=] mg acetate/mg carbon of IP.

The data from the batch experiment were used to estimate the values of the kinetic parameters in the model. A modified non-linear least squares fitting method was used and the least-squares objective was to select the best kinetic parameter values so as to minimise the squared residuals between the experimentally measured concentrations of the glucose, lactate, propionate and acetate and the respective predicted concentrations. Biogas production was not included in the least-squares objective equation because this model aims only at the prediction of the dissolved COD removal. The GAMS modelling language was used to formulate the optimisation problem (Brooke *et al*., 1996).

The proposed model was solved assuming that the biomass concentration remained constant during the batch experiment. This is a reasonable assumption, given the fact that the expected biomass growth attributed to the consumption of glucose fed (with the low biomass yield of the anaerobic bacteria) was negligible compared to the initial biomass concentration (14 g VSS/l). Also, the duration of the experiment was comparatively small (48 h). The model exhibited a mathematically stable convergence, yielded reasonable kinetic parameter values and adequately matched the concentration response curves for glucose, lactate, propionate and acetate (Fig. 2(a) and (b)).

The predicted biogas production at time t of the batch experiment is equal to:

$$\begin{aligned}\mathrm{PBP} = \int_0^t (& Y^{5}_{\mathrm{CH_4Ac}} \cdot r5 + Y^{5}_{\mathrm{CO_2Ac}} \cdot r5 + Y^{4}_{\mathrm{CO_2Pr}} \\ & \cdot r4 + Y^{3}_{\mathrm{CO_2Ac}} \cdot BE3 \cdot r3 + Y^{2}_{\mathrm{CO_2Lac}} \cdot r2)\mathrm{d}t\end{aligned} \tag{9}$$

where PBP is the model prediction for the biogas production, [=] l of produced biogas/digester volume.

The model predicts less methane production than it is experimentally observed (Fig. 2(c)). This happens because the model does not consider the production of methane by H_2-utilising methanogens.

Optimal kinetic parameters obtained from the simulation process are given in Table 2. Typical values (according to the literature) for the maximum specific consumption rates are: 1800 mg/g h for glucose consumption (Ghosh and Klass, 1978);

Table 2. Estimated values of the kinetic parameters

Parameter	Value	Units
$m_{\max 1}$	197.94	mg Gl (g biomass h)$^{-1}$
$m_{\max 2}$	2.88	mg Lac (g biomass h)$^{-1}$
$m_{\max 3}$	4.82	mg C IP (g biomass h)$^{-1}$
$m_{\max 4}$	0.52	mg Pr (g biomass h)$^{-1}$
$m_{\max 5}$	1.87	mg Ac (g biomass h)$^{-1}$
$Ks1$	46	mg Gl l^{-1}
$Ks2$	11	mg Lac l^{-1}
$Ks3$	31	mg C IP l^{-1}
$Ks4$	14	mg Pr l^{-1}
$Ks5$	32	mg Ac l^{-1}
$CE1$	0.137	mg Lac (mg Gl)$^{-1}$
$DE1$	0.345	mg C IP (mg Gl)$^{-1}$
$AL2$	0	mg Pr (mg Lac)$^{-1}$
$AL3$	0.41	mg Pr (mg C IP)$^{-1}$
$BE2$	0.66	mg Ac (mg Lac)$^{-1}$
$BE3$	0.61	mg Ac (mg C IP)$^{-1}$

1912 mg/g h for lactate utilisation (Lee *et al.*, 1974); 212 mg/g h for propionate (Lawrence and McCarty, 1969); and 150 mg/g h for acetate consumption (van den Berg, 1977). Expectedly, the latter values are significantly higher in comparison with the respective values given in Table 2 because the $m_{\max\, i}$ values obtained from the literature are equal to $\mu_{\max\, i}/Y_{x/i}$ and do not include the factor f_i. The above typical values are expressed in mg/(g biomass) h, where biomass is only a specific group of bacteria such as methanogens. On the contrary, the values for the present simulation process were based on the assumption that biomass is the total bacterial mass contained in the batch digester. In addition, the values given in Table 2 are related to the total biomass concentration (as VSS) even if a considerable portion of the digester VSS content is non-viable biomass (which is the case for the anaerobic digesters with high solids retention time), or is the biomass of different bacterial groups than these taken into consideration in this model. Finally, the optimal value of coefficient *AL*2 was found to be zero, suggesting that the biodegradation of lactate leads only to the production of acetate.

PABR experimental results

The measured dissolved COD concentration in each of the four compartments during a switching period of one, 1.5 and two days is shown in Fig. 4

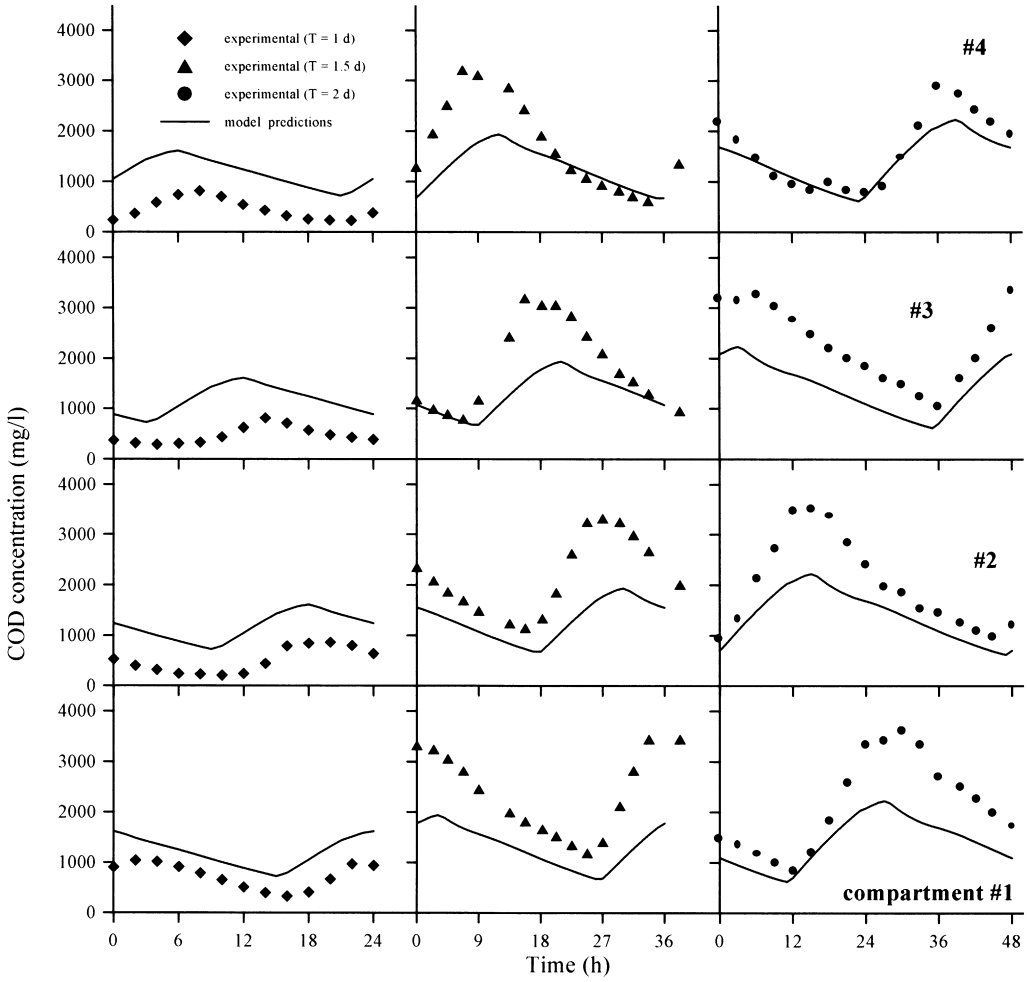

Fig. 4. Experimental results for the COD concentration in each compartment of the PABR under SPS at switching periods (T) of one, 1.5 and two days and the respective model predicted values. For T = 1 d, compartment no. 3 was the effluent one between time 0 and 6, compartment no. 2 between time 6 and 12, compartment no. 1 between time 12 and 18 and compartment no. 4 between time 18 and 24. Similarly, compartment no. 3 was the effluent one between time 0 and 9, compartment no. 2 between time 9 and 18, compartment no. 1 between time 18 and 27 and compartment no. 4 between time 27 and 36 for T = 1.5 d. For T = 4 d, compartment no. 1 was the effluent one between time 0 and 12, compartment no. 4 between time 12 and 24, compartment no. 3 between time 24 and 36 and compartment no. 2 between time 36 and 48.

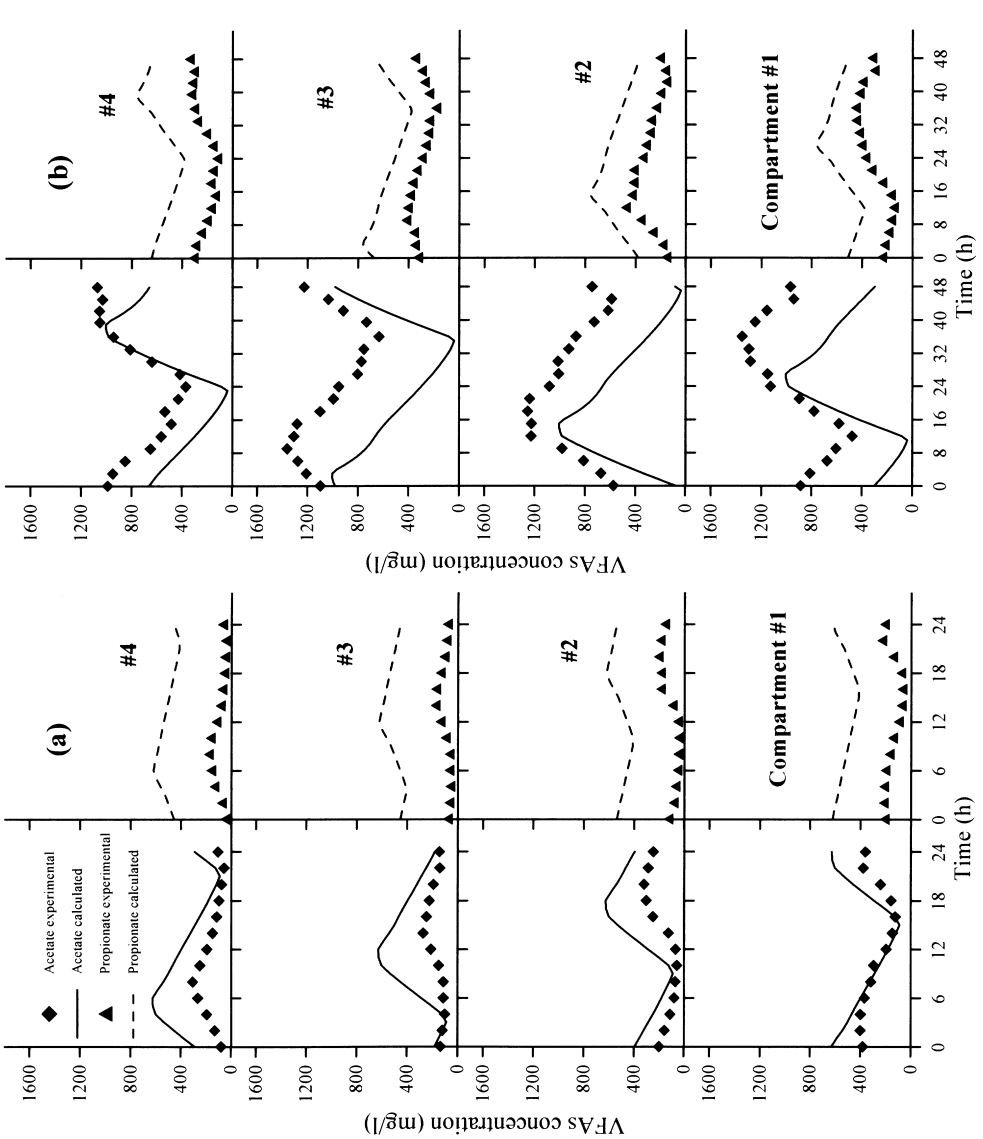

Fig. 5. Experimental results for the VFAs concentration in each compartment of the PABR under SPS at switching periods of one and two days and the respective model predicted values.

and the VFAs concentration in each of the four compartments during a switching period of one and two days is shown in Fig. 5. The values at the start of a period are equal with those at the end of the same period (*stable periodic state*, SPS). For each compartment the COD and the VFAs values are located on a wave-like curve. The four curves are almost identical verifying an SPS. Each curve is transposed for T/4 in relation with the curve that corresponds to the previous compartment, because four changes of the influent and effluent compartment occur during a time of one switching period (four compartment PABR). Note that higher switching periods lead to larger amplitude oscillation of the COD (Fig. 4) and the VFAs (Fig. 5) concentrations in each compartment. Note (Fig. 4) that the COD concentration at the effluent is almost always equal to the lowest COD value in the four compartments (the COD value of the harvesting compartment).

Model development for the PABR

Subsequently, the kinetic model for glucose consumption, which was developed based on the batch kinetic experiment, was used for the development of a dynamic model for the prediction of the PABR behaviour under constant operating conditions (SPS), as well as of the response of the PABR to organic loading disturbances. The key assumption of the dynamic model is that the hydraulic behaviour of a four compartment PABR is equivalent with the behaviour of four CSTRs in series as far as the substrates and products are concerned, whereas the biomass is assumed to be retained in the compartments of the PABR by precipitation. According to this assumption the glucose, lactate, IP, propionate and acetate concentration in each one of the four compartments equals the respective concentration of the effluent stream from the same compartment. In contrast, the biomass concentration of the effluent stream from each one of the four compartments will be equal to $(1-\boldsymbol{\delta})X$ if the biomass concentration in the same compartment is X, where $\boldsymbol{\delta}$ is a real number (with values between 0 and 1) from now on called the *biomass retention factor*.

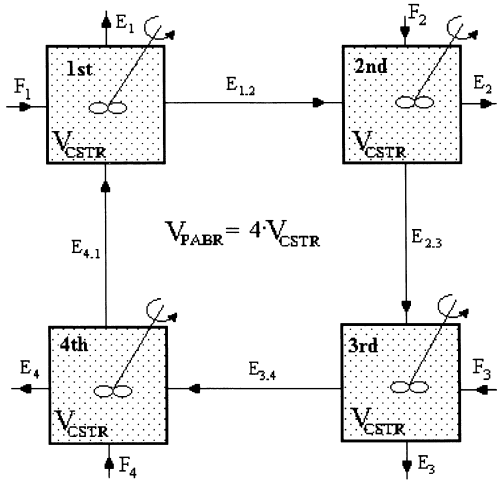

Fig. 6. A circular series of four CSTRs that is assumed equivalent to a four compartment PABR as far as the substrates and products are concerned.

Figure 6 shows a circular series of four CSTR, which is assumed equivalent to a four compartment PABR. F_j is the influent stream of the PABR when the compartment j is the feeding one ($j = 1$, 2, 3 or 4), E_j is the effluent stream of the PABR when the compartment j is the effluent one, and $E_{j,\,(j+1)}$ is the flow stream between compartment j and compartment $j+1$. Because of the circular flow pattern, one should have in mind that $j+1$ is equal to 1 for $j = 4$, and $j-1$ is equal to 4 for $j = 1$. The values of the dimensionless factors F_j, E_j and $E_{j,\,(j+1)}$ may be either 0 or 1 and are switched periodically with time as the role of the four compartments changes periodically.

Consider the parameter vector $\mathbf{VF} = (F_1\ F_2\ F_3\ F_4\ E_1\ E_2\ E_3\ E_4\ E_{1,2}\ E_{2,3}\ E_{3,4}\ E_{4,1})$. Then:

1. $\mathbf{VF} = (1\ 0\ 0\ 0\ 0\ 0\ 0\ 1\ 1\ 1\ 1\ 0)$ when the first compartment (Fig. 6) is the feeding and the fourth is the effluent one.
2. $\mathbf{VF} = (0\ 1\ 0\ 0\ 1\ 0\ 0\ 0\ 0\ 1\ 1\ 1)$ when the second compartment is the feeding and the first is the effluent one.
3. $\mathbf{VF} = (0\ 0\ 1\ 0\ 0\ 1\ 0\ 0\ 1\ 0\ 1\ 1)$ when the third compartment is the feeding and the second is the effluent one.
4. $\mathbf{VF} = (0\ 0\ 0\ 1\ 0\ 0\ 1\ 0\ 1\ 1\ 0\ 1)$ when the fourth compartment is the feeding and the third is the effluent one.

Consequently, the mass balances for the anaerobic biodegradation of glucose to biogas in a PABR simulated with four CSTR type digesters in series (Fig. 6) may be compactly written in the form:

$$\begin{bmatrix} [\mathrm{Gl}]^0 & [\mathrm{Gl}]_j & [\mathrm{Gl}]_j & [\mathrm{Gl}]_{j-1} & -R^j_{\mathrm{Gl}} \\ 0 & [\mathrm{Lac}]_j & [\mathrm{Lac}]_j & [\mathrm{Lac}]_{j-1} & R^j_{\mathrm{Lac}} \\ 0 & [\mathrm{IP}]_j & [\mathrm{IP}]_j & [\mathrm{IP}]_{j-1} & R^j_{\mathrm{IP}} \\ 0 & [\mathrm{Pr}]_j & [\mathrm{Pr}]_j & [\mathrm{Pr}]_{j-1} & R^j_{\mathrm{Pr}} \\ 0 & [\mathrm{Ac}]_j & [\mathrm{Ac}]_j & [\mathrm{Ac}]_{j-1} & R^j_{\mathrm{Ac}} \\ 0 & (1-\boldsymbol{\delta})X_j & (1-\boldsymbol{\delta})X_j & (1-\boldsymbol{\delta})X_{j-1} & R^j_X \end{bmatrix} \times \begin{bmatrix} 4\cdot D\cdot F_j \\ -4\cdot D\cdot E_j \\ -4\cdot D\cdot E_{j,\,j+1} \\ 4\cdot D\cdot E_{j-1,\,j} \\ 1 \end{bmatrix} = \begin{bmatrix} \mathrm{d}[\mathrm{Gl}]_j/\mathrm{d}t \\ \mathrm{d}[\mathrm{Lac}]_j/\mathrm{d}t \\ \mathrm{d}[\mathrm{IP}]_j/\mathrm{d}t \\ \mathrm{d}[\mathrm{Pr}]_j/\mathrm{d}t \\ \mathrm{d}[\mathrm{Ac}]_j/\mathrm{d}t \\ \mathrm{d}X_j/\mathrm{d}t \end{bmatrix} \quad (10)$$

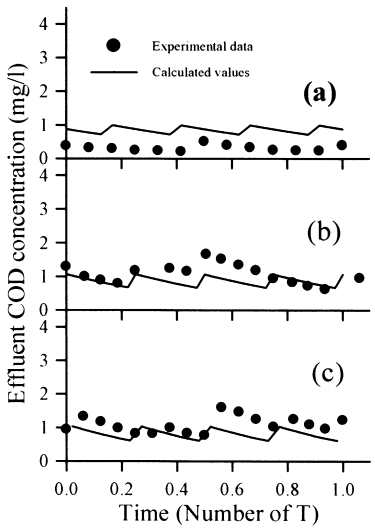

Fig. 7. The optimal values of the calculated effluent COD concentrations during the time of one period are graphically compared with the experimental results from the anaerobic digestion of glucose in the 15 l PABR. (a) $T = 1$ d, (b) $T = 1.5$ d and (c) $T = 2$ d.

where $[Gl]^0$ is the influent glucose concentration, $[Gl]_j$, $[Lac]_j$, $[IP]_j$, $[Pr]_j$, $[Ac]_j$ and X_j are the glucose, lactate, IP, propionate, acetate and biomass concentrations in the compartment j, D is the dilution rate (the inverse of the HRT), $[=]$ h^{-1}, $R^j_{Gl} = r1_j$ (rate of glucose consumption in the compartment j), $R^j_{Lac} = CE1 \cdot r1_j - r2_j$ (rate of lactate production in the compartment j), $R^j_{IP} = DE1 \cdot r1_j - r3_j$ (rate of IP production in the compartment j), $R^j_{Pr} = AL2 \cdot r2_j + AL3 \cdot r3_j - r4_j$ (rate of propionate production in the compartment j), $R^j_{Ac} = BE2 \cdot r2_j + BE3 \cdot r3_j + Y^4_{Ac\ Pr} \cdot r4_j - r5_j$ (rate of acetate production in the compartment j) and $R^j_X = CE1 \cdot r1_j \cdot Y^1_{X\ Lac} + AL3 \cdot r3_j \cdot Y^3_{X\ Pr} + AL2 \cdot r2_j \cdot Y^2_{X\ Pr} + BE2 \cdot r2_j \cdot Y^2_{X\ Ac} + BE3 \cdot r3_j \cdot Y^3_{X\ Ac} + r4_j \cdot Y^4_{X\ Pr} + r5_j \cdot Y^5_{X\ Ac}$ (rate of biomass production in the compartment j).

The methane production rate may be calculated by:

$$Q_{CH_4} = \sum_j (Y^5_{CH_4Ac} \cdot r5_j), \quad [=]\frac{1CH_4}{1\ d} \qquad (11)$$

The value of $\boldsymbol{\delta}$ was estimated by fitting the above mathematical model to the values of the effluent COD concentration of the 15-l PABR under three different SPSs at switching periods of one, 1.5 and two days, respectively. A least squares fitting method was used, where the system of differential equations [equation (10)] was solved by a fourth-order Runge–Kutta routine. Since the kinetic parameters of the model had already been determined during the simulation process of the batch kinetic experiment, the least-squares objective was to select the best $\boldsymbol{\delta}$ value (with no kinetic parameters manipulation), so as to minimise the squared residuals between the experimentally measured and the respective predicted values of the mean effluent COD concentration for the three different SPSs. In Fig. 7 the optimal values of the calculated effluent COD concentrations during the time of one period are graphically compared with the experimental results from the anaerobic digestion of glucose in the 15 l PABR. The optimal $\boldsymbol{\delta}$ value (with a precision of three decimal digits) obtained from the fitting process was 0.936.

The developed dynamic model was validated by comparing its predictions for the anaerobic digestion of glucose in the PABR with the experimental results for the COD and VFAs concentration. The model is capable of predicting adequately the amplitude oscillation of the COD (Fig. 4) and the VFAs (Fig. 5) concentrations in each compartment of the PABR in SPS for a biomass retention factor $\boldsymbol{\delta} = 0.936$. Finally, the prediction of the model for the biomass concentration is about 34 g/l and thus in good correspondence with the aforementioned experimental results (31 g/l).

Simulation of the PABR behaviour

Next, the model was used for the simulation of the PABR behaviour for several SPSs, as well as for the prediction of the PABR response to changes of the HRT. For assessment of the PABR performance and stability characteristics, the mean rate of organic matter (COD) removal as a function of the HRT for a given feed concentration is shown in Table 3. It can be seen that an optimum value for the HRT exists for every value of the period. In addition, for small enough HRTs, the mean COD removal rate is greater at shorter periods of switch-

Table 3. The mean methane production rate and the mean rate of COD removal (optimum values in bold letters) as a function of the HRT of a four compartment PABR for different values of period (T [=] d). Influent COD concentration 15 g/l

$T = \ll$	$T = 1$	$T = 4$	$T = 12$	$T = \gg$	HRT (d)	$T = \ll$	$T = 1$	$T = 4$	$T = 12$	$T = \gg$
0.4156	0.4198	0.4206	0.4206	**0.4211**	6	2483	2498	2501	2501	**2503**
0.4895	0.4973	**0.4991**	0.4974	0.4786	5	2941	2963	**2969**	2962	2877
0.5711	0.5798	**0.5826**	0.5760	0.4504	4	3513	3532	**3540**	3520	3114
0.5977	**0.5984**	0.5967	0.5862	0.3387	3	**4153**	4143	4137	4104	3363
0.5689	0.5687	0.5579	0.5288		2	**5259**	5216	5187	5121	
Methane production rate (l/l d)						Mean rate of COD removal (mg/l d)				

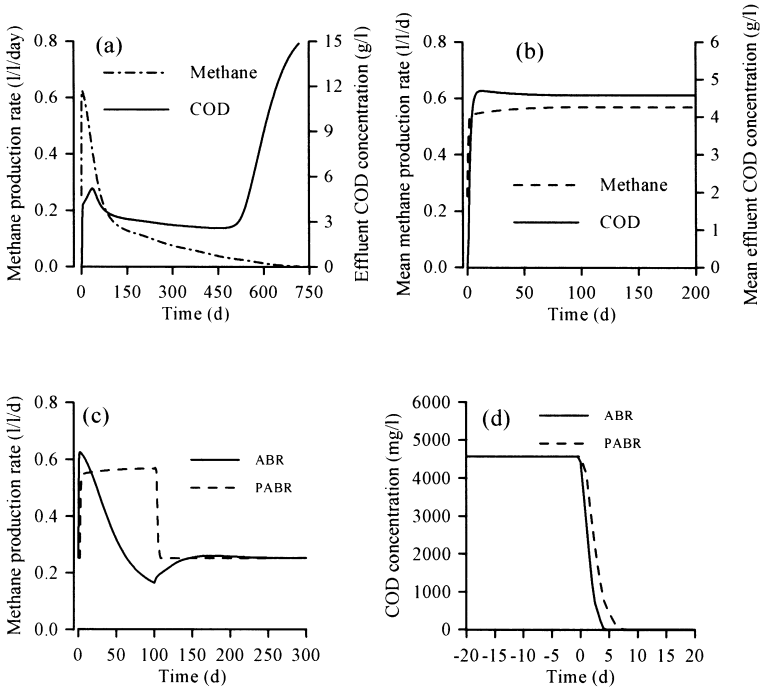

Fig. 8. Predicted response of: (a) an ABR to a step decrease in the HRT from 10 to two days; (b) a PABR (with a switching period of one day) to the same step decrease in the HRT; (c) a PABR to the same step decrease in the HRT without switching (ABR), as well as with a switching period of one day and to the reverse step change after 100 days operation at two days HRT; (d) a PABR to a step increase of the HRT (from two to 10 days) without switching, as well as with a switching period of one day.

ing, whereas for large HRTs it is larger at longer switching periods. Finally the PABR tends to behave as a UASBR, as the switching frequency becomes high enough ($T = \ll$). The equivalent UASBR is then of equal volume to the total volume of the four individual compartments. The same exact behaviour is predicted for the mean methane production rate (see Table 3), whereas again for every value of the period there is an optimum HRT. Here, it may also be seen that for small values of the HRT, the mean methane production rate is greater at shorter periods of switching and exactly the reverse is true for large values of the HRT. Finally, these conclusions and general trends are valid regardless of the influent COD concentration (see Table 4).

In order to assess the relative merits of the PABR when it comes to stability, the following simulations were undertaken. When a PABR is operated without switching of the feeding point (namely as an ABR), it fails when a step decrease in the HRT from 10 to two days is imposed, due to methanogen washout (see Fig. 8(a)). The PABR, however, when operated with periodic switching of the feeding point (T = 1 d), approaches an SPS when exposed to the same step change. Thus, it is possible to maintain a continued operation in spite of the large drop of the HRT (see Fig. 8(b)). When the same PABR is exposed to the reverse step change in the HRT after 100 days operation at two days HRT (before the methanogens have completely washed out), it returns back to the initial steady state. This reversion is more efficient if the PABR is operated with periodic switching of the feeding point (Fig. 8(c)). In the case of zero switching frequency, the methanogens have almost completely washed out from the first three compartments and they need more time to recover. On the contrary, the response of a PABR at SPS, which is exposed to the same step increase of the HRT, is more efficient if it simultaneously will start to be operated without switching of the feeding point (Fig. 8(d)). There will be enough time for the bacteria to remove more organic content from the first three compartments.

Table 4. The mean methane production rate (l/l d) as a function of the influent COD concentration of a four compartment PABR for different values of switching period (T) and HRT

T = 1	T = 4	T = 12	COD (g/l)	T = 1	T = 4	T = 12
0.2529	0.2531	0.2533	15	0.5687	0.5579	0.5288
0.5060	0.5063	0.5068	30	1.1495	1.1268	1.0695
0.7591	0.7595	0.7604	45	1.7293	1.6957	1.6104
HRT = 10 d				HRT = 2 d		

The predictions of the above developed model for the performance of the PABR in SPS, as well as for the reactor response in a step change of the HRT, are qualitatively similar to those using Smith's model (Skiadas and Lyberatos, 1998). This proves that the predictions for the behaviour of the PABR are not sensitive to the particular model structure, at least qualitatively. Given that a series of several CSTRs provides greater substrate conversion than a CSTR of equal volume for reactions with Monod kinetics (Bailey and Ollis, 1986), the compartmentalised structure of the PABR gives the possibility of optimising the COD removal rate as a function of the OLR by the manipulation of the switching frequency. When the resulted biomass dilution rate is smaller than the maximum biomass growth rate in each of the four PABR compartments, the COD removal is higher at a PABR operated at zero frequency of switching the feed point (as a ABR). In contrast, when the biomass dilution rate is relatively high but not higher than the overall biomass production rate, the COD removal is higher at a PABR operated at high frequency of switching the feed point (as an UASBR). For every intermediate value of the OLR there is a value of the switching frequency (between zero and infinite) for which the COD removal rate is maximised (see Tables 3 and 4).

The model predicts less methane production than it was experimentally observed due to the neglected production of methane from H_2 and CO_2. Nevertheless, the usefulness of this model is not reduced since it aims at the prediction of the COD removal during the anaerobic wastewater treatment in PABR.

CONCLUSIONS

A dynamic model for the anaerobic digestion of glucose in the Periodic Anaerobic Baffled Reactor was developed. The key assumption of the model is that the hydraulic behaviour of a four compartment PABR is equivalent with the behaviour of four CSTR in series, as far as the dissolved components are concerned, whereas the biomass is allowed to be retained in the compartments of the PABR by precipitation. The accumulation of biomass is simulated assuming that the biomass concentration of the effluent stream from each one of the four compartments will be equal to $(1 - \boldsymbol{\delta})X$ if the biomass concentration in the same compartment is X. The optimal value of the *biomass retention factor* $\boldsymbol{\delta}$ was estimated (with no kinetic parameters manipulation) by fitting the model to the values of the effluent COD concentration of a glucose fed 15-l PABR under different SPSs. The model is capable of predicting adequately the experimentally measured values of the COD concentration in each compartment of the PABR in SPS, the effluent COD concentration, as well as the biomass concentration in the reactor.

The simulations of the PABR behaviour employing the new model for the anaerobic digestion of glucose in the PABR showed that for large values of organic loading, the PABR is expected to perform better when operated at a high frequency of switching feed point, namely it behaves as a UASBR, whereas for smaller values of the organic loading the PABR should be operated at smaller frequencies approaching that of an ABR. Also, the simulations showed that depending on the loading rate, which in principle may be variable, it is possible that the switching frequency should be manipulated accordingly, allowing for the PABR to be operated as an ABR, a UASBR or at an intermediate mode. Consequently, the PABR is best suited for handling time-varying loading rates since it allows for maximal conversion rates at all times.

The PABR should prove a useful high rate anaerobic system of high flexibility and it deserves further study and characterisation. On the other hand, the above developed model should be a useful tool for the future designing of a pilot scale PABR; despite that, its validity and prediction capacity are limited to the conditions under which the experiments were conducted. Apparently, the constant $\boldsymbol{\delta}$ assumption over the four compartments is not quite precise. Further experiments need to be carried out (preferably in pilot scale) to determine the parameter $\boldsymbol{\delta}$ as a function of the PABR operational parameters such as volumetric and organic loading rate.

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REFERENCES

Bachmann A., Beard V. L. and McCarty P. L. (1982) Comparison of fixed-film reactors with a modified sludge blanket reactor. *Proceedings of the First International Conference on Fixed-Film Biological Processes* **II**, 1192–1211.

Bachmann A., Beard V. L. and McCarty P. L. (1985) Performance characteristics of the anaerobic baffled reactor. *Wat. Res.* **19**, 99–106.

Bailey J. E. and Ollis D. F. (1986) Design and analysis of biological reactors. In *Biochemical Engineering Fundamentals*. McGraw-Hill.

Barber W. P. and Stuckey D. C. (1999) The use of the anaerobic baffled reactor (ABR) for wastewater treatment: a review. *Wat. Res.* **33**, 1559–1578.

Bauchop T. and Elsden S. R. (1960) The growth of microorganisms in relation to their energy supply. *Journal of General Microbiology* **23**, 45–469.

Brooke A., Kendrick D. and Meeraus A. (1996) *GAMS Release 2.25: A User's Guide*. GAMS Development Corporation, Washington, DC.

Costello D. J., Greenfield P. F. and Lee P. L. (1991) Dynamic modelling of a single-stage high-rate anaerobic reactor—I. Model derivation. *Wat. Res.* **25**, 847–858.

Gavala H. N., Skiadas I. V. and Lyberatos G. (1999) On

the performance of a centralised digestion facility receiving seasonal agroindustrial wastewater. *Wat. Sci. Technol.* **40**(1), 339–346.

Ghosh S. and Klass D. L. (1978) Two-phase anaerobic digestion. *Process Biochemistry* **13**, 15–24.

Grobicki A. and Stuckey D. C. (1991) Performance of the anaerobic baffled reactor under steady state and shock loading conditions. *Biotechnol. Bioeng.* **37**, 344–355.

Grobicki A. and Stuckey D. C. (1992) Hydrodynamic characteristics of the anaerobic baffled reactor. *Wat. Res.* **26**, 371–378.

Josefsson B. (1983) Rapid spectrophotometric determination of total carbohydrates. In *Methods of Seawater Analysis*, 2nd ed., eds K. Grassoff, M. Ehrhardt and K. Kremling, pp. 340–342. Verlag Chemie GmbH, D-6940 Weinheim.

Lawrence A. W. and McCarty P. L. (1969) Kinetics of methane fermentation in anaerobic treatment. *Journal WPCF* **41**, R1–R17.

Lee I. H., Fredrickson A. G. and Tsuchiya H. M. (1974) Diauxic growth of Propionibacterium shermanii. *Appl. Microbiol.* **28**, 831–835.

Lettinga G., van Velsen A. F. M., Hobma S. W., de Zeeuw W. J. and Klapwijk A. (1980) Use of the Upflow Sludge Blanket (USB) reactor concept for biological wastewater treatment. *Biotechnol. Bioeng.* **22**, 699–734.

Nachaiyasit S. and Stuckey D. C. (1997a) The effect of shock loads on the performance of an anaerobic baffled reactor (ABR), 1. Step changes in feed concentrations at constant retention time. *Wat. Res.* **31**, 2737–2747.

Nachaiyasit S. and Stuckey D. C. (1997b) The effect of shock loads on the performance of an anaerobic baffled reactor (ABR), 2. Step and transient hydraulic shocks at constant feed strength. *Wat. Res.* **31**, 2747–2755.

Pullammanappallil P. (1993) Modelling and control of the anaerobic digestion process. Ph.D. thesis, University of Florida, USA.

Skiadas I. V. (1998) The Periodic Anaerobic Baffled Reactor (in Greek). Ph.D. thesis, University of Patras, Greece.

Skiadas I. V. and Lyberatos G. (1998) The periodic anaerobic baffled reactor. *Wat. Sci. Technol.* **38**(89), 401–408.

Smith P. H., Eordeaux F. M., Goto M., Shiralipour A., Wilke A., Andrews J. F., Ide S. and Barnett M. W. (1988) Biological production of methane from biomass. In *Methane from Biomass. A Treatment Approach*, eds W. H. Smith and J. R. Frank, pp. 291–334. Elsevier, London.

van den Berg L. (1977) Effect of temperature on growth and activity of a methanogenic culture utilising acetate. *Can. J. Microbiol.* **23**, 898–902.