DE GRUYTER OPEN
Print ISSN: 1312-2622; Online ISSN: 2367-5357
DOI: 10.1515/itc-2017-0022

Mathematical Modelling and Extremum Seeking Control of Cascade of Two Bioreactors for Production of Hydrogen and Methane

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Key Words: *Extremum seeking control; cascade control; anaerobic digestion bioreactors; biogas production optimization; non-linear models.*

Abstract. *A mathematical model of a cascade of two continuously stirred anaerobic bioreactors is presented in this paper and the extremum seeking control is applied on it. The dilution rate of the first bioreactor is chosen as control action and the joint biogas flow rate both bioreactors is the measured output to be maximized. The concentration of inlet organics is accepted as the disturbance. The correction of the working volume of the second bioreactor is studied as the inner loop of the cascade control system. The outer control loop is represented by the extremum seeking controller, which finds the optimum control action and reacts to the disturbance. Computer simulation studies show the feasibility of this scheme.*

1. Introduction

The human population is constantly growing and with it, the environmental pollution and energy demands are increasing. Dumping the used materials generates problems with their safe storage and simultaneously their value for modern circular world economy is lost. Keeping the raw materials longer in circulation will mitigate environmental pollution and will make our world looks better in several ways.

Anaerobic digestion of organic wastes (AD) is a relatively cheap method for realization of two tasks: depollution of organic wastes and production of energy in the form of biogas (hydrogen and methane) at the same time [1]. The outlet material (digestate) can be used for fertilization of farmlands and other territories. That is why it is important to find ways of increasing the performance of the AD process and maintain the stability of the processes [11,12].

The effectiveness of the AD processes depends on many factors such as the inlet material, physical and chemical conditions in the bioreactors, bioreactor types and the microorganisms. Due to these diverse factors and the difficulties in measuring important indicators in real-time or the high price of such systems, which can be used for modelling and control of the process, it is very difficult to operate biogas installations with high performance. The extremum seeking control (ESC) does not require process model to find optimum control action, so ESC is very suitable for controlling biogas installations [2-5]. Chaining two AD bioreactors in cascade system leads to dual digestion by different microorganisms which increase transformation of organics into hydrogen and methane.

The aim of the paper is examining the possibility of using ESC controller on cascade of two bioreactors with non-linear mathematical models and the studying of overall performance of the cascade system in the presence of disturbance in the inlet organic concentration. The impact of a more complex model of the first bioreactor on system performance is also examined.

2. Anaerobic Digestion Process

The production of hydrogen in addition to the wide spread methane production is conditioned by gaining economic importance of the hydrogen in today's world. Burning of methane is accompanied by releasing of carbon dioxide which has significant effect on global warming. In *table 1* are given the typical biogas components concentrations.

Table 1. Typical chemical composition of the biogas

Gas	Concentration, % Vol
Methane – CH_4	50-80
Hydrogen – H_2	5-10
Carbon dioxide – CO_2	20-50
Water vapor – H_2O	2-10
Nitrogen – N_2	0-2
Hydrogen sulfide – H_2S	0-0.4

The AD processes consist of four main steps: hydrolysis, acidogenesis, acetogenesis and methanogenesis. Each of these steps is conducted by separate microorganism. These steps go simultaneously in the bioreactor and lead to formation of diverse products. The pathways for producing different products are several and can alter under the influence of conditions in the bioreactor. Transformations of organic compounds in the branches of the diagram given on *figure 1* take places with different rates and efficiency, due to different microorganism involved.

Complex organic substances entering the bioreactor can't be used directly by hydrogen and methane producing microorganisms. During first step, the hydrolysis, the long organic molecules are cut to shorter ones via enzymes secreted by bacteria. Next steps convert this products to even shorter ones (acidogenesis and acetogenesis). The last step, methanogenesis, converts acetates into methane. This gas is produced also from hydrogen and carbon dioxide released in the previous steps. Another pattern is the conversion of acetate into hydrogen and carbon dioxide and vice versa by another type of microorganisms. From the diagram on figure 1 is obvious that biogas production by AD of organic wastes have potential for optimization by microorganisms' selection, bioreactor conditions and processed materials.

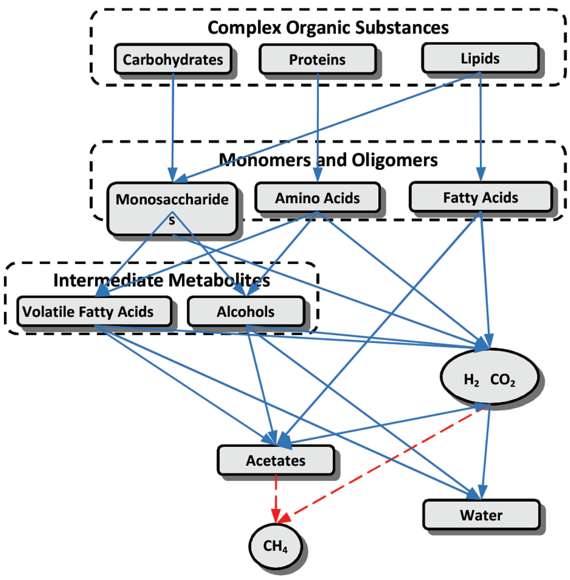

Figure 1. General diagram of the AD process

Another way for efficiency boosting is the separation of the AD steps in two different bioreactors each with optimum conditions tuned for given microorganisms [4,8]. Each of them has exceptive environmental requirements which lead to sub-optimal process performance if only one bioreactor is used. This means that the cost of the biogas will be higher and it won't be economically attractive. It is known that the application of two-phase process considerably increases biogas production. Diagram of a typical two-phase cascade system of bioreactors is given on *figure 2*.

The aim of such system is hydrogen production to take place only in the first bioreactor and methane production only in the second bioreactor. Organic wastes are first fed in the hydrogen bioreactor and after that they are transferred to the second bioreactor for consecutive conversion of remaining organics into methane. This scheme provides better extraction of organic pollutants than the single bioreactor scheme. This leads to more biogas produced and lowering to the greater extend the organic contents in the output product.

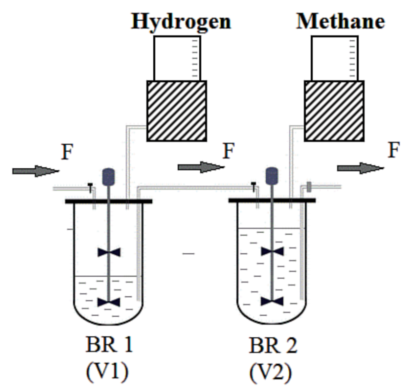

Figure 2. Diagram of a cascade of two bioreactors for separate production of hydrogen and methane

Except the selection of suitable microorganisms in the two bioreactors, it is necessary to comply with some technological constrains in order the cascade system to function in the best possible way. The specific growth rates of the microorganisms producing methane is significantly lower than that of the microorganisms in the hydrogen bioreactor. If the inlet flow of the reactor is too high, there won't have enough time for the methanogenic microorganisms to grow and they will be washed out by the output flow of the bioreactor. If the inlet flow of the first bioreactor is kept also low, this will strongly limit the hydrogen yield. The solution of this problem is to make the second bioreactor with higher volume, so the washout effect is avoided.

In order to achieve also the maximum methane yield, it is necessary to determine the how large the second bioreactor in comparison to the hydrogen one must be. The ratio of the working volumes, have to be such that the methane bioreactor works in its optimal working point when the hydrogen bioreactor is in its optimum point. The inner control loop of the cascade system is represented by the working volume of the second bioreactor. The determination of the optimum dilution rate of the inlet organic substrate of the first bioreactor is done by ESC controller.

3. Extremum Seeking Control

The ESC is a type of optimal control, which is applied in situations where plant model and/or objective function are not completely known, but input-output signals are measurable and this function has an extremum. The aim of this approach is through constant change of the control input to search for such value, that the objective function is maximized or minimized. This is done with the addition of external perturbation signal to the input signal of the plant, which generates variations in the output signal. The updated control signal is calculated on the basis of the change in the output signal.

There are known many algorithms for ESC but for some of them the stability is not mathematically proven. One of the frequently studied versions of this algorithm is the one using periodic external perturbation signal with sinusoidal form [2,3,5].

The perturbation signal has to be weak, but to generate enough change in the output. The form of the signal can be different including rectangular and even stochastic. The speed of convergence depends also on normalized power of the perturbation signal [10]. The plant must be stable, but it is allowed to change in time. The diagram of this algorithm is shown on *figure 3*.

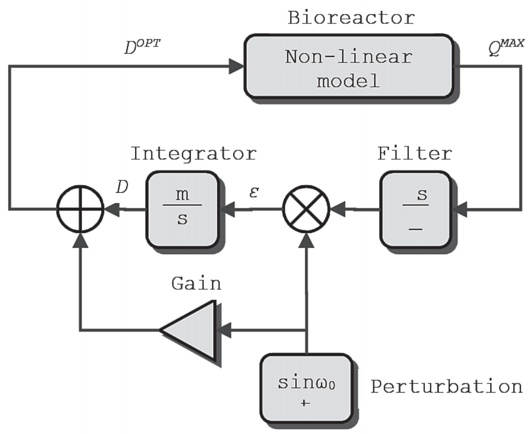

Figure 3. Diagram of sinusoidal ESC algorithm

Operating principle of the ESC control is the following. After suitable scaling of the external signal according to the plant, it is summed with the current control input D.

This signal generates periodic variations in output signal Q, which is passed through a high-pass filter eliminating the DC component. The filtered output signal is multiplied by the primary perturbation signal. After that the signal ε is passed on to the integrator, which updates the control signal D in the direction where the gradient decreases. The signal D is also scaled with the coefficient m.

A low-pass filter can be added before the integrator which passes only the DC component of the demodulated signal ε. In that case the calculated gradient will be exact, while if only integrator is used, the estimated gradient will not be completely accurate, because of the higher harmonics.

When the coefficient m > 0, the algorithm is searching for maximum of the objective function and when m < 0 the minimum is searched. When ε has positive value, the work point of the system is on the left of the maximum and vice versa. When the smooth function Q(D) has negative second derivative, it has a maximum and in the case of positive second derivative, it has minimum.

The parameters for tuning the ESC controller are coefficient m, the cut-off frequency of the high-pass filter h, the amplitude and a frequency ω0 of the periodic perturbation signal. The smaller the amplitude is, the smaller the residual error and output variations are, but the possibility for stopping at local extremum is higher and the speed of convergence is lower. Higher values of m lead to higher speed of convergence. The frequency h of the filter has to be sufficiently lower than that of the perturbation signal. The higher the ω0 is, the effect of the perturbation on the plant will be lower, but it has to stay in the frequency pass band of the plant.

4. Cascade System Model

The studied models are based on the mass balance of the process [6,7]. They are simplified and no inhibition nor microorganisms' death or any other features of AD process are taken into account.

By definition D = F / V and F = DV. From *figure 2* is obvious that $F = D_1V_1 = D_2V_2$ or

$$(1)\quad V_2 = \frac{D_1}{D_2}V_1 = KV_1 .$$

This means that the working volume of BR_2 is K times that of the BR_1. It is known that the specific growth rate of methanogens is considerably lower than that of the hydrogen producing microorganisms, so $D_1 > D_2$ and $K > 1$. After determining the optimum values D_1^{OPT} and D_2^{OPT} the value of K bringing BR_2 to its optimal working point can be calculated [9].

In this paper the following two models of the first bioreactor (BR_1) are considered:

$$(2)\quad \begin{aligned}
\frac{dS_1}{dt} &= -\frac{1}{Y_1}\mu_1 X_1 + D_1\left(S_1^{IN} - S_1\right)\\
\frac{dX_1}{dt} &= \mu_1 X_1 - D_1 X_1\\
\frac{dAc_1}{dt} &= \frac{1}{Y_2}\mu_1 X_1 - D_1 Ac_1\\
\mu_1 &= \frac{\mu_1^{MAX} S_1}{K_1^S + S_1}\\
Q_{H2} &= Y_{H2}\mu_1 X_1
\end{aligned}$$

$$(3)\quad \begin{aligned}
\frac{dS_0}{dt} &= -\beta X_1 S_0 + D_1(Y_P S_0^{IN} - S_0)\\
\frac{dS_1}{dt} &= -D_1 S_1 + \beta X_1 S_0 - \frac{1}{Y_1}\mu_1 X_1\\
\frac{dX_1}{dt} &= \mu_1 X_1 - D_1 X_1\\
\frac{dAc_1}{dt} &= \frac{1}{Y_2}\mu_1 X_1 - D_1 Ac_1\\
Q_{H2} &= Y_{H2}\mu_1 X_1\\
\mu_1 &= \frac{\mu_1^{MAX} S_1}{K_1^S + S_1}
\end{aligned}$$

The used notations are:

S_0,S_1 – organics concentration in the BR_1 [g/l];
S_0^{IN}, S_1^{IN} – organic concentration in the inlet flow of BR_1 [g/l];
X_1 – biomass concentration in the BR_1 [g/l];
Ac_1 – acetate concentration in BR_1 [g/l];
QH_2 – hydrogen flow rate per hour [dm3/l.h];
μ_1 – specific growth rate of hydrogen producing microorganisms [h^{-1}].

Model (2) describes a one-step transformation of organic substrate into hydrogen and acetate by one type of microorganisms. Model (3) adds hydrolysis as first step, which is conducted by the same microorganisms.

The bioreactors are operated in continuous mode where the transient processes are finished, so we can find the equations for the above variables in the steady-state, by nullifying the differential equations. After some other mathematical transformations we get the two systems of algebraic equations for both models which give the values as functions of model parameters and the two input signals, D_1 and S^{IN}.

The input-output static characteristics of the bioreactors Q(D) are important for the extremum seeking control. The coordinates of their maximum are calculated by nullifying the first derivative of Q(D) for several values of S^{IN}.

The model of the second bioreactor in the cascade (BR_2) is given in (4).

$$\begin{aligned} &\frac{dX_2}{dt} = \mu_2 X_2 - D_2 X_2 \\ (4)\quad &\frac{dAc_2}{dt} = -\frac{1}{Y_3}\mu_2 X_2 + D_2\left(Ac_1 - Ac_2\right) \\ &\mu_2 = \frac{\mu_2^{MAX} Ac_2}{K_2^{S} + Ac_2} \\ &Q_{CH4} = Y_{CH4}\mu_2 X_2 \end{aligned}$$

It describes again a one-step transformation of the inlet acetate into methane by single type of microorganisms.

The used notations are:

X_2 – biomass concentration in BR_2 [g/l];

Ac_2 – acetate concentration in BR_2 [g/l];

Ac_1 – inlet acetate from BR_1 [g/l];

Q_{CH4} – methane yield per hour [dm^3/l.h];

μ_2 – specific growth rate of methanogens [h^{-1}].

The corresponding equations for D_1^{OPT} and D_2^{OPT} are given in (5) and (6), respectably. The equations of Q(D) for the models of BR_1 and BR_2 respectably, are given in (7) and (8). The expressions for S_1, Ac_1 and Ac_2 in the steady-state mode are not given, but they can be expressed by model parameters and input signals in question. The value of D_1^{OPT} for the second model of BR_1 is numerically determined due to impossibility of Symbolic Math toolbox to find solution.

$$(5)\quad D_1^{OPT} = \mu_1^{MAX}\left(1 - \sqrt{\frac{K_1^{S}}{S_1^{IN} + K_1^{S}}}\right)$$

$$(6)\quad D_2^{OPT} = \mu_2^{MAX}\left(1 - \sqrt{\frac{K_2^{S}}{Ac_1 + K_2^{S}}}\right)$$

$$(7)\quad Q_{H2} = Y_1 Y_{H2} D_1\left(S_1^{IN} - S_1\right)$$

$$(8)\quad Q_{CH4} = Y_3 Y_{CH4} D_2\left(Ac_1 - Ac_2\right)$$

5. Simulation Studies

The computer simulations of the cascade system are done in Matlab/Simulink environment version 2009b and 2016a. The mathematical transformations are done with Symbolic Math Toolbox in the same products.

The models of both bioreactors are not calibrated due to the scarce experimental data. Because of that, example values for the model parameters are used, which leads to complex values in some of the simulations [11].

Simulations with two variants of the cascade system are made. The first variant uses first model of BR_1 and the second variant uses the second, more complex, model of BR_1. The model of BR_2 is the same for the two variants of the cascade system. In *table 2* are given model parameters for both bioreactors and in *table 3* the parameters of the ESC controller are given. They are chosen heuristically for the first model of BR_1.

Table 2. Bioreactors model parameters

Y_1	Y_2	Y_{H2}	μ_1^{MAX}	K_1^S	β	Y_P
0.08	1	1	0.568	3.914	1	1
Y_3	Y_{CH4}	μ_2^{MAX}	K_2^S			
0.24	18.7	0.0083	0.22			

Table 3. ESC controller parameters

Amplitude *a*	Frequency *ω₀*	Frequency *h*	Gain *m*
0.04 h^{-1}	0.6 rad/s	0.5 rad/s	0.1

5.1. Volumetric Coefficient K

The input-output static characteristics of the three models for two values of S^{IN} are given on *figures 4-6*, respectably. In *table 4* are given the calculated values of the important system parameters.

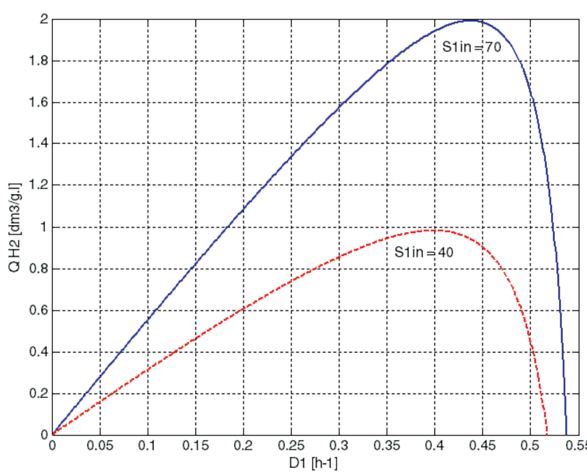

Figure 4. I/O static characteristics of BR1 model 1

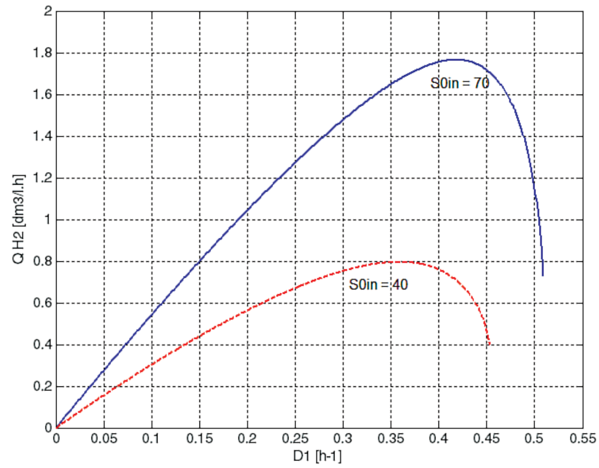

Figure 5. I/O static characteristics of BR_1 model 2

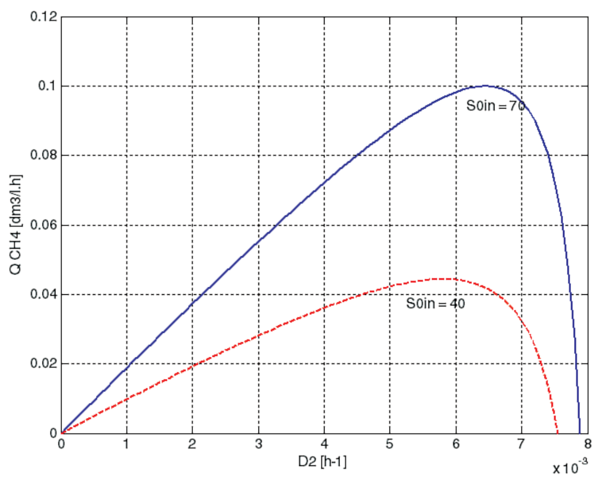

Figure 6. I/O static characteristics of BR2

Table 4. Values of D^{OPT}, D^{WASH} and Q^{MAX}

S^{IN} [g/l]	D_1^{OPT} [h^{-1}]	D_1^{WASH} [h^{-1}]	Q_1^{MAX} [dm^3/l.d]	D_2^{OPT} [h^{-1}]	D_2^{WASH} [h^{-1}]	Q_2^{MAX} [dm^3/l.d]
Variant 1						
70	0.437	0.538	1.991	0.0065	0.0079	0.110
40	0.398	0.517	0.986	0.0059	0.0076	0.051
Variant 2						
70	0.418	0.510	1.770	0.0065	0.0079	0.100
40	0.359	0.454	0.796	0.0058	0.0076	0.045

From *figures 4-6* it is obvious that the input-output characteristics have only global maximum and it is in the admissible range for control input D. The coordinates of extremum is shifting down and left with lowering the organics concentration of the inlet flow S^{IN}. The slope after the maximum is considerably steeper and this can quickly render the process nonoperational, because further small increments of D lead to large decrease in Q.

Making the model of BR_1 a little more complex lead to lowering biogas flow rate, achieved at lower dilution rates also. The form of characteristics remained the same. The one on *figure 5* is not complete, because the remaining part is complex, due to the model parameters.

From equations (5) and (6) for D^{OPT} is obvious that they are functions of S^{IN} and Ac_1, but these variables are bound with the model of BR_1. Therefore, the coefficient K will depend on the input signals S^{IN} and D_1 of BR_1. The characteristics $K(S^{IN},D_1)$ for the two variants of cascade system and two values of D_1 are given on *figures 7* and *8*. The two values of D_1 correspond to the optimum values for the two organic concentrations S^{IN}, before and after the disturbance in S^{IN}.

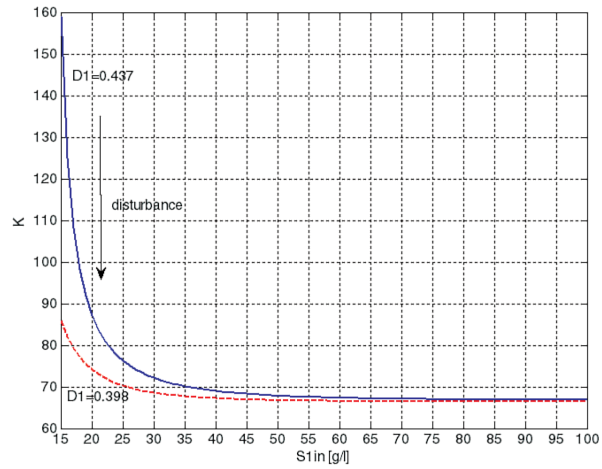

Figure 7. Characteristics $K(S^{IN},D_1)$ for variant 1

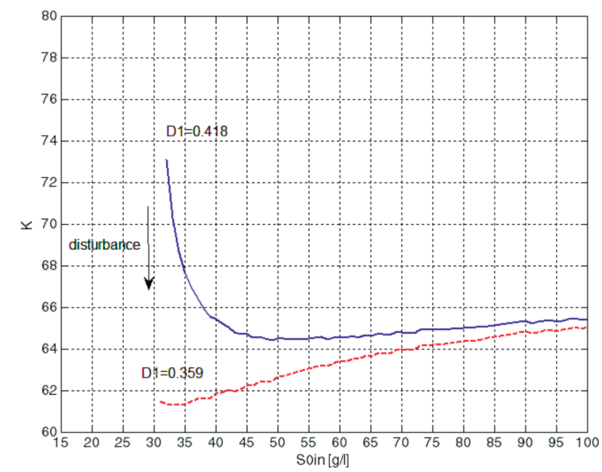

Figure 8. Characteristics $K(S^{IN},D_1)$ for variant 2

As can be seen from *figures 7* and *8*, K has very close values for high input concentrations, especially for variant 1. The change in K for variant 2 is a little higher for the range of S^{IN} = 40-70 g/l. When the S^{IN} changes, this leads to change in D_1^{OPT}, so the optimum point shifts to the lower line in both figures. The calculated values of K before and after disturbance in S^{IN} are given in *table 5*.

Table 5. Values of K for the two variants and disturbance in S^{IN}

	Before	**After**
Variant 1	67.085	67.245
Variant 2	64.775	61.836

For variant 1, the change in K is 0.24% and there is no observed change is biogas flow rate Q_{CH4} before and after disturbance in the case of unchanged K. For variant 2, the change in K is 4.54% and the decrease in Q_{CH4} after disturbance is 1.54%. Here, the working point remains on the left of the maximum of the I/O static characteristic of BR_2, where the decrease of biogas flow is slower.

When K is higher after disturbance, this means that the working point of BR_2 remains on the right side of the maximum and vice versa, if no measures are taken to correct it. Therefore, the first situation is more problematic because BR_2 gets closer to dangerous zone, where washout of microorganisms can occurs.

For the studied models of bioreactors the coefficient K remains almost the same for relatively large diapason of S^{IN} and it is not mandatory to use additional controller to correct the working volume of the second bioreactor. The drop in biogas flow rate Q is very little if K keeps its first value, but if the disturbance in S^{IN} is larger, K gets sufficiently different and this can causes the process in BR_2 to stop or to function far from optimum working point.

5.2. Extremum Seeking Control

The objective function to be maximized in this paper is accepted as:

$$A = Q_{H2} + Q_{CH4} \rightarrow \max.$$

As it was shown, if the little drop in Q_{CH4}, due to the suboptimal value of K, is neglected, the above function can be modified to include biogas flow of the first bioreactor only and this will be enough for optimum results of the cascade system for relatively large disturbances in S^{IN} and the objective function obtain the form:

$$A = Q_{H2} \rightarrow \max$$

The effect of ESC controller is tested for both variants of the cascade system, starting from left and right of the maximum. The starting values of D_1 is 0 and the highest possible for which the process stays vital.

On *figures 9* and *10* are given the trajectories of the working points of the two variants of system in the phase plane Q-D. Two simulations are performed starting with different $D_1(0)$.

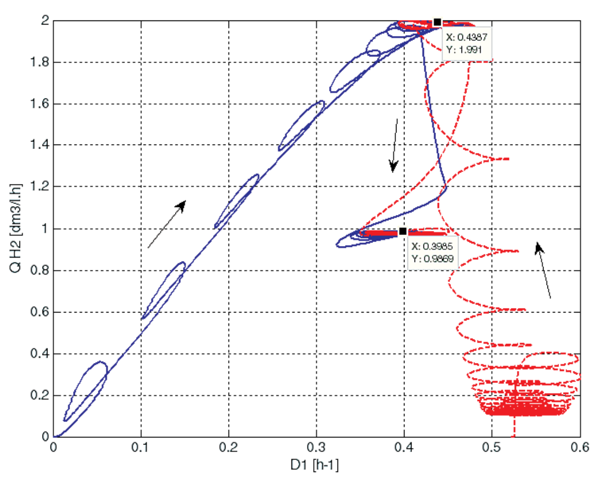

Figure 9. BR_1 process with ESC control for variant 1 in phase plane, $D^{RIGHT}(0) = 0.522$

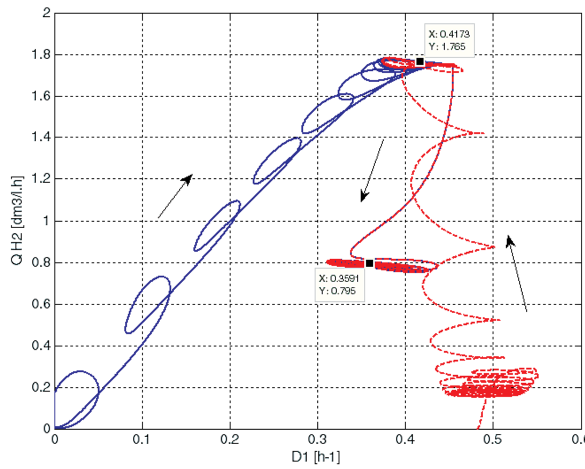

Figure 10. BR_1 process with ESC control for variant 2 in phase plane, $D^{RIGHT}(0) = 0.482$

From *figures 9* and *10* it can be seen that even when the process start far from the optimum value in the danger zone, the ESC controller succeeds in finding the best value for D_1 for both variants.

In *table 6* are given some quality metrics of the cascade system for the two variants with ESC controller and the open loop system. The steady-state time of H_2 is longer with ESC controller, partly because of the negative wave of the perturbation signal and partly of the controller parameters. They can be tuned, so the steady-state time is shortened. When the start is from the right the steady-state time is significantly longer for both biogases. Methane is getting to the steady-state faster for variant 2.

Table 6. Biogas flow with and without ESC

	Steady-state H_2, h	Steady-state CH_4, h	Biogas yield after disturbance	
			H_2, l/h	CH_4, l/h
	Variant 1			
No ESC	20	125	0.942	0.0400
ESC left	63	95	0.982	0.0507
ESC right	257	1500	0.982	0.0507
	Variant 2			
No ESC	20	80	0.708	0.0270
ESC left	62	75	0.809	0.0447
ESC right	165	878	0.809	0.0447

For variant 2, the difference in the flow rate of the methane (39.6%) is caused by suboptimal coefficient K and dilution rate D_1 when no ESC is used. For variant 1, the difference is 21.1%. The difference in the hydrogen flow rate is 4.1% for variant 1 and 12.5% for variant 2. From these figures can be seen that the more complex model of BR_1

leads to larger loss in the biogas yields, then the first model, when no ESC is used.

In *table 7* are given the degree of biodegradation in the two bioreactors for both variants of the cascade system. The ESC control recovered the degree of biodegradation after the disturbance for both variants. The gain in the process efficiency when ESC is used is larger for variant 2. The negative impact of the disturbance is greater for the second bioreactor.

When using perturbation signal with amplitude of 0.04 h^{-1} (9.2% before and 10.1% after perturbation), periodic variations of hydrogen and methane are given in *table 8*. The perturbation is from 70 to 40 g/l (step decrease of 43%).

Table 7. Degree of biodegradation in both bioreactors in the cascade system

	Before disturbance		After disturbance	
	BR$_1$	BR$_2$	БР$_1$	БР$_2$
	Variant 1, %			
No ESC	75	83	62	63
ESC	75	83	70	78
	Variant 2, %			
No ESC	70	82	49	55
ESC	70	83	65	82

Table 8. Periodic variations in the output of the bioreactors

	BR$_1$, %		BR$_2$, %	
	Before	After	Before	After
Variant 1	0.70	0.60	0.90	0.10
Variant 2	1.40	2.10	0.08	0.07

The ESC behavior is studied also in the case of varied parameters of model 2 of the BR_1. The two examined coefficients are connected with the hydrolysis step, β and Y_P. Their values are given in *table 9*. The results from simulations are presented on *figure 11*.

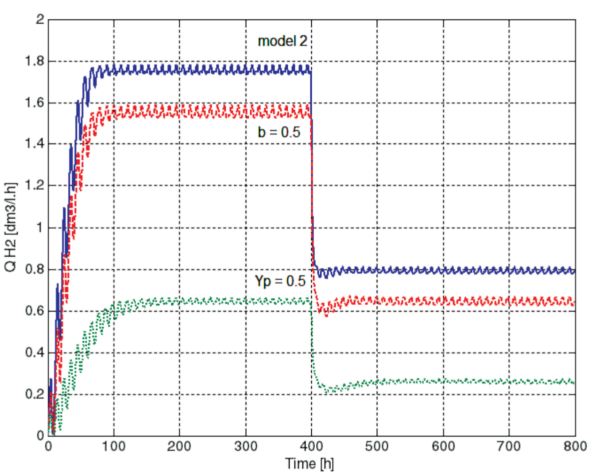

Figure 11. ESC control of BR1 and varied model parameters in the time domain

Table 9. Values of Q_1^{MAX} and D_1^{OPT} before disturbance for model 2 and varied parameters

Coefficient	Q_1^{MAX}, $dm^3/l.h$	D_1^{OPT}, h^{-1}
Model 2	1.775	0.418
$Y_P = 0.5$	0.659	0.341
β = 0.5	1.571	0.396

It is obvious that these changes in parameters have effect mainly on the biogas flow rate and not on the dynamics of the bioreactor. So, the previously configured for the first model of BR1, ESC controller gives very good results even for those models. The influence of YP is much greater than that of β, for both, biogas flow rate and dilution rate. The ESC control succeeds in finding the optimal control action for these models too. This means that the ESC control has the properties of a robust control system

6. Conclusion

In the paper was discussed the problem of improving biogas energy production of AD processes in a cascade of continuously stirred tank bioreactors with hydrogen and methane production. For this task simple mathematical models of bioreactors were adopted. It was shown that the ESC control strategy can be suitable solution for this task and that for the studied bioreactor models it is not mandatory to use another controller for the inner loop of the cascade system correcting the working volume of the second bioreactor in order to obtain close to the maximum system performance.

The ESC found optimal dilution rate of the substrate when started from 0 and close to the washout value of D_1. The algorithm updated the control signal to the new optimal value in the presence of disturbance in the inlet organics concentration S^{IN}.

The ESC controller was tuned for the first model of BR_1, but it achieved good performance without being retuned for the second model too and even with changed model parameters. This shows that the ESC approach is viable solution for bioreactors control where many variables are hard to measure and that it has robust properties.

All studied in this paper bioreactor models are simplified and they do not account for many real-life effect such as inhibition by substrate, existing of more microorganisms groups and alternative pathways for substrate transformation. These features will have significant effects on the ESC control system performance and optimal volumetric coefficient determination.

The existing research papers have shown that this algorithm can be further improved by different modifications and to acquire even better results [13].

Acknowledgement

The authors gratefully acknowledge the financial support of this work by the Bulgarian National Science Fund, contract No. DFNI-E02/13.

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Manuscript received on 17.02.2017

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