Formalization of target invariants and designing an adaptive control system for the model of anaerobic biological wastewater treatment

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Abstract. A model of a two-step anaerobic fermentation in a bioreactor-mixer, whose mathematical description is a system of nonlinear mathematical equations, is discussed. The purpose is to design an algorithm of an energy-saving control relying on the principles of nonlinear adaptation on target manifolds with an attractive property, which are referred to as invariants or invariable laws of the target system behavior for the object under study. A necessary preliminary step is the formalization of possible target invariants in the form of prescribed (desired) laws of the controlled object behavior. An example is given of designing a vector regulator with a compensation of random disturbances over the control channel in a system of anaerobic biological waste water treatment.

1. Introduction
Several effective design and engineering solutions for the systems of anaerobic purification, based on an in-depth analysis of the features of anaerobic fermentation processes and mathematical modeling of the bio-methanogenesis, were advanced in [1-6].

More recently (based on [1-4]), an international IWA Anaerobic Digestion Task Group proposed a generalized model of the anaerobic fermentation kinetics ADM-1 [5, 6], which today represents a tool providing the most complete and detailed description of the principal stages of conversion of organic pollutants and intermediates of biodegradation.

The purpose of this research is to formalize the invariants (laws of behavior of a weakly formalized object in a steady state) for the system of anaerobic biological wastewater treatment from the point of view of the possibilities of the synergetic control theory (SCT) [7], which implements the principles of physical control theory [8].

2. Formulation of the problem of setting invariants for organizing an adaptive control design for anaerobic biological wastewater treatment
Let the initial substance of volume \( V \) be fed into a bioreactor at rate \( Q(t) \), concentration of nutrient organic substances \( S_{o}(t) \) and biomass \( B_{o}(t) \), and let an equivalent amount of liquid be removed (see anaerobic fermentation model, ADM1).
Use \( \theta(t) \) to denote the operating temperature in the bioreactor, and \( k_i(\theta) \) - the kinetic parameters of the process, taking the law of their variation given by

\[
k_i(\theta) = k_{35^\circ C} \exp\left(c(\theta - 35^\circ C)\right)
\]

[9], where \( k_{35^\circ C} \) is the value of the parameter at the normal temperature of the biomass.

Consider a system of equations of the anaerobic biological wastewater treatment dynamics for a two-stage process (figure 1) of anaerobic fermentation in a bioreactor-mixer acquiring the following form [1-7]:

\[
\begin{align*}
\dot{S}(t) & = \frac{Q(t)}{V} \left(S_{in}(t) - S(t)\right) - k_1(\theta)B_1(t) - k_2(\theta) \frac{S(t)B_1(t)}{k_3(\theta) + S(t)}, \\
\dot{B}_1(t) & = -\frac{Q(t)}{V} B_1(t) + k_4(\theta) \frac{S(t)B_1(t)}{k_3(\theta) + S(t)}, \\
\dot{P}(t) & = -\frac{Q(t)}{V} P(t) + k_4(\theta)B_1(t) + k_6(\theta) \frac{S(t)B_1(t)}{k_3(\theta) + S(t)} - k_7(\theta)B_2(t) - k_8(\theta) \frac{P(t)B_2(t)}{k_9(\theta) + P(t)}, \\
\dot{B}_2(t) & = -\frac{Q(t)}{V} B_2(t) + k_{10}(\theta) \frac{P(t)B_2(t)}{k_9(\theta) + P(t)}, \\
\dot{G}(t) & = -G(t) + k_{11}(\theta) \frac{P(t)B_2(t)}{k_9(\theta) + P(t)} k_{12}(\theta), \\
\dot{\theta}(t) & = \zeta_1(t) + u_1(t), \\
\dot{Q}(t) & = \zeta_2(t) + u_2(t), \\
k_i(\theta) & = k_{35^\circ C} \exp\left(c(\theta - 35^\circ C)\right),
\end{align*}
\]

Figure 1. Flowchart of conversion of organic wastewater pollutants in an anaerobic bioreactor.

The examples of anaerobic biological wastewater treatment invariants and the algorithm of nonlinear adaptation presented below demonstrate a possibility in principle of an analytical synthesis of an adaptive regulator with a compensation of disturbances, without being regarded as a final result.
Note that for the algorithm of nonlinear adaptation used here it is critical that the dimensionalities of the control and the set invariants coincide.

3. Target invariants for anaerobic biological wastewater treatment

1. The main purpose of a bioreactor functioning in the wastewater purification system is to reduce the concentration of the initial organic pollution $S_{in}$ to (or lower than) a specified guideline value $S^*$. In so doing, it is desirable to convert the pollutants to a biogas. If $G^*$ is the design amount of biogas, which could be generated from the set amount of the initial substance, then the formal model of the control target will be given by

$$
\psi_1^*(t) = S(t) + P(t) - S^* \to 0;
\psi_2^*(t) = G(t) - G^* \to 0.
$$

2. The stability-indicating parameter of the process of anaerobic fermentation is the content of organic acids in the reaction medium, which are intermediate products of the process. The limiting concentration of organic acids $P^*$, $P(t) \leq P^*$ can be determined for the anaerobic biomass, at which inhibition of the purification process starts. Therefore, the respective control targets will be as follows:

$$
\psi_1^*(t) = P(t) - P^* \to 0;
\psi_2^*(t) = S(t) - S^* \to 0.
$$

3. Anaerobic bioreactors, in addition to the systems of wastewater treatment, are used in biogas production units. Then the control target will be given by the following:

$$
\psi_1^*(t) = P(t) - P^* \to 0 \text{ (minimization of } P(t), \ P(t) \leq P^*); \\
\psi_2^*(t) = G(t) - G^* \to 0 \text{ (maximization of } G(t)).
$$

4. An increased amount of gas does not always improve the energy efficiency of the system due to higher energy consumption on heating the reactor.

Supplement the anaerobic biological wastewater treatment model with an energy efficiency index $E = \frac{E_G - E_{heating}}{E_{heating}}$, where $E_G$ is the amount of energy that can be potentially produced from biogas, $E_{heating}$ is the energy spent on heating the bioreactor, determined in the general case from the thermal system equation. Then, the target invariant for the waste water treatment system will be given by

$$
\psi_1^*(t) = S(t) - S^* \to -0; \\
\psi_2^*(t) = E(t) \to \max; \ (\psi_2^*(t) = E(t) \to 1-);
$$

and for the biogas plants is reasonable to use it in the form

$$
\psi_1^*(t) = P(t) - P^* \to 0; \ P(t) \leq P^*; \\
\psi_2^*(t) = E(t) \to \max.
$$

4. Fundamental concepts and definitions of SCT

Fundamental concepts and definitions related to the algorithm of nonlinear adaptation on a target manifold used here (based on the formalism of system’s invariants and SCT) are following.

The phase flow $x(t, x_0, t_0)$ of a system $\dot{x} = f(x) + u$, $x \in \mathbb{R}^n$, $u \in \mathbb{R}^m$, $m \leq n$ defines the law of motion in every point of the phase space of an autonomous system of differential equations.
The imaging point of the system in its state space is set by the values of the state vector coordinates at fixed time $t$.

Sets $V \subseteq \mathbb{R}^n$ are referred to as invariant sets with respect to the flow $x_f(t, x_0, t_0)$, if $x_f(t, x_0, t_0) \in V$ for any $x_0 \in V$ for all $t > t_0$, where $x_f(x_0, t_0) \rightarrow (x, t) \in V$.

Set $V$ is referred to as attractive, if it is a closed and invariant set.

Macrovariables are certain (user)-defined functions $\psi(x)$ of the object coordinates, whose equality to zero $\psi(x) = 0$ determines the target (desirable) set of states.

A classical formulation of the problem of control on a target manifold includes 1) control object, set by a system of ODEs or a system of difference equations for the continuous and the discrete problems of control, respectively; 2) control aim in the form of an analytically formulated equation $\psi(x) = 0$; 3) satisfaction of the following requirements: the set of states, obeying the description $\psi(x) = 0$, is an invariant manifold; the solutions to the initial system of equations are limited; there is a regime of object’s stabilization in the neighborhood of $\psi(x) = 0$.

A classical method of analytical design of aggregated regulators (ADAR) [7] control is a (vector) variable $u^i(x(t)) = (u_1^i, ..., u_m^i)$ that provides a solution for a continuous variational problem $(\Phi, \psi)$:

$$\Phi = \int_0^\infty \sum_{i=1}^m \left( \psi_i^2 + w_i^2 \psi_i^2(t) \right) dt \rightarrow \min$$

under the constraint of $\psi(x(t)) = 0, t \rightarrow \infty$, $\psi(x(t)) = (\psi_1(x(t)), ..., \psi_m(x(t)))$.

The mathematical apparatus for the method of analytical design of aggregated regulators is based on the results of theoretical mechanics (e.g., [10]), in particular if the variational problem $(\Phi, \psi)$ is given by

$$\Phi(\psi) = \int_0^\infty \left( \phi^2(\psi) + w^2 \psi^2 \right) dt \rightarrow \min, \psi \rightarrow 0, \phi(\psi) > 0, \forall \psi \neq 0, \phi(0) = 0,$$

then the solutions to the functional equation $w\psi + \phi(\psi) = 0$ would determine the stationary extremals ensuring a maximum for functional $\Phi$. Here we consider only the case $\phi(\psi) = \psi$.

Statement 1. Equation (8) is a consequence of the Euler-Lagrange equation for the functional $\Phi(\psi) = \int_0^\infty (\psi^2 + w^2 \psi^2) dt \rightarrow \min$.

Proof. The Euler-Lagrange equation is:

$$2\psi - \frac{d}{dt} \left( 2w^2 \psi \right) = 0, \quad w^2 \ddot{\psi} - \psi = 0.$$

We multiply the last equality by $\psi$ and integrate the left and right sides. Thus, we get

$$w^2 \dot{\psi}^2 - \psi^2 = C.$$

Taking into account that $\psi(t) = 0, \dot{\psi}(t) = 0, t \rightarrow \infty$, we have $C = 0$:

$$\left( w\psi + \psi \right) \left( w\dot{\psi} - \psi \right) = 0.$$
The asymptotic stability property is possessed by the solutions of the equation

\[ w \psi + \psi = 0. \] (8)

**Remark 1.** The physical meaning of the functional (7) is transparent: it reaches the target of control at a given velocity determined by the parameter \( w \).

5. **Implementation algorithm of target invariants for anaerobic biological wastewater treatment**

Consider case (2), introducing the notations

\[ S = (x; u + \zeta), x \in \mathbb{R}^2, u, \zeta \in \mathbb{R}^2, x = (S, B_1, P, B_2, G, \theta, Q). \]

**Step 1.** Phase space extension aimed at transforming the initial system into a closed system in order to compensate for disturbances; the description will be obtained in the following form:

\[ S_E = (x_E; u + z), x_E = (S, B_1, P, B_2, G, \theta, Q, z_1, z_2), \dot{z}_i(t) = \eta_i \psi_i^*(t), \eta_i = \text{const} > 0, i = 1, 2 \] (9)

From now on, system \( S_E \) is referred to as the initial system for synthesizing a vector regulator.

The functions \( z_1 \) and \( z_2 \) model the disturbances \( \zeta_1 \) and \( \zeta_2 \), respectively.

**Remark 2.** Omit variable \( t \) and other arguments, where this would not distort the understanding of the text.

**Step 2.** Introduce the auxiliary macrovariables \( \psi_1, \psi_2 \) (in order to transfer the control functions from the variables \( \theta(t), Q(t) \) to the internal control variables \( \phi_i(S, B_1, P, B_2, G, z_1, z_2), i = 1, 2 \), respectively.

\[ \psi_1 = \theta - \phi_1(S, B_1, P, B_2, G, z_1, z_2), \]
\[ \psi_2 = Q - \phi_2(S, B_1, P, B_2, G, z_1, z_2). \]

**Step 3.** Write equation \( T_i \psi_i(t) + \psi_i = 0, \ i = 1, 2 \) of the form of (8) for the partial quality functional \( \Phi_i(\psi^i) \), \( \psi^i = (\psi_1, \psi_2) \) and substitute into them

\[ T_1 \psi_1(t) + \psi_1 = T_1 \dot{\theta} - T_i \phi_1 + \psi_1 = 0, \]
\[ T_2 \psi_2(t) + \psi_2 = T_2 \dot{Q} - T_2 \phi_2 + \psi_2 = 0, \] (10)

where

\[ \dot{\phi}_i = \dot{\phi}_i(S, B_1, P, B_2, G, z_1, z_2) = \frac{\partial \phi_i}{\partial S} \dot{S} + \frac{\partial \phi_i}{\partial B_1} \dot{B}_1 + \frac{\partial \phi_i}{\partial P} \dot{P} + \frac{\partial \phi_i}{\partial B_2} \dot{B}_2 + \frac{\partial \phi_i}{\partial G} \dot{G} + \frac{\partial \phi_i}{\partial z_1} \dot{z}_1 + \frac{\partial \phi_i}{\partial z_2} \dot{z}_2, \ i = 1, 2, \]

or, considering equations (9), obtain

\[ \phi_i = \phi_i(S, B_1, P, B_2, G, z_1, z_2) + \frac{\partial \phi_i}{\partial S} f_S + \frac{\partial \phi_i}{\partial B_1} f_{B_1} + \frac{\partial \phi_i}{\partial P} f_P + \frac{\partial \phi_i}{\partial B_2} f_{B_2} + \frac{\partial \phi_i}{\partial G} f_G + \frac{\partial \phi_i}{\partial z_1} \eta_1 \psi_1^* + \frac{\partial \phi_i}{\partial z_2} \eta_2 \psi_2^*, \ i = 1, 2, \] (11)

where \( f_S, f_{B_1}, f_P, f_{B_2}, f_G \) are the right-hand parts of the description for \( \dot{S}, \dot{B}_1, \dot{P}, \dot{B}_2, \dot{G}, \dot{z}_1 \) and \( \dot{z}_2 \), respectively, in system \( S_E \).
Equations (10) yield the formulas for the external vector control:

\[ u_i = \phi_i - T_i^{-1} \psi_i - z_i, \quad i = 1, 2. \]  

Expressions (12) define the regulator structure for (1) to an accuracy of the unknown functions \( \phi_1, \phi_2 \) and their partial derivatives

\[ \frac{\partial \phi_1}{\partial S}, \frac{\partial \phi_1}{\partial B_1}, \frac{\partial \phi_2}{\partial B_2}, \frac{\partial \phi_1}{\partial G}, \frac{\partial \phi_2}{\partial \bar{z}_1}, \frac{\partial \phi_2}{\partial \bar{z}_2}, \quad i = 1, 2. \]

**Step 4.** Decompose the basic model (9) on manifold \( \psi_1 = 0, \psi_2 = 0 \) and obtain a system of equations, which would be the initial system for a further synthesis of the internal controls \( \phi_1 \) and \( \phi_2 \).

In (9) replace

\[ \psi_1 = \psi_2 = 0, \\theta = \phi_1, \\Theta = \phi_2, \eta_i = \text{const} > 0, \quad i = 1, 2, \]

or more specifically

\[ \dot{\psi}_1 = (\dot{\psi}_1, \dot{\psi}_2), \quad \dot{\phi}_1 = \Theta_1, \quad \Theta_2 = \phi_2, \quad \eta = \text{const} > 0, \quad i = 1, 2, \]  

\[ \phi_1 = (\phi_1, \phi_2), \quad \phi_2 = \phi_2, \quad \eta_i = \text{const} > 0, \quad i = 1, 2, \]

or more specifically

\[ \dot{S}(t) = \frac{\phi_2(t)}{V} \left( S_m(t) - S(t) \right) - k_1(\phi_1)B_1(t) - k_2(\phi_2)S(t), \]

\[ \dot{B}_1(t) = -\frac{\phi_2(t)}{V} B_1(t) + k_4(\phi_1) \frac{S(t)B_1(t)}{k_3(\phi_1) + S(t)}, \]

\[ \dot{P}(t) = \frac{\phi_2(t)}{V} P(t) + k_5(\phi_1)B_2(t) + k_6(\phi_1) \frac{S(t)B_2(t)}{k_3(\phi_1) + S(t)} - k_7(\phi_1)B_2(t) - k_8(\phi_2) \frac{P(t)B_2(t)}{k_3(\phi_1) + P(t)}, \]

\[ \dot{B}_2(t) = -\frac{\phi_2(t)}{V} B_2(t) + k_{10}(\phi_1) \frac{P(t)B_2(t)}{k_3(\phi_1) + P(t)}, \]

\[ \dot{G}(t) = \frac{\phi_2(t)}{V} \left( G(t) + k_{11}(\phi_1) \frac{P(t)B_2(t)}{k_3(\phi_1) + P(t)} \right), \]

\[ \dot{z}_1(t) = \eta_1 \psi_1(t), \quad \eta_1 > 0, \quad \dot{z}_2(t) = \eta_2 \psi_2, \quad \eta_2 > 0, \]

\[ k_1(\phi_1) = k_{35C} \exp \left( c \left( \phi_1 - 35^\circC \right) \right). \]

From now on, system (14) would be the initial system in the algorithm for synthesizing a vector regulator for object (1).

**Step 5.** Introduce a macrovariable \( \psi^2 = (\psi_3, \psi_4) \) and write an equation of the form of (8) for the partial quality functional \( \Phi_2(\psi^2), \psi^2 = (\psi_3, \psi_4) \)

\[ T_3 \psi_3 + \psi_3 = T_4 \left( \psi_4 + \mu_1 \bar{z}_1 \right) + \psi_3 = 0, \quad \psi_3 = \psi_4 + \mu_1 \bar{z}_1, \]

\[ T_4 \psi_4 + \psi_4 = T_1 \left( \psi_1 + \mu_2 \bar{z}_2 \right) + \psi_4 = 0, \quad \psi_4 = \psi_1 + \mu_2 \bar{z}_2. \]

Substituting the derivatives of the target macrovariables \( \psi_1(t) = S(t) + P(t) - S^*, \psi_2(t) = G(t) - G^* \) into (15), considering (14), obtain \( f_s, f_p, f_G \) are the right-hand parts of the descriptions for \( \dot{S}(t), \dot{P}(t) \) and \( \dot{G}(t) \), respectively, in system (14) a system of quadratic algebraic equations in terms of two unknown quantities \( \phi_1 \) and \( \phi_2 \).
\[
\frac{\phi_2}{V} \left( S_m - S - P \right) + \phi_1 \left( h_5 - h_1 \right) B_1 + \left( h_6 - h_2 \right) \frac{SB_1}{h_3 \phi_1 + S} - h_7 B_2 - \frac{h_8 PB_2}{h_9 \phi_1 + P} = \\
= -T_3^{-1} \mu_1 z_1 - \left( \mu_1 \eta_1 + T_3^{-1} \right) \left( S + P - S^* \right),
\]

\[
h_1 \phi \frac{PB_2}{h \phi_1 + P} h_2 \phi_1 = -T_4^{-1} \mu_2 z_2 + G^* + \psi^* \left( 1 - \mu_2 \eta_2 - T_4^{-1} \right).
\]

\[
\tilde{\phi}_1 = \exp \left( c \left( \varphi - 35^\circ C \right) \right), h_i = k_i 35^\circ C.
\]

Determine from (16) functions \( \phi_1 \) and \( \phi_2 \) and their partial derivatives. The synthesis of a regulator for the control object (1) (2) has been completed. The final control system acquires the form of a set of equations (1), (2), (11), (12), and (16).

**Remark 3.** Such parameters \( (T_1, T_2) \) as a duration of reaching the vicinity of the target state require careful selection for the given individual characteristics of the models (1)-(2) and (17).

**Statement 2.** Control \( u = u_{NAD} \), if any, ensures an asymptotic stability for the controlled object (1) in the neighborhood of \( \psi(t) = 0, t \to \infty \).

### 5.1. Results of numerical simulation of the object control

Let us consider the example of application of the control design technique presented in Section 5 for a given target invariant \( (G \to G^*) \) by means of a temperature control set \( \Theta \) in the bioreactor.

In this case, the control system will take the form

\[
S = \left( x; u + \zeta, \zeta \in R^7 \right), u, \zeta \in R^t, x = \left( S, B_1, P, B_2, G, \Theta, Q \right),
\]

\[
u = \phi - T_1^{-1} (\theta - \varphi) - z, z(t) = \eta \int \psi^* (t) dt, \varphi = c^{-1} \ln (\bar{\phi}) + 35^\circ C,
\]

\[
\phi(G, z) = Y \left( e \bar{\phi} \right)^{-1} \left( \left( 1 - T_2^{-1} \right) f_\mu - T_2^{-1} \mu_2 \eta \psi^* \right), \psi^* (t) = G(t) - G^*,
\]

\[
\tilde{\phi} = \frac{\tilde{C} P (h_9 + h_{12}) + P \sqrt{\Theta}}{2 h_2 (h_1 PB_2 - h_9 \tilde{C})}, \tilde{C} = \left( 1 - T_2^{-1} \right) G + T_2^{-1} \left( G^* - \mu z \right),
\]

\[
\tilde{G} = \frac{K \left( h_9 PB_2 - h_9 \tilde{C} \right) + h_9 \Theta}{2 h_2 \sqrt{\Theta}}, h_1 = 0.94, h_2 = 0.332, h_3 = 1.5, h_4 = 0.059, h_5 = 0.78, h_6 = 0.215, h_7 = 0.03, h_8 = 0.95
\]

\[
h_9 = 0.4, h_{10} = 0.023, h_{11} = 0.02, h_{12} = 0.06.
\]

The initial conditions for state variables are as follows (conventional units)

\[
S(0) = S_0 (0) = 10, B_1 = B_2 = 0.25, Q(0) = 0(0) = 35, G(0) = P(0) = 0, V = 1000.
\]
Figure 2. Trajectories of a variable $G(t)$ under different temperature conditions ($\theta=\text{const}$) in a system without control ($u=0$).

Figure 3. Biogaz flow change $G(t)$; $G^* = 2.5 \cdot 10^{-4}$ is a target value.

Figure 4. The trajectory of a regulated variable $\theta(t)$ according to the classical ADAR method (if we do not consider the disturbance).

Figure 5. Regulated temperature trajectories under conditions of constant disturbance $\zeta = 1, 10$.

Figure 6. Behavior of a control variable under conditions of constant and harmonic disturbances, $A = 10$, $\delta(t) = \pi/25$.

Figure 2 (object (1) without control) denotes that a target value of biogas can be expected at the temperature range ($45 \leq \theta \leq 50$) under the given initial conditions.

The resulting control (figures 3, 4) ensures the achievement of a set value with the expected dynamics of the temperature regime.

Figures 5, 6 show the graphs of the trajectories of a controlled variable and the control itself for different types of disturbances, which indicate the acceptable quality of the constructed regulator (17).

Thus, the constructed control for such a nonlinear multidimensional multi-connected object provides robust properties of the target system that operates under uncertainty. The numerical solution of algebraic equations (16) that arise in the process of regulator synthesis introduces an additional disturbance due to the existence of unstable limit states of the object (1).
6. Conclusion

The formulation of the problem of control, based on the description (1) and the reasonable invariants (2)-(7), deserves a separate consideration and a study of the issues related to each of them consisting in the following:

- mathematical conditions of a possible linear synthesis a correctness of the physical values of all variables of the target system;
- necessary and sufficient conditions of an existence of a single or multiple solution forms for the control variables;
- a physical interpretation of the local functionals accompanying the regulator synthesis and a practical implementation of the resulting control systems.

Finally, a quality solution of the tasks of data assurance of the control over a complex object anaerobic biological wastewater treatment needs the information on the complete state vector of this object. In the object studied in this work not all coordinates are available for an immediate change; for part of the coordinates in real systems this is either technically difficult to implement or physical impossible, since the rate and quality of biochemical reactions are affected by multiple factors, not all of which are included into the model. Therefore, the presence of unmodelled dynamics not only is possible but can also play an undesirable role resulting in an unstable state of anaerobic biological wastewater treatment.

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