Hybrid Intelligent Inverse Optimal Control for Methane Production in an Anaerobic Process

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Abstract

Anaerobic processes are very attractive because of their waste treatment properties and their capacity for transforming waste materials in order to generate methane, which can be used as a renewable energy source. A hybrid intelligent control strategy for an anaerobic process is proposed in this work; the structure of this strategy is as follows: a) a control law calculates dilution rate and bicarbonate addition in order to track a methane production reference trajectory; this control law is based on speed-gradient inverse optimal neural control, b) a nonlinear discrete-time recurrent high-order neural observer is used to estimate biomass concentration, substrate degradation and inorganic carbon, and c) a Takagi-Sugeno supervisor, which detects the process state, selects and applies the most adequate control action, allowing a smooth switching between open loop and closed loop. The applicability of the proposed scheme is illustrated via simulations considering a completely stirred tank reactor.

Keywords:
Anaerobic process, methane production, hybrid intelligent control, neural observer, inverse optimal neural control, Takagi-Sugeno supervisor

Introduction

Motivated by the rapid growth of electricity demand, considering the depletion of fossil fuels, and due to increased environmental awareness, developed countries began to investigate the potential of renewable energy sources.1–3 In recent years, with varying degrees of success, different renewable energy sources have been and continue to be studied for electric power generation, among them, geothermal, biomass, solar, wind, hydropower by micro-turbines and tidal waves.4–6 Research on the optimization of energy generation in hybrid systems, which use different renewable sources, are discussed by Liang et al.7 and Marwali et al.8 Biomass is attractive as a potential energy resource, and it is an important fuel in several developing countries.9 There are different reasons for biomass utilization as an energy source. One of them is that the amount of traditional petroleum sources for conventional fuels is not unlimited, while biomass is potentially renewable.10 Another reason is that replacing fossil fuels with biomass would reduce the net carbon dioxide emissions that are contributing to the greenhouse warming of Earth.11 Moreover, biomass fuels have a reasonable heat of combustion, and they usually have low sulfur, nitrogen and ash content as compared to many coals and oils.12 Biomass may be converted into a variety of energy forms including heat (via burning), steam, electricity, hydrogen, ethanol, methanol, and methane.13–16 Anaerobic digestion is a biological process by which organic matter (substrate) is degraded by anaerobic bacteria (biomass), in the absence of oxygen. Such degradation produces biogas, consisting primarily of methane (CH4) and carbon dioxide (CO2), and stable organic residues. Anaerobic digestion is a complex and sequential process which occurs in four basic stages: hydrolysis, acidogenesis, acetogenesis and methanogenesis.17 Each stage has specific dynamics; hydrolysis, acidogenesis and acetogenesis are fast stages in comparison with methanogenesis, which is the slowest one; it imposes the dynamics of the process and is considered as the limiting stage. For this paper, the process is developed in a continuously stirred tank reactor (CSTR), with immobilized bacteria on a solid support. A variety of factors affect the rate of diges-
tion and biogas production, such as pH, temperature and overloads.\textsuperscript{18} In addition, some variables and parameters are hard to measure due to economic or technical constraints. Then, estimation and control strategies are required in order to guarantee adequate performance.\textsuperscript{19} In biological processes, there exist hardly measurable or nonmeasurable variables which are necessary for process control. Different biogas sensors have been developed in order to measure CH\textsubscript{4}.\textsuperscript{20–22} However, substrate and biomass measures are more restrictive. A discrete-time recurrent high-order neural observer (RHONO) for nonlinear systems, which model is assumed to be unknown is proposed by Alansis et al.\textsuperscript{23} and Belmonte-Izquierdo et al.\textsuperscript{24} This neural observer is based on a discrete-time recurrent high-order neural network (RHONN) trained with an extended Kalman filter (EKF)-based algorithm, using a parallel configuration. In this paper, the RHONO structure is modified in order to obtain a better estimation. The objective is to estimate biomass concentration, substrate degradation and inorganic carbon in the anaerobic process. The training of the RHONO is performed on-line. The variables are estimated from CH\textsubscript{4} and dioxide flow rates, which are commonly measured in this process. It is assumed that pH, YCH\textsubscript{4}, YCO\textsubscript{2} and the process inputs are on-line measured. Neural networks are considered as good candidates for nonlinear systems applications, which deal with uncertainties, and are attractive due to their simpler implementation, robustness and the capacity to adjust their parameters on-line; additionally, the knowledge of the model is not strictly necessary.\textsuperscript{25} In order to control the anaerobic process, a speed-gradient inverse optimal neural control is considered;\textsuperscript{26} which is developed on the basis of the above mentioned neural observer. The controllers are designed to regulate bicarbonate in the reactor by two control actions: a base supplying (\(b_{\text{base}}\)) and dilution rate (\(D_{\text{dil}}\)) changes. Speed-gradient inverse optimal neural control is an adequate and novel algorithm in biological systems.\textsuperscript{27} The aim of the inverse optimal control is to avoid the solution of the HJB (Hamilton-Jacobi-Bellman) equation,\textsuperscript{28,29} diminishing implementation complexity.\textsuperscript{30} A fuzzy supervisor is implemented in order to apply control actions to reject large disturbances on input substrate and to track a methane reference trajectory production. A Takagi-Sugeno supervisor\textsuperscript{31,32} detects the process state, selects and applies the most adequate control action, allowing a smooth switching between open loop and closed loop. The process works in open loop in presence of small disturbances. For large disturbances, the supervisor allows the control actions to be applied avoiding washout; after that, the process returns to open loop operation. In general, the supervisor improves the performances of the anaerobic process and is feasible for application in real processes, since the control scheme shows a good compromise between efficiency and complexity.

**Mathematical model**

A functional diagram of anaerobic digestion is proposed by Betetu\textsuperscript{33} as shown in Fig. 1. Biomass is classified as: \(X_1\), corresponding to hydrolytic, acidogenic and acetogenic bacteria, and \(X_2\), which represents methanogenic bacteria. On the other hand, the organic load is classified in \(S_1\), the components equivalent glucose, which model complex molecules and \(S_2\), the components equivalent acetate, which represent the molecules directly transformed in acetic acid. This classification allows the process to be represented by a fast stage, which involves hydrolysis, acidogenesis and acetogenesis and a slow stage, which corresponds mainly to methanogenesis.

![Functional diagram of the anaerobic digestion](image)

Thus, a discrete-time nonlinear mathematical model of the process is deduced in Carlos-Hernandez et al.\textsuperscript{17} On one side, the biological phenomena are modeled by ordinary differential equations (1), which represent the dynamic part of the process as:

\[
X_{1,k+1} = X_{1,k} + (\mu_{1,k} - k_d) X_{1,k},
\]

\[
S_{1,k+1} = S_{1,k} - R_k \mu_{1,k} X_{1,k} + D_k (S_{1,in,k} - S_{1,k}),
\]

\[
X_{2,k+1} = X_{2,k} + (\mu_{2,k} - k_d) X_{2,k},
\]

\[
S_{2,k+1} = S_{2,k} - R_k \mu_{2,k} X_{2,k} + D_k (S_{2,in,k} - S_{2,k}),
\]

\[
IC_{k+1} = IC_k + R_1 R_3 \mu_{2,k} X_{2,k} + R_3 \mu_{1,k} X_{1,k} - \\
\lambda_k R_1 R_3 \mu_{2,k} X_{2,k} + D_k (IC_{in,k} - IC_k),
\]

\[
Z_{k+1} = Z_k + D_k (Z_{in,k} - Z_k),
\]

where \(\mu_{1,k}\) is the growth rate (Haldane type) of \(X_{1,k}\) (h\textsuperscript{-1}) at step \(k\), \(\mu_{2,k}\) the growth rate (Haldane type) of
\[ X_{2,k} (h^{-1}), k_{dj} \] the death rate of \( X_{1,k} (h^{-1}) \), \( k_{dj} \) the death rate of \( X_{2,k} (h^{-1}) \), \( D_k \) the dilution rate (h^{-1}), \( S_{1mk} \) the fast degradable substrate input (mol L^{-1}), \( S_{2mk} \) the slow degradable substrate input (mol L^{-1}), IC inorganic carbon (mol L^{-1}), \( Z \) the total of cations (mol L^{-1}), \( IC_{\text{in,k}} \) the inorganic carbon input (mol L^{-1}), \( Z_{\text{in,k}} \) the input cations (mol L^{-1}), \( \lambda_k \) is a coefficient considering law of partial pressure for the dissolved CO2 and \( R_1, \ldots, R_6 \) are the yield coefficients.

The growth rate for \( X_{1,k} \) and \( X_{2,k} \) are described by equations (2) and (3) respectively:

\[ \mu_{1,k} = \frac{\mu_{1_{\text{max}}} S_{1,k}}{k_{s1} + S_{1,k} + \frac{S_{1,k} HS}{k_{i1}}} \]  
\[ \mu_{2,k} = \frac{\mu_{2_{\text{max}}} S_{1,k}}{k_{s2} + HS + \frac{HS^2}{k_{i2}}} \]

where \( \mu_{1_{\text{max}}} \) and \( \mu_{2_{\text{max}}} \) are the maximum growth rate for the \( X_{1,k} \) and \( X_{2,k} \) biomasses respectively, \( k_{s1} \) (mol L^{-1}) and \( k_{i1} \) (mol L^{-1}) are the growth saturation for the biomasses, \( k_{s2} \) (mol L^{-1}) and \( k_{i2} \) (mol L^{-1}) are the inhibition constants by substrate excess, \( HS \) is non ionized acetic acid (mol L^{-1}), and \( S_{1,k} \) (mol L^{-1}) is slow stage substrate.

On the other side, the physical-chemical phenomena (acid-base equilibriums and material conservation) are modeled by algebraic equations (4).

\[ HS + S^- - S_2 = 0, \]
\[ H^+ S^- - K_a HS = 0, \]
\[ H^+ B - K_b CO_{2d} = 0, \]
\[ B + CO_{2d} - IC = 0, \]
\[ B + S^- - Z = 0, \]

where \( HS \) is non ionized acetic acid (mol L^{-1}), \( S \) ionized acetic acid (mol L^{-1}), \( H^+ \) ionized hydrogen (mol L^{-1}), B measured bicarbonate (mol L^{-1}), \( CO_{2d} \) dissolved carbon dioxide (mol L^{-1}), \( K_a \) is an acid-base equilibrium constant, \( K_b \) is an equilibrium constant between \( B \) and \( CO_{2d} \).

Finally, the gaseous phase (CH4 and CO2) is considered as the process output:

\[ Y_{CO_{2d},k} = \lambda_k R_2 R_3 u_{2,k} X_{2,k} \]  
\[ Y_{CH_4,k} = R_1 R_2 \mu_{2,k} X_{2,k} \]

\( \lambda \) is a pressure partial coefficient for CO2 defined as:

\[ \lambda_k = \frac{CO_{2d}}{P_i K_h - CO_{2d}} \]

where \( P_i \) is atmospheric pressure (Pa), \( K_h \) is a gases Henry constant (mol L^{-1} Pa^(-1)) and \( CO_{2d} \) defined as before. Biomass growth, substrate degradation and CO2 are good indicators of CH4 production and biological activity inside the reactor. These variables can be used for monitoring the process and to design an inverse optimal neural control.

**Discrete time neural observer**

A nonlinear discrete-time recurrent high-order neural observer (RHONO) for unknown nonlinear systems in the presence of external disturbances and parameter uncertainties is described in Alanis et al.\(^{23}\) This observer is based on a discrete-time recurrent high-order neural network (RHONN) trained with an extended Kalman filter (EKF) based algorithm. Let us consider the next nonlinear system, which is assumed to be observable:

\[ x_{k+1} = F(x_k, u_k) + d_k, \]
\[ y_k = h(x_k), \]

where \( x \in \mathbb{R}^n \) is the state vector of the system, \( u \in \mathbb{R}^m \) is the input vector, \( y \in \mathbb{R}^p \) is the output vector, \( h(x(k)) \) is a nonlinear function of the system states, \( d(w) \in \mathbb{R}^n \) is a disturbance vector and \( F(\cdot) \) is a smooth vector field and \( F(\cdot) \) its entries; hence (8) can be also expressed component-wise as:

\[ x_k = [x_{1,k}, \ldots, x_{i,k}, \ldots, x_{n,k}]^T, \]
\[ d_k = [d_{1,k}, \ldots, d_{i,k}, \ldots, d_{n,k}]^T, \]
\[ x_{i,k+1} = F_i(x_k, u_k) + d_{i,k}, \]
\[ y_k = h(x_k). \]

For system (9), a Luenberger-like neural observer is proposed, with the following structure:

\[ \tilde{x}_k = [\tilde{x}_{1,k}, \ldots, \tilde{x}_{i,k}, \ldots, \tilde{x}_{n,k}]^T, \]
\[ \tilde{x}_{i,k+1} = w_i^T z_i(\tilde{x}_k, u_k) + g_{wi} e_k, \]
\[ \hat{y}_k = h(\tilde{x}_k); \quad i = 1, \ldots, n, \]

with \( g_{wi} \in \mathbb{R}^p \), \( u_i \) is the external input vector to the NN and \( z_i \) is a function of states and inputs to each neuron; the weight vectors are updated on-line with a decoupled extended Kalman filter (EKF). The output error is defined by:

\[ e_k = y_k - \hat{y}_k, \]

and let us define the \( w_i \) estimate as \( w_i \); then, the weights estimation \( w_{i,k} \) and state observer \( \tilde{x}_{i,k} \) errors are stated, respectively, as
For more details on the design and the stability analysis of this RHONO, we refer the reader to the results presented in Sanchez et al.\textsuperscript{35}

In this paper, considering the RHONO advantages mentioned in section 1 and due to the requirement of nonmeasurable variables estimation for discrete-time speed gradient inverse optimal neural control, we propose the use of a discrete-time RHONO structure, which estimates the variables of the methanogenesis stage: biomass ($X_{z,k}$), substrate ($S_{z,k}$) and inorganic carbon ($IC_k$); the biomass is used in the supervisor structure; the substrate and the inorganic carbon are estimated for comparison (with real measures) in future researches. The observability property of this anaerobic digestion process is analyzed by Alcaraz-Gonzalez et al.\textsuperscript{36} It is concluded that substrates ($S_{1,k}$ and $S_{2,k}$), biomasses ($X_{1,k}$ and $X_{3,k}$) and inorganic carbon ($IC_k$) are observable states. In Fig. 2, the proposed observer scheme is displayed and its formulation is shown by equations (14).

\begin{equation}
\tilde{w}_{i,k} = w_{i,k} - w_i^*(12)
\end{equation}
\begin{equation}
\tilde{x}_{i,k} = x_{i,k} - \hat{x}_{i,k}. (13)
\end{equation}

where $w_i$ is the respective on-line adapted weight vector; $\tilde{x}_{i,k}$, $S_{2,k}$ and $IC_k$ are the estimated states; $S(\cdot)$ is the sigmoid function defined as $S(x) = \alpha \tanh(\beta x)$, $S(\cdot)$ is the square of the sigmoid function; $(g_{m1}, g_{m2}, g_{m3})$ are the Luenberger-like observer gains, $e_i$ is the output error, $D_{in,k}$, $S_{2in,k}$ and $b_{in,k}$ are defined as before.

**EKF training algorithm**

The Kalman filter (KF) provides an efficient computational solution to estimate the state of a linear dynamic system with additive state and output white noises.\textsuperscript{35} For KF-based NN training, the network weights become the states to be estimated. In this case, the error between the NN output and the measured plant output can be considered as additive white noise. If, however, the model is nonlinear, the use of KF can be extended through a linearization procedure; the resulting filter is the well-known EKF. Since the NN mapping is nonlinear, an EKF-type is required. The training goal is to find the optimal weight values, which minimize the prediction error. In this work, an EKF-based training algorithm\textsuperscript{37-40} described by (15) is used.

\begin{equation}
w_{i,k+1} = w_{i,k} + \eta_iK_i,k e_{i,k},
\end{equation}
\begin{equation}
K_i,k = P_i,k H_{i,k} M_{i,k},
\end{equation}
\begin{equation}
P_{i,k+1} = P_{i,k} - K_i,k H_{i,k}^T P_{i,k} + Q_{i,k},
\end{equation}
\begin{equation}
M_{i,k} = \left[ R_{i,k} + H_{i,k}^T P_{i,k} H_{i,k} \right]^{-1},
\end{equation}
\begin{equation}
e_{i,k} = y_k - \hat{y}_k, \quad i = 1, \ldots, n
\end{equation}

where $e_i \in R^n$ is the observation error, $P_{i,k} \in R^{i \times Li}$ is the prediction error covariance matrix at step $k$, $w_{i} \in R^{Li}$ is the weight (state) vector, $L_{i}$ is the respective number of neural network weights, $y \in R^n$ is the plant output, $\hat{y}_{i} \in R^n$ is the NN output, $\eta_i$ is the learning rate, $K_{i,k} \in R^{i \times nP}$ is the Kalman gain matrix, $Q_{i,k} \in R^{i \times Li}$ is the NN weight estimation noise covariance matrix, $R_{i,k} \in R^{nP \times i}$ is the error noise covariance, and $H_{i,k} \in R^{i \times P}$ is the matrix for which each entry ($H_{ij}$) is the derivative of the $i$-th neural output with respect to $j$-th NN weight, ($w_j$).

\begin{equation}
\tilde{x}_{2,k+1} = w_{11}S(\tilde{x}_{2,k}) + w_{12}S^2(\tilde{x}_{2,k}) + w_{13}S(I^C_k) + w_{14}S^2(I^C_k) + w_{21}S^2(\tilde{x}_{2,k}) D_{in,k} + w_{23}S(I^C_k) + w_{24}S^2(I^C_k) D_{in,k} + w_{31}S(\tilde{x}_{2,k}) + w_{32}S^2(\tilde{x}_{2,k}) S_{2in,k} + g_{m1}e_{k},
\end{equation}
\begin{equation}
\tilde{S}_{2,k+1} = w_{21}S(\tilde{S}_{2,k}) + w_{22}S^2(\tilde{S}_{2,k}) + w_{23}S(I^C_k) + w_{24}S^2(I^C_k) + w_{31}S(\tilde{x}_{2,k}) + w_{32}S^2(\tilde{x}_{2,k}) S_{2in,k} + g_{m2}e_{k},
\end{equation}
\begin{equation}
\tilde{I}_{C,k+1} = w_{31}S(I^C_k) + w_{32}S^2(I^C_k) + w_{33}S(\tilde{x}_{2,k}) + w_{34}S^2(I^C_k) D_{in,k} + w_{35}S^2(I^C_k) b_{in,k} + g_{m3}e_{k},
\end{equation}

**Speed-gradient inverse optimal neural control**

As mentioned above, speed-gradient inverse optimal neural control is an adequate algorithm,
whose application in biological systems is novel.\textsuperscript{27}

The aim of the inverse optimal control consists of designing a stabilizing feedback control law, based on an a priori known control Lyapunov function (CLF) which ensures that the stabilizing control law optimizes a cost functional.\textsuperscript{30} Let us consider the affine in the input discrete-time nonlinear system:

\[
x_{k+1} = f(x_k) + g(x_k) u_k
\]

where \(x \in \mathbb{R}^n\) is the state of the system, \(u \in \mathbb{R}^m\) is the control input, \(f(x)\) and \(g(x)\) are smooth maps with \(f(x) \in \mathbb{R}^n, g(x) \in \mathbb{R}^{n \times m}, k \in \mathbb{Z}^* = \{0, 1, 2, \ldots\}\). \(f(0) = 0\) and \(\text{rank } [g(x)] = m \ \forall x \neq 0\). In Ornellas et al.\textsuperscript{30} the following cost functional is associated with system (16):

\[
V(z_k) = \sum_{n=k}^{N} (l(z_n) + u_k^T R_C(z_n) u_n)
\]

where \(z_n = x_n - x_n^d\) with \(x_n^d\) as the desired trajectory for \(x_n^d; z_n \in \mathbb{R}^n\); \(V(z): \mathbb{R}^n \to \mathbb{R}^n; I(z): \mathbb{R}^n \to \mathbb{R}^n\) is a positive semidefinite function and \(R_C(z): \mathbb{R}^n \to \mathbb{R}^{n \times n}\) is a real symmetric positive definite weighting matrix. The cost functional (17) is a performance measure.\textsuperscript{42} The entries of \(R_C(z_n)\) can be functions of the state system in order to vary the weighting on control efforts according to the state value.\textsuperscript{42} Considering state feedback control, we assume that the full state \(x_k\) is available. Equation (17) can be rewritten as

\[
V(z_k) = l(z_k) + u_k^T R_C(z_k) u_k + \sum_{n=k}^{N} (l(z_n) + u_n^T R_C(z_n) u_n) = \sum_{n=k}^{N} V(z_k) + V(z_{k+1})
\]

where \(V(z_{k+1})\) depends on both \(x_{k+1}\) and \(u_k\) by means of \(x_{k+1}\) in (16). In order to establish the conditions that the optimal control law must satisfy, we define the discrete-time Hamiltonian \(H\)\textsuperscript{43} as

\[
H(z_k, u_k) = l(z_k) + u_k^T R_C(z_k) u_k + V(z_{k+1}) - V(z_k)
\]

A necessary condition that the optimal control law \(u_k\) should satisfy is \(\partial H / \partial u_k = 0\),\textsuperscript{42} which is equivalent to calculate the gradient of (19) with respect to \(u_k\), then

\[
= 2R_C(z_k) u_k + \frac{\partial V(z_{k+1})}{\partial u_k} = \frac{\partial V(z_{k+1})}{\partial u_k} = 2R_C(z_k) u_k + \frac{\partial V(z_{k+1})}{\partial u_k} = 2R_C(z_k) u_k + \frac{\partial V(z_{k+1})}{\partial u_k}
\]

Therefore, the optimal control law is formulated as

\[
u_k^* = -\frac{1}{2} R^{-1}(z_k) g^T(x_k) \frac{\partial V(z_{k+1})}{\partial z_{k+1}}.
\]

For control law (21) in order to ensure trajectory tracking of system (16), a discrete-time CLF is proposed,\textsuperscript{30} with the form:

\[
V_c(z_k) = \frac{1}{2} z_k^T P_k z_k, \quad P_k = P_k^T > 0
\]

This will be achieved by defining an appropriate matrix \(P_k\); moreover, it will be established that the control law (21) with (22), which is referred to as the inverse optimal control law, optimizes a cost functional of the form (17). Consequently, the control law takes the following form:

\[
u_k^* = -\frac{1}{2} \left( R_C(z_k) + \frac{1}{2} g^T(x_k) P_k g(x_k) \right)^{-1} \times
\]

\[
x^T g(x_k) P_k f(x_k, x_{d,k+1})
\]

\(P_k\) and \(R_C(z_k)\) are positive definite and symmetric matrices; thus, the existence of the inverse in (23) is assured. To compute \(P_k\), which ensures stability of the system (16) with (23), the speed-gradient (SG) algorithm is used. Control law (23) at every time step depends on the matrix \(P_k\). Let us define the matrix \(P_k\) at every time step \(k\) as:

\[
P_k = p_k P_C
\]

where \(P_C = P_C^T > 0\) is a given constant matrix and \(p_k\) is a scalar parameter to be adjusted by the SG algorithm.\textsuperscript{26} Then, (23) is transformed into:

\[
u_k^* = -\frac{p_k}{2} \left( R_C(z_k) + \frac{1}{2} g^T(x_k) P_k g(x_k) \right)^{-1} \times
\]

\[
x^T g(x_k) P_k f(x_k, x_{d,k+1})
\]

The dynamic variation of parameter \(p_k\) in (24) results in

\[
p_{k+1} = p_k + \frac{8}{(2R_C(z_k) + p_k g^T(x_k) P_k g(x_k))^{\frac{3}{2}}}
\]

which is positive for all time step \(k\) if \(p_0 > 0\). Therefore, positiveness for \(p_k\) is ensured and requirement \(p_k = p_k^T > 0\) for (24) is guaranteed. With the control Lyapunov function as defined by (22) and \(p_k = \overline{p}\) (\(\overline{p}\) is a constant value when the SG algorithm converges) the control law is inverse optimal in the sense that it minimizes the cost functional (17),
which is proposed such that \( l(z_k) \) ponders the states and \( R_c(z_k) \) ponders the control.\(^{26}\)

In order to apply the control law (25) to the anaerobic process, the following analysis is required, for which the proposed RHONO is presented as an affine system:

\[
\begin{align*}
 f_1(\dot{X}_{2,k}, \dot{IC}_k) &= w_{11}S(\dot{X}_{2,k}) + w_{12}S^2(\dot{X}_{2,k}) + w_{13}S(\dot{IC}_k) + g_{m1}\varepsilon_k, \\
 f_2(\dot{S}_{2,k}, \dot{IC}_k) &= w_{21}S(\dot{S}_{2,k}) + w_{22}S^2(\dot{S}_{2,k}) + w_{23}S(\dot{IC}_k) + w_{24}S^2(\dot{S}_{2,k})S_{2in,k} + g_{m2}\varepsilon_k, \\
 f_3(\dot{X}_{2,k}, \dot{IC}_k) &= w_{31}S(\dot{IC}_k) + w_{32}S^2(\dot{IC}_k) + w_{33}S(\dot{X}_{2,k}) + g_{m3}\varepsilon_k, \\
 G_{11}(\dot{X}_{2,k}) &= w_{14}S^2(\dot{X}_{2,k}), \\
 G_{12}(\dot{X}_{2,k}) &= w_{15}S^2(\dot{X}_{2,k}), \\
 G_{21}(\dot{S}_{2,k}) &= w_{24}S^2(\dot{S}_{2,k}), \\
 G_{22}(\dot{S}_{2,k}) &= w_{25}(\dot{S}_{2,k}) = 0, \\
 G_{31}(\dot{IC}_k) &= w_{34}S^2(\dot{IC}_k), \\
 G_{32}(\dot{IC}_k) &= w_{35}S^2(\dot{IC}_k).
\end{align*}
\]

\[
\begin{align*}
 f_1(\dot{X}_{2,k}) &= f_1(\dot{X}_{2,k}), \\
 f_2(\dot{X}_{2,k}) &= f_2(\dot{X}_{2,k}), \\
 f_3(\dot{X}_{2,k}) &= f_3(\dot{X}_{2,k}).
\end{align*}
\]

According to (25), the inverse optimal control law is formulated as

\[
\begin{align*}
 u^*_k &= D_{in,k} = -\frac{1}{2} \left( R_{c1}(z_k) + \frac{1}{2} g_{i1}(\dot{X}_{2,k}) P_{1,k} g_{i1}(\dot{X}_{2,k}) \right)^{-1} \left( 2 g_{i1}(\dot{X}_{2,k}) P_{1,k} f(x) \right) \times \\
 & \quad \times g_{i1}(\dot{X}_{2,k}) P_{1,k} f(x),
\end{align*}
\]

\[
\begin{align*}
 u^*_{inc,k} &= -\frac{1}{2} \left( R_{c2}(z_k) + \frac{1}{2} g_{i2}(\dot{X}_{2,k}) P_{2,k} g_{i2}(\dot{X}_{2,k}) \right)^{-1} \left( 2 g_{i2}(\dot{X}_{2,k}) P_{2,k} f(x) \right) \times \\
 & \quad \times g_{i2}(\dot{X}_{2,k}) P_{2,k} f(x),
\end{align*}
\]

where the positive definite matrix \( P_{inc} = p_{inc} P_c \) is calculated by the SG algorithm, \( R_c(z_k) \) is a constant matrix, \( g_{i1}(\dot{X}_{2,k}) \) and \( f(x) \) are matrices as in (27)-(28) and

\[
f(x, x_{\delta,k+1}) = f(x) - f_{ref}(x, x_{\delta,k+1}).
\]

The tracking of a desired trajectory, defined in terms of the plant state \( x_{\delta,k} \) formulated as (1) can be established as the following inequality:

\[
\| x_{i,k} - x_{\delta,k} \| \leq \| x_{i,k} - \dot{x}_{i,k} \| + \| x_{i\delta} - \dot{x}_{i,k} \|.
\]

where \( \| . \| \) stands for the Euclidean norm, \( \dot{x}_{i,k} \) is the observed state, \( x_{\delta,k} \) is the desired trajectory signal, \( x_{i\delta} \) is a small positive constant.

An on-line neural observer trained with extended Kalman filter based on (15) ensures (32), while (33) is guaranteed by a discrete controller developed using the inverse optimal control technique.

### Hybrid intelligent control scheme

Anaerobic digestion is able to work adequately without control for an interval of operating conditions and even in presence of small disturbances. However, for large disturbances, a control law is required in order to maintain process stability. Then, supervision of key variables is a very important task. The \( ODL/X_2 \) is the quantity of organic load that a unit of biomass can treat in a working day and is important regarding process stability.\(^{17}\) It is defined as:

\[
ODL/X_2 = D_{in,k} A_2 S_{20}/\dot{X}_2
\]

where \( D_{in,k} \) is the dilution rate (h\(^{-1}\)), \( A_2 \) a disturbance amplitude on the substrate input \( S_{20} \) (mol L\(^{-1}\)), \( S_{20} \) the initial value of the substrate \( X_2 \) (mol L\(^{-1}\)) and is the estimated biomass \( X_2 \) (mol L\(^{-1}\)).

In the presence of a disturbance in \( S_{20} \), \( ODL/X_2 \) can abruptly increase up to a value, which exceeds the conditions of stability limits (critical value); therefore the process tends to washout, that means, the absence of active microorganisms and then the increase of nontreated substrate. If \( ODL/X_2 \) is above its critical value, then a control law must be applied in order to allow biomass growth, and hence, diminishing \( ODL/X_2 \) and stabilizing the system. In contrast, if the \( ODL/X_2 \) is under its critical value then the system can work in open loop. Depending on the \( ODL/X_2 \) value, commutation between operating modes (open loop, closed loop) is done by a Takagi-Sugeno fuzzy supervisor.\(^{45}\) This commutation takes place progressively in order to avoid abrupt switching. The fuzzy set is defined as in Fig. 3.
The Takagi-Sugeno algorithm is used to define the supervisor. From empirical knowledge, each fuzzy set is associated with a control action; then three fuzzy inference rules are deduced:

- If $ODL/X_2$ is LOW then $u = \text{open loop}$
- If $ODL/X_2$ is AVERAGE then $u = b_{\text{inc,k}}$ action
- If $ODL/X_2$ is HIGH then $u = D_{\text{inc,k}}$ action

The structure of the hybrid intelligent control is shown in Figure 4.

The main advantage of this control scheme is to combine different control actions in order to minimize their drawbacks and profit from their advantages: dilution rate ($D_{\text{inc,k}}$) changes reject larger disturbances and supplying a base ($b_{\text{inc,k}}$) allows the process to track reference methane production. The operation mode in open loop works satisfactorily in the presence of small disturbances, which represents saving of energy. Consequently, the most adequate control action is applied in order to avoid washout.

**Simulation results**

The whole control strategy for the anaerobic process is implemented using Matlab™ and parameter values are presented in Tables 1, 2 and 3. The observer is initialized at random values to verify the estimation convergence. In order to test the observer sensitivity to input changes, a disturbance of...
50 % S2 in increase in the input substrate is incepted at \( t = 200 \) hours. The performance of the proposed RHONO and the input disturbance substrate is illustrated in Fig. 5.

It is clear that the biomass, substrate, and inorganic carbon are well estimated. Additionally, robustness of the proposed RHONO is tested in the presence of a 80 % disturbance in \( 200 < t < 500 \), different initial conditions and parameters variation in the biomasses growth. A 10 % negative variation in the maximum rate growth of the hydrolytic, acidogenic and acetogenic bacteria (\( \mu_{1\text{max}} \)) and a 10 % positive variation in the maximum rate growth of the methanogenic bacteria (\( \mu_{2\text{max}} \)). Parameter values are in Table 4 and the performance of the proposed RHONO is illustrated in Fig. 6.

System states are well estimated and the robustness of the proposed RHONO to parameters variations is verified. Thus, the proposed neural observer is a good alternative to estimate those important states of the considered anaerobic process. Model and observer validation are found in Belmonte et al.46

As mentioned in section 5, the inverse optimal neural control algorithm requires reference trajectories. In a previous work48 anaerobic system was controlled in the presence of disturbances with a PI L/A controller which avoided inhibition; the process presented a suitable behavior which was reflected in trajectories for methane production. Therefore these trajectories represent an adequate dynamic behavior of the anaerobic process for growth biomass and methane production in the presence of disturbances and are smooth. Hence, they are selected as reference trajectories for inverse optimal neural control. The hybrid control scheme is tested in the presence of a 100 % distur-

Table 3 – Controller parameters

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
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<td>( R_{C2} )</td>
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<tr>
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<td>( P_{C1,12} )</td>
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<td>( P_{C2,12} )</td>
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<tr>
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<td>( P_{C2,13} )</td>
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<tr>
<td>( P_{C1,21} )</td>
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<td>( P_{C2,21} )</td>
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<td>( P_{C1,22} )</td>
<td>0.05E4</td>
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<td>( P_{C1,23} )</td>
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<td></td>
<td>( P_{C2,32} )</td>
<td>629</td>
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<tr>
<td>( P_{C1,33} )</td>
<td>0.05E4</td>
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<td>( P_{C2,33} )</td>
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<tr>
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<td>1600</td>
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<td>( S_{S2} )</td>
<td>500</td>
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</tbody>
</table>

Fig. 5 – State estimation for a 50 % disturbance
Fig. 6 – State estimation for parameters variation

Fig. 7 – Trajectories tracking states for a 100% disturbance
Bance on $S_{2in}$, incepted at $t = 200$ hours. Trajectories tracking for states and $YCH_4$ are illustrated below.

When the disturbance is introduced in the input substrate, an adequate control law must be applied in order to allow biomass growth, and hence, diminishing $ODL/X_2$ and stabilizing the system. As can be seen the process operates in open loop because disturbance is small; this is because $ODL/X_2$ belongs to the associated fuzzy set corresponding to open loop (Fig. 3). This situation implies that the anaerobic digestion process is able to work adequately without control in the presence of this small disturbance. Thus, trajectory tracking for the states is achieved as illustrated in Fig. 7 and the error approaches zero in steady state. The $YCH_4$ is calculated with equation (6), which is based on the system observed states. As can be seen, the reference is reached; Fig. 8 displays the inputs $b_{m,k}$ and $D_{in,k}$. The proposed hybrid control scheme is also tested introducing a 150 % disturbance in $S_{2in}$ incepted at $t = 200$ hours, as illustrated in Fig. 9.

For this case, the supervisor operates in closed loop because the disturbance is large and closed loop control is required. During disturbance, $ODL/X_2$ increases its value until reaching a level corresponding to HIGH fuzzy set. Therefore the system goes to closed loop operation mode applying control action $D_{in,k}$. During the evolution process, $ODL/X_2$ diminishes its level and starts to belong to HALF fuzzy set. Thus control action $b_{inc,k}$ is applied and the control action $D_{in,k}$ is stopped. Finally, $ODL/X_2$ diminishes its value until belonging to the fuzzy set associated to open loop. This situation implies that the disturbance has been rejected completely. Under these last conditions, supervisor stops the action $b_{inc,k}$ and the process returns to its operation in open loop. Thus, trajectory references for the states are reached with error approaching 206 K. J. GURUBEL et al., Hybrid Intelligent Inverse Optimal Control for Methane ..., Chem. Biochem. Eng. Q. 27 (2) 197–210 (2013)

Fig. 8 – Input signals for a 100 % disturbance

Fig. 9 – Trajectories tracking states for a 150 % disturbance
also, $YCH_4$ reaches its reference and the corresponding error approaches zero at steady state. Fig. 10 displays the control signals $b_{inc,k}$ and $D_{in,k}$.

The proposed hybrid control scheme is also tested introducing a 200% disturbance in $S_{2in}$ incepted at $t=200$ hours, as illustrated below. As can be seen in Fig. 11, the proposed scheme detects a large disturbance and applies the adequate control action until the disturbance is rejected. Thus trajectory tracking is efficient and the error approaches zero at steady state. $YCH_4$ reference is reached with a small error at steady state as is illustrated in Fig. 11. Fig. 12 displays the control signals $b_{inc,k}$ and $D_{in,k}$. System operation is ensured due to the control strategy applied, even though a large disturbance is incepted. For the case of disturbances larger than 200% in $S_{2in}$, the oscillation induced by the observer prevents the supervisor from controlling the process. Therefore, the system tends to washout; a critical value exists for which the supervisor cannot control the bio-process due to the magnitude of the disturbances.
Finally, controller tolerance to change of the system parameters is tested; such variation is incepted as a disturbance in the bacteria concentration, $\mu_{1\text{max}}$ and $\mu_{2\text{max}}$ as presented in Table 4, and a disturbance in the input substrate of 200 % $S_{2\text{in}}$ increase incepted at $t=200$ h as in Fig. 11. Performance of the system is illustrated in Fig. 13.

### Table 4 – Parameter values variation

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X_{2,1}$</td>
<td>0.0116</td>
<td>mol L$^{-1}$</td>
</tr>
<tr>
<td>$S_{2,1}$</td>
<td>0.0052</td>
<td>mol L$^{-1}$</td>
</tr>
<tr>
<td>$I_C$</td>
<td>0.1386</td>
<td>mol L$^{-1}$</td>
</tr>
<tr>
<td>$\mu_{1\text{max}}$</td>
<td>0.1845</td>
<td>h$^{-1}$</td>
</tr>
<tr>
<td>$\mu_{2\text{max}}$</td>
<td>0.0188</td>
<td>h$^{-1}$</td>
</tr>
</tbody>
</table>

As illustrated in Fig. 13, the closed loop performance presents a transient state error which is due to parameters variation in rate growths that affect directly the kinetic; the control scheme acts in order to track the trajectory which is achieved at steady state with a small error. The control trajectories are illustrated in Fig. 14.

System states are well estimated and the robustness of the proposed RHONO to parameters variations is verified. Thus, the proposed neural observer is a good alternative to estimate those important states of the considered anaerobic process. Model and observer validation are found in Belmonte et al.$^{46}$ Fuzzy PI control for the same process is discussed in Belmonte et al.$^{46}$ There, the goal was not to track specific trajectories, but to avoid washout. PID control is unsuitable for time-varying trajectory tracking. Due to these two facts, comparison with these control schemes is not included in this paper.
Conclusions

In this paper, a hybrid intelligent control scheme for an anaerobic wastewater treatment process is proposed in order to produce methane and avoid washout. A nonlinear discrete-time recurrent high-order neural observer (RHONO) is used to estimate the biomass concentration, substrate degradation, and inorganic carbon; then this observer is transformed into an affine mathematical model with the aim of applying speed-gradient inverse optimal control. Once this model is obtained, an inverse control law, based on it, is developed. The fuzzy supervisor detects biological activity inside the tank reactor, on the basis of estimated biomass, and applies a control action. The goal is to force the system to track desired reference, which is achieved; simulation results show how the hybrid intelligent control is able to stabilize the methane production along desired trajectories in the presence of disturbances, and avoiding washout. Thus, control action fulfills the objectives of rejecting disturbances, and of obtaining a high efficiency of the process, which is reflected in a good production of biogas. This research will be pursued in order to evaluate the application in real-time of the proposed control scheme to an anaerobic prototype process.

ACKNOWLEDGMENT

This work was supported by CONACyT projects 131678 and 105844.

List of symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>YCH₄</td>
<td>methane production, mol h⁻¹</td>
</tr>
<tr>
<td>YCO₂</td>
<td>carbon dioxide production, mol h⁻¹</td>
</tr>
<tr>
<td>D_in</td>
<td>dilution rate, h⁻¹</td>
</tr>
<tr>
<td>b_in</td>
<td>provided bicarbonate, mol L⁻¹</td>
</tr>
<tr>
<td>X₁</td>
<td>hydrolytic, acidogenic and acetogenic bacteria, mol L⁻¹</td>
</tr>
<tr>
<td>X₂</td>
<td>methanogenic bacteria, mol L⁻¹</td>
</tr>
<tr>
<td>S₁</td>
<td>fast degradable substrate, mol L⁻¹</td>
</tr>
<tr>
<td>S₂</td>
<td>slow degradable substrate, mol L⁻¹</td>
</tr>
<tr>
<td>IC</td>
<td>inorganic carbon, mol L⁻¹</td>
</tr>
<tr>
<td>S₁_im</td>
<td>fast degradable substrate input, mol L⁻¹</td>
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<tr>
<td>S₂_im</td>
<td>slow degradable substrate input, mol L⁻¹</td>
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<tr>
<td>IC_im</td>
<td>inorganic carbon input, mol L⁻¹</td>
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<td>Zₐ</td>
<td>input cations</td>
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<td>λ</td>
<td>pressure partial coefficient</td>
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<td>Rₚ</td>
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<td>ionized hydrogen, mol L⁻¹</td>
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<td>dissolved carbon dioxide, mol L⁻¹</td>
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<td>Kₐ</td>
<td>acid-base equilibrium constant</td>
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<tr>
<td>Kₖ</td>
<td>equilibrium constant between B and CO₂d</td>
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<td>Ẋ₂</td>
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<td>Ẋ₂</td>
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<tr>
<td>eₖ</td>
<td>output error, mol h⁻¹</td>
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<tr>
<td>eₖ,k</td>
<td>observation error, mol h⁻¹</td>
</tr>
<tr>
<td>R P</td>
<td>espacio euclidiano de dimisión P</td>
</tr>
<tr>
<td>Xₖ₊₁</td>
<td>discrete state of the system</td>
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<tr>
<td>V(...)</td>
<td>Lyapunov function</td>
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<tr>
<td>J</td>
<td>cost function</td>
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<tr>
<td>OD/Lₙ/X₂</td>
<td>quantity of organic load treated by biomass</td>
</tr>
<tr>
<td>A₂</td>
<td>disturbance amplitude, mol L⁻¹</td>
</tr>
</tbody>
</table>

Abbreviations

TS – Takagi-sugeno
CSTR – continued stirred tank reactor
NN – neural network
RHONO – recurrent high-order neural observer
RHONN – recurrent high-order neural network
KFE – Kalman extended filter
SG – speed-gradient

References

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