Abstract - Bioethanol is the most widely used liquid biofuel. Because of its economic and industrial relevance, improvements of bioethanol production have been addressed from different disciplines. In this paper the control of a general class of CSTRs for bioethanol production is addressed via a practical robust model-based control approach. The controller design is able to suppress complex behavior and reject typical disturbances to the bioethanol processing.

Keywords: Bioethanol production; CSTRs; Robust control; Modeling error compensation.

I. INTRODUCTION

The term biofuel is referred to as liquid or gaseous fuels for the transport sector that are predominantly produced from biomass. Biofuels generally offer many benefits including sustainability, reduction of greenhouse gas emissions, regional development, reduction of rural poverty, and fuel security. A variety of fuels can be produced from biomass resources including liquid fuels, such as ethanol, methanol, biodiesel, Fischer-Tropsch diesel, and gaseous fuels, such as hydrogen and methane. The most commonly used biofuel is ethanol, which is produced from sugarcane, corn, and other grains (Chiaramonti, 2007; Demirbas, 2009; Sanchez and Cardona, 2007).

Bioethanol production can be carried out in batch, fed-batch and continuous bioreactors. Batch and feed-batch operation are widely used in biotechnological processes (Roels, 1982; Cho et al. 1982; Nipkow et al. 1986; Sanchez and Cardona, 2007). Advantages of the batch and fed-batch operation include: simplicity of equipment, the ability to clean completely between batches, and years of operating experience. Continuous bioreactors on the other hand, have the built-in flexibility for control of temperature, biomass growth and all the other process parameters that influence the outlet product concentration. Continuous bioreactors are desired to operate at a steady state in order to achieve a desired product quality, however, they are very challenging units for both open-loop and closed loop operation, because process variables are usually unknown, slow attainment of steady state, potential instability of operation and for the complexity of the underlying biochemical reactions (Roels, 1982; Femat et al., 2007; Garhyan and Elnashaie, 2004; Wu and Chang, 2007; Crook et al., 1980). For instance, nonlinear oscillations in continuous bioreactors are a well-known phenomenon leading to practical difficulties in design and operation. In particular, this undesired behavior negatively affects downstream process units and also often fails to meet desired product quality specifications (Roels, 1982; Chiaramonti, 2007).

During the last years, significant improvements have been done in the bioethanol industry in order to make it economically more competitive (Margaritis and Kilonzo, 2005; Chiaramonti, 2007; Demirbas, 2009; Sanchez and Cardona, 2007). However, the economical feasibility of the bio-ethanol industry is still questioned, and therefore much effort should be oriented to the optimization and control of the process. Control policies are required to maintain the specific product quality, to suppress the influence of process disturbances, to switch from one product quality to other at minimal production loss, to stabilize the bioreactor in case of cyclic behavior and to optimize the economic process performance.

In this work, we introduce a simple robust control approach to control a general class of models of CSTRs for bioethanol production. Robust feedback control seems to be essential for biotechnological processes as it permits to deal with model uncertainties related to model parameters. Although the bioethanol processing literature is vast, few papers on control studies are available (Ishizaki et al. 1994; Choi et al. 1996; Nagy, 2007), and to the authors’ knowledge there is no general framework for the synthesis of practically implementable robust feedback controllers for continuous production of bioethanol. For the robust control design we consider the modeling error compensation approach (MEC). The proposed MEC approach leads to relatively simple control structures and easy-to-use tuning guidelines. The underlying idea behind MEC control designs is to lump the input-output uncertainties into a term whose trajectory is estimated and compensated via a suitable algorithm.
This MEC approach has the following advantages over adaptive and IMC methods: (i) The performance of a model-based adaptive control is limited by the accurateness of the model used to describe complex interactions in microorganisms, (ii) model uncertainty can be explicitly addressed; (iii) the nonlinear process model is directly incorporated in the control design, allowing for the nonlinearity of the bioreactor model to be taken into account; (iv) tedious (even difficult) algebraic manipulations for control laws due to the complex bioreactor model, which may occur when using, for example, feedback linearization or IMC approaches, are avoided; and (v) control input saturation constraints on the control input can be incorporated.

This work is organized as follows. In Section 2, for the sake of clarity of presentation, some generalities of bioethanol production are described, and the case studies are also presented. In Section 3, the robust feedback control approach is presented and applied for the case studies. In Section 4 numerical simulations shown the closed-loop performance of the proposed robust control approaches for the case studies. Finally, conclusions are given in Section 5.

II. PROCESS DESCRIPTION AND MODELING OF BIOETHANOL PRODUCTION IN CSTRS

Process description
Ethanol is the most widely used liquid biofuel. It is produced by fermentation of sugars, which can be obtained from natural sugars (e.g., sugar cane, sugar beet), starches (e.g., corn, wheat), or cellulosic biomass (e.g., corn stover, straw, grass, wood). The most common feedstock is sugar cane or sugar beet, and the second common feedstock is corn starch. Currently, the use of cellulosic biomass is very limited due to expensive pretreatment the crystalline structure of cellulose required for breaking. Bioethanol is already an established commodity due to its ongoing non-fuel uses in beverages, and in the manufacture of pharmaceuticals and cosmetics. Bioethanol can be used as a 10% blend with gasoline without need for any engine modification. However, with some engine modification, bioethanol can be used at higher levels, for example, E85 (85% bioethanol) (Chiaramonti, 2007; Demirbas, 2009; Sanchez and Cardona, 2007).

Microorganisms for ethanol fermentation can best be described in terms of their performance parameters and other requirements such as compatibility with existing products, processes, and equipment. The performance parameters of fermentation are: temperature range, pH range, alcohol tolerance, growth rate, productivity, osmotic tolerance, specificity, yield, genetic stability, and inhibitor tolerance (Chiaramonti, 2007; Demirbas, 2009; Sanchez and Cardona, 2007).

Case study 1: Oscillatory CSTR for bioethanol production
The first case study consists of a CSTR that displays oscillatory behavior. The occurrence of oscillations in biological reactors has been well documented experimentally and theoretically (Femat et al., 2007; Garhyan and Elnashaie, 2004; Wu and Chang, 2007; Crook et al., 1980). For ethanol production, simulation and experimental results have shown that the average conversion of sugar and the average yield/productivity of ethanol are sometimes higher for periodic and chaotic attractors than for the corresponding steady states despite the fact that, during oscillations, the values of the state variables fall below the average values of the oscillations for some time (Garhyan and Elnashaie, 2004).

We consider the fermentation of ethanol using Zymomonas mobilis in a bioreactor as described in (Garhyan and Elnashaie, 2004). The model considers four state variables, namely, the dynamic behavior of the system is described by the following differential equations, an internal key component $x_1$, the cell concentration $x_2$, the substrate concentration $x_3$, and the product (ethanol) concentration, $x_4$. The internal component considers that the biomass as being divided into compartments containing specific groupings of macromolecules (e.g., protein, DNA, and lipids), and a relatively simple unsegregated, structured model was suggested on the basis of the introduction of an internal
key compound of the biomass. The activity of this compound is expressed in terms of the concentrations of substrate, product, and the compound of the biomass itself.

\[
\begin{align*}
    x_1 &= \left( \frac{k_1 - k_2}{\mu_{\text{max}}} - x_3 - x_4^2 \right) \frac{\mu_{\text{max}} x_2 x_1}{k_3 + x_1} - \frac{\mu_{\text{max}} x_2 x_1}{k_3 + x_1}, \\
    x_2 &= \frac{\mu_{\text{max}} x_2 x_1}{k_4 + x_1} x_2 + D(x_{2in} - x_2) \\
    x_3 &= -\frac{1}{Y_{s/x}} \frac{\mu_{\text{max}} x_2 x_1}{k_5 + x_1} x_2 - m_s x_2 - D x_3 + D x_{3in} \\
    x_4 &= \frac{1}{Y_{p/x}} \frac{\mu_{\text{max}} x_2 x_1}{k_6 + x_1} x_2 + m_p x_2 + D(x_{4in} - x_4)
\end{align*}
\]

where \( D \) is the dilution rate, \( x_{3in} \) is the substrate concentration in the feed stream, \( Y_{s/x} \), \( Y_{p/x} \), \( \mu_{\text{max}} \), \( k_1 \), \( k_2 \), and \( k_3 \) are kinetic parameters. Both inputs \( D \) and \( x_{3in} \) can affect the dynamic behavior, such that the model may evolve into a stable steady state, a limit cycle, or chaotic behavior. For the following parameter values, \( D=0.04605 \), \( x_{3in}=200 \), \( x_{3in}=x_{3in}=0 \), \( Y_{s/x}=0.024498 \), \( Y_{p/x}=0.0526315 \), \( m_s=1.1 \), \( m_p=2.16 \), \( \mu_{\text{max}}=1 \), \( k_4=4 \), \( k_5=16 \), \( k_6=0.497 \), and \( k_7=0.00383 \), model (1) displays a periodic oscillatory behavior. A detailed description of this model and a complete stability analysis are given in (Garhyan and Elnashaie, 2004).

Case study 2: Stable CSTR for bioethanol production

As a second case we consider a CSTR with a single stable steady-state behavior which incorporates various nonlinear characteristics of the process, such as the oxygen mass transfer, detailed energy balance, complex reaction kinetics, the temperature dependence of the kinetic parameters as well as the effect of ionic strength and temperature on the mass transfer coefficient of oxygen (Nagy, 2007).

The reactor is modeled as a continuous stirred tank with constant substrate feed flow. There is also a constant outlet flow from the reactor that contains the product, substrate as well as biomass. The reactor contains three distinct main components (Nagy, 2007): (i) the biomass, which is a suspension of yeast fed into the system and evacuated continuously, (ii) the substrate, which is solution of glucose, which feeds the micro-organism (Saccharomyces cerevisiae) and (iii) the product (ethanol), which is evacuated together with the yeast. In order to have a quasi-steady-state regarding the biomass, a low dilution rate \( (F_i/V) \) is necessary, that is, the dilution rate must not exceed the biomass production rate. Consequently, the process has a very slow dynamics. Together with the yeast, inorganic salts are added. These are necessary compounds for the formation of coenzymes. The inorganic salts due to the "salting-out" effect have also strong influence upon the equilibrium concentration of oxygen in the liquid phase (Nagy, 2007; Garhyan and Elnashaie, 2004).

The dynamic behavior of the system is described by a model that considers seven state variables, namely, the reactor volume \( x_j \), the biomass \( x_2 \), the substrate \( x_3 \), the substrate \( x_4 \), the dissolved oxygen \( x_5 \), the reactor temperature \( x_6 \), and the jacket temperature \( x_7 \).

\[
\begin{align*}
    x_1 &= F_i - F_x \\
    x_2 &= \frac{\mu_{s,max} x_4}{k_1 + x_1} x_2 - m_s x_2 - D x_3 + D x_{3in} \\
    x_3 &= \frac{\mu_{p,max} x_4}{k_2 + x_1} x_3 - m_p x_2 + D(x_{4in} - x_4) \\
    x_4 &= \frac{1}{Y_{s/x}} \frac{\mu_{s,max} x_4}{k_5 + x_1} x_2 + m_s x_2 + D(x_{4in} - x_4) \\
    x_5 &= k_{b} (x_s \cdot x_3) - \frac{1}{Y_{s/x}} \frac{\mu_{o,2,\text{max}} x_5}{k_4 + x_1} x_2 \\
    x_6 &= x_{6in} + 273 - \frac{F}{V} x_6 + \frac{\Delta H}{32 \rho_s C_{p,s}} \\
    x_7 &= \frac{F}{V} x_{7in} + \frac{K_T A_T}{V \rho_s C_{p,s}} (x_6 - x_7)
\end{align*}
\]

where inputs of the system are the flows \( F_i \), \( F_x \), the substrate input concentration \( x_{3in} \), and the reactor and jacket input temperatures, \( x_{6in} \) and \( x_{7in} \), respectively. Additional relationships and a detailed description of this model and parameter values are given in (Nagy, 2007).

Numerical simulations (not shown) have shown that variations in the input concentration have no significant effects on the ethanol concentration. On the other hand, effects of the change in the inlet reactor temperature, input flow to the reactor and input flow to the jacket leads to much more significant changes in bioethanol concentration. The manipulation of input reactor conditions is impractical as they are determined from downstream units. Thus, the manipulation of the input flow to the reactor jacket is suitable for this case study.
The general class of CSTRs for bioethanol production

For control design purposes, we consider the following class of mathematical model for continuous crystallizers,

\[
d\frac{y}{dt} = f_1(y, z) + g(y, z)u + \psi(y, z) + \phi(t) \\
d\frac{z}{dt} = f_2(y, z)
\]  

(3)

Where \( f_1(y, z) \in \mathbb{R} \), \( f_2(y, z) \in \mathbb{R}^{n-1} \) and \( g(y, z) \in \mathbb{R} \) are smooth functions of their arguments, \( y \) is the measured and controlled variable, \( z \) is the internal state, \( u \) is the control input, and \( \psi(y, z) \) represents unmodeled dynamics and \( \phi(t) \) external perturbations.

Several published models of CSTRs for bioethanol production can be described by model (3) (Nagy, 2007; Roels, 1982; Nipkow et al. 1986). On the other hand, for more complex models of continuous bioreactors, such as case study 2, input-output model approximation approaches can be used to derive simple linear models that can be described by (3).

III. SIMPLE ROBUST FEEDBACK CONTROL DESIGN

In this section the control problem for the class of CSTRs for bioethanol production is presented. A simple practical robust control approaches based on modeling error compensation (MEC) ideas is then designed.

Control problem

The control problem consists in the control of the output variable \( y \) to a desired reference \( y_{ref}(t) \) via manipulation of an the control input \( u \).

The control problem description is completed by the following assumptions:

A1 The measurement of the variable to be controlled \( y \), is available for control design purposes.

A2 Nonlinear functions \( f(y, z) \) and \( g(y, z) \) are uncertain, and can be available rough estimates of these terms.

The following comments are in order:
A1 is a reasonable assumption. Even in the absence of such measurements, a state estimator can be designed. A2 considers that nonlinear functions \( f(y, z) \) and \( g(y, z) \) can contain uncertain parameters, or in the worst case the whole terms are unknown. Indeed, parameters in bioprocesses have a high degree of uncertainties, as these parameter values commonly are estimated from experimental data, which contain errors due to both the estimation procedure adapted to fit data and the experimental errors of the data themselves (Sanchez and Cardona, 2007).

Robust control design based on MEC approach

Sun et al. (1994) proposed a robust controller design method for single-input/single-output (SISO) minimum-phase linear systems. The design approach consists of a modeling error compensator (MEC). The central idea is to compensate the error due to uncertainty by determining the modeling error via plant input and output signals and uses this information in the design. In addition to a nominal feedback, another feedback loop is introduced using the modeling error and this feedback action is explicitly proportional to the parametric error which is the source of uncertainty. The MEC approach was extended for a class of linear time-varying and nonlinear linearizable lumped parameter systems with uncertain and unknown terms by Alvarez-Ramirez and Suarez (2000) and Alvarez-Ramirez (1999), where instead of designing a robust state feedback to dominate the uncertain term, the uncertain term is viewed as an extra state that is estimated using a high-gain observer. The estimation of the uncertain term gives the control system some degree of adaptability. The extension of the MEC approach to distributed parameter systems has been applied by Puebla (2005) and Puebla et al. (2009) for a class of biological distributed parameter systems.

Consider the class of CSTRs for bioethanol production (3). Define the modeling error function \( \eta \) as,

\[
\eta = f_1(y, z) + \psi(y, z) + \phi(t)
\]

(4)

System (3) can be written as,

\[
\frac{dy}{dt} = \eta + g(y, z)u
\]

(5)

Let \( e = y - y_{ref} \) be the regulation error and consider the inverse dynamics control law,

\[
u = -\bar{g}(y, z)^{-1}(\eta - \frac{dy_{ref}}{dt} + \tau_c^{-1}e)
\]

(6)

where \( \tau_c > 0 \) is a closed-loop time constant. Under the inverse-dynamics control law (6), the closed-loop system dynamics is \( de/dt = -\tau_c^{-1}e \), so that the error dynamic behavior is given as \( e(t) = e(0) \exp(-t/\tau_c) \). In this way, the asymptotic convergence \( e(t) \rightarrow 0 \), and so \( y \rightarrow y_{ref} \), is guaranteed.

In order to implement the control input an estimate of the real uncertain term is computed using a high-gain reduced-order observer, which after some direct algebraic manipulations can be written as,
\[
\frac{dw}{dt} = -\vec{g}(y, z)u - \vec{\eta} \\
\vec{\eta} = \tau_e^{-1}(w + e)
\]  

(7)

where \( \tau_e > 0 \) is the estimation time constant. The final form of the controller is given by the feedback function (6) and the modeling error estimator (7). The resulting feedback controlled depends only on the measure \( y \) and the estimated values of uncertain terms \( g(y, z) \).

The above model-based control approach has only two control design parameters, i.e., \( \tau_c \) and \( \tau_e \). The closed-loop parameter \( \tau_c \) can be chosen as the inverse of the dominant frequency of the open-loop dynamics. On the other hand, the estimation parameter \( \tau_e > 0 \), which determines the smoothness of the modeling error can be chosen as \( \tau_e < (1/2) \tau_c \).

IV. NUMERICAL SIMULATIONS

In this section, numerical experiments are presented for both case studies. In the first case a tracking problem is addressed with the MEC control approach based on the non-linear model (1). For the second case a regulatory problem is formulated based on an approximate first-order model obtained from step-response of nonlinear model (2).

Tracking of a periodic reference

Consider the bioreactor model (1) with the MEC scheme (6) and (7). The control objective is the enforcing of the natural oscillatory behavior to track a sinusoidal reference for the substrate concentration \( y \) via the manipulation of the feed substrate concentration. Control law is turned on at \( t = 400 \) time units. We have set the controller parameters as \( \tau_c = 0.5 \) and \( \tau_e = 0.1 \). In this case, we introduce an oscillatory reference with different properties of the open-loop behavior in order to possibly exploit other levels of mean productivity. Indeed, it has been reported that the best production policy in terms of the ethanol concentration, yield, and productivity for this case is a periodic attractor (Garhyan and Elnashaie, 2004).

Fig. 1 shows the control performance for the tracking of substrate concentration \( y \) and the corresponding control input. Fig. 1 shows that closed-loop system provides a stable transition from the open-loop oscillations to new simple periodic oscillations. It can be seen from Fig. 1, that in order to obtain a new oscillatory behavior, the external control input evolves towards a quasi-periodic behavior. The fermenter can be forced into a new sustained oscillatory behavior from natural oscillatory behavior by the periodic variation of the feed substrate concentration at a fixed dilution rate.

Regulation of a stable steady-state behavior

In the second case, the control objective is the regulation of the bioreactor temperature with the feedback controller based on an approximate first-order model via the manipulation of the jacket reactor temperature.

To test the robustness of the proposed controller under uncertainties in the nominal parameters of the transfer functions (these uncertainties are associated with the modeling error induced by external disturbances and unmodelled nonlinearities), numerical experiments shown below were computed with estimated values of the parameters \( k_p \) and \( \tau_0 \) with a + 15-20 % of the nominal parameter values obtained from the curve reaction method. The control parameters were set according to the tuning guidelines described above and are given as \( \tau_c = 15.0 \), and \( \tau_e = 7 \). The control action was connected at \( t = 250 \) h.

Figure 2 shows the control performance for the regulation of the reactor temperature \( y \) and the corresponding control input. In this case, the regulation value of 32.5 C is set. A set point change to 30.0 C at \( t = 400 \) h is also shown in Figure 2. Reactor temperature influences the reactor’s performance via the equilibrium concentration of oxygen, the mass transfer coefficient for oxygen, and the maximum specific growth rate, which in turn influences the bioethanol concentration (Nagy, 2007).

Notice that the control input show a step-type response with a slight peak. The controlled variable shows smooth transitions to achieve the desired set-points. The stabilization times for both references are around 50.
Thus, it is noted that the controller can successfully regulate the reactor temperature with a good closed-loop performance despite significant uncertainties in the parameters of the transfer function obtained from the simple-step identification process.

V. CONCLUSIONS

A simple robust practical controller is designed for the control of a general class of CSTRs for bioethanol production. The control design is based on modeling compensation approach ideas. In the MEC approach the uncertainty that exists in a system is explicitly quantified and utilized as such in further stages of controller design. Both forcing of a periodic reference and regulation of a desired set point are achieved with good closed-loop references. The periodic reference can be suitable as such oscillations might enhance the performance, and designing the system to behave periodically would be not detrimental. However, if the oscillatory behavior deteriorates the reactor performance, this behavior should be suppressed. Despite that our control approach has been presented for two case studies, the extension to more complex models should be straightforward as it is based on minimum systems information.

REFERENCES


