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Software sensors design for the simultaneous saccharification and fermentation of starch to ethanol

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HIGHLIGHTS

- The estimator is developed based on knowledge of only one on-line measurable variable.
- Local stability, observability and controllability analysis.
- It is presented a nonlinear observer to perform the estimation process of the bioreactor.
- The observer's convergence was analyzed employing stability theory.

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ABSTRACT

A local analysis of stability and observability of the ethanol process are determined for continuous operation. It is found that the process is stable and noncompletely observable in the selected steady states. The analysis of observability was studied in terms of the observability matrix rank conditions. Furthermore, we design a nonlinear observer in order to estimate the observable state variables. The software sensor (state estimator) is developed considering only one measurable variable, the glucose concentration, and taking in account model uncertainties, which is a realistic issue. Some sufficient conditions for the existence of the proposed observer are obtained, which guarantee the convergence of the proposed methodology. The maximum ethanol production conditions are obtained by manipulating the dilution rate with optimal initial substrate concentration and the observable subspace is determinate which allows estimating six state variables (starch concentration, susceptible starch concentration, ethanol concentration, biomass concentration, glucose concentration and enzyme concentration). Numerical simulations are provided to show the effectiveness of the proposed observer where a comparison with a standard sliding-mode observer is done.

1. Introduction

Actually the key role that process design plays during the development of cost-effective technologies is recognized through the analysis of major trends in process synthesis, modeling, simulation and optimization, e.g. the related to ethanol and biodiesel productions [1–6]. In particular, for biochemical processes their optimal performances depend on available information. Because these variables are frequently associated to the process output quality, they are very important for the process control and monitoring. For this reason it is of great attention deliver additional information about process variables, which is accurately the role of the software sensor [7–9].

However, the development and especially the implementation of advanced monitoring and control strategies on real bioprocesses are difficult because of absence of reliable instrumentation for the biological state variables, i.e. the substrates, biomass, and product concentrations; for example, required quality of monitored data, precision data, time delay, frequency of sampling, are a function of the accuracy of bio-sensors, usually require more sophisticated measurement devices, which can have several drawbacks, e.g. sterilization, discrete-time (and often rare) samples, relatively long processing (analysis) time, in many cases the state variables, are not on-line (and real-time), this is related to high cost sensors and extreme operating conditions, these facts together with the nonlinearity and parameter uncertainty of the bioprocesses

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requires an enhanced modeling effort and modern state estimation and identification strategies [10,11].

A solution to these latter problems can be found through the design of software sensors, this estimation approach takes based combine some available measurement devices to provide signals as dissolved oxygen, glucose, pH and temperature and a mathematical model, in order to provide in continuous time estimates of nonmeasured variables on-line, the estimation algorithm is called a state observer [12–14].

Kadlec et al. [15] defined a software sensor as a grouping of the words "*software*", for the reason that the models are generally computer programs (algorithm), and "*sensors*", because the models are delivering similar information as their hardware equivalents. The first class of observers including classical observers like Luenberger, Kalman observers, and nonlinear observers (e.g., [16,17]) are based on perfect knowledge of the model structure. Classical observers, particularly the extended Kalman filter, have found applications in several bio-processes [18]. As it is well known, the extended Kalman filter is employed for nonlinear systems where model uncertainties and noisy measurements are presents. However the extended Kalman filter is based on a linear representation of the process model to construct the corresponding Riccati equation of the covariance of the estimation error in order to update the observer's gain, therefore when large nonlinearities are present the convergence properties cannot be warranted anymore.

The research work reported by Koshkouei and Zinober [19], Kravaris et al. [20], Veloso et al. [21] for nonlinear observer designs have been proposed for several special classes of nonlinear systems. Adaptive observers are used to provide estimates of the plant's states and of the system parameters simultaneously. Several studies on state reconstruction and software sensors of microbial growth processes have been reported in the literature [22–24].

Besides, from several years ago the process control engineers have perceived the main advantages of named sliding-mode control, such that robustness to matched disturbances and a finite time convergence were offset by a undesirable side effect, named chattering [25,26], caused mainly by unmodeled cascade dynamics. The latter increases the system's relative degree and perturbs the ideal sliding mode, which exists in the system with the original (ideal) input–output dynamics [27,28]. In order to overcome the chattering problem in the sliding-mode, higher order sliding mode (HOSM) control was introduced in Levant [29] systematized the second-order sliding mode algorithms and obtained estimates of their accuracy. However, design of new types of HOSM controllers still remained complicated. Recently, generalized algorithms for designing universal arbitrary-order HOSM controllers have been developed based on the homogeneous [30] and quasi-homogeneous [31] properties of HOSM dynamics.

Furthermore, observability is a clearly critical issue in dynamic systems in general and in chemical and biochemical systems in particular (e.g., Morari and Stephanopoulos [32]). The test of a system's observability is a necessary prerequisite to the estimation of states. Because of the nonlinear aspects of their dynamics, stability and observability analysis is rather complex in (bio-chemical) process applications. However, for nonlinear systems, the theory of observers is not nearly as neither complete nor successful as it is for linear systems. The design of observability conditions for nonlinear systems is a challenging problem (even for accurately known systems) that has received a considerable amount of attention.

The main issue of this work is under the frame of sliding-mode theory, where it is proposed an alternative smooth bounded nonlinear observer which contains a sigmoid function coupled with the discontinuous sign function as output injection in order to diminish the chattering problem.

From the above it is locally analyzed the stability and observability properties of a simultaneous saccharification and fermentation of starch of ethanol model. Several combinations of measured outputs are analyzed in order to show the corresponding observability conditions of the process. The convergence properties of the proposed nonlinear observer are tested through numerical simulation.

2. Methodology

Ethanol can be produced by biologically catalyzed reactions. Several reports and reviews have been published on the production of ethanol fermentation by microorganisms, as well as some bacteria, yeasts, and fungi have been used. The conventional ethanol fermentation processes using liquefied starch as substrate comprise two separate operations which have significant consequences viz. costs; the saccharification of starch and ethanol fermentation. In contrast, the simultaneous saccharification and fermentation (SSF) process combines these two steps into one to offer the potential of an increased rate of hydrolysis. In this cost-effective alternative process, the product inhibition on saccharification of glucose can be diminished since the glucose produced from oligosaccharides is consumed immediately by the cells and converted into ethanol. The development simultaneous saccharification and fermentation starch to ethanol (SSFSE) has been studied intensively [33,34,37].

Mathematical models are often used to describe the basic characteristics of the enzymatic hydrolysis. In order to increase starch conversion efficiency several kinetics models have been developed e.g. specific fermentation rates and production yield by polynomial approximation, it was assumed that the biomass, ethanol and glucose concentration are functions of time. On the other hand, in cybernetic modeling the crucial parts are the key enzyme synthesis rates description and the enzyme balance equation [38,39]. Nakasaki et al. [35] reported dynamic modeling of immobilized cell reactor for application to ethanol fermentation from glucose. Kurosawa et al. [36] reported ethanol production from starch by an immobilized mixed culture system of *Aspergillus awamori* and *Saccharomyces cerevisiae*. Most researchers focused on, a mathematical model of direct ethanol production from starch in immobilized recombinant amylase-producing yeast culture was proposed for estimating the dynamic behavior of cell growth, starch degradation, glucose accumulation, ethanol production, and glucoamylase synthesis by immobilized yeast. Some investigators developed mathematical models that included the enzyme deactivation during the hydrolysis of the insoluble substrate. Fan and Lee [40] and Gan et al. [41] developed more complicated models whose solutions cannot be solved analytically. Fan and Lee analyze the functions of the three kinds of enzymes in the cellulase system. Kobayashi and Nakamura [42] presented a model based on following items. In direct fermentation using glucoamylase-producing recombinant yeast, glucoamylase, synthesized by recombinant yeast breaks down starch to glucose; the yeast can convert the glucose into ethanol. The rate of glucoamylase synthesis of recombinant yeast is expressed in basis of the diauxic growth model that represents catabolite repression and enzyme induction. Finally Nag et al. [43] evaluated, a detailed kinetic model based on ordinary differential equations for the degradation pathways for starch synthesized in plants and green algae, which to our knowledge is the most complete such model reported to date, this model detailed contains 17 metabolites, 6 enzymes, 2 transporter proteins, and 3 inhibitors that participate in 9 reactions characterized by 63 enzyme kinetic and binding parameters.

However, the above mentioned models are complicated because (1) the models are a higher order and some of them are described by partial differential equations; (2) there are too many parameters and these parameters cannot be uniquely determined.