Robust Software Sensor Design for the State Estimation in a Sulfate-Reducing Bioreactor

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Abstract—The goal of this work is to present a class of state observer in order to infer unavailable concentrations in a sulfate-reducing bioreactor containing an anoxic culture of \textit{Desulfovibrio alaskensis} 6SR from the measurements of the sulfate concentration. The methodology is applied to the corresponding sulfate-reducing model considering modeling uncertainties. The proposed observer design presents a proportional term plus a sigmoid function structure. The model’s observability was locally analyzed by the observability matrix test, concluding that the sulfate-reducing bioreactor is detectable. A sketch of proof of the observer’s convergence is depicted in order to show the asymptotic convergence characteristics. Numerical experiments provide an overview about the superior performance of the proposed observer methodology compared to a sliding-mode and high order sliding mode observers.

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INTRODUCTION

The increasing demand of high performance technologies for biotechnology applications leads to a constant pressure to develop more efficient, quality and environmentally friendly bioprocesses. In order to meet such demand the use of bioreactors offer a class of processes which are adequate to generate specialized products, however the high nonlinear behavior of these kind of process lead to important difficulties in operation, control, monitoring and optimization. One of the major problems in the bioreactor operation is that on-line measurements are limited, thus making impossible to follow the dynamic behavior of the main variables of the system. This problem is related with the cost, time processing and/or the efficiency of physical sensors; therefore, this situation leads to an incomplete understanding of the dynamic inside the reactor and make unable to take steps to ensure a suitable production for the closed-loop system [1]. A complementary solution to infer the physically unmeasured states is to implement a mathematical algorithm known as virtual sensor or state observer which, from the known system information (measurable outputs) and the nominal plant model itself, a reconstruction can be made, at least partially, of the state vector [2]. The study of such algorithms began with the works of Luenberger, D.G. [3] and Kalman, R.E. [4] for linear dynamic systems and have been proven extremely useful, especially for on-line monitoring, fault detection and observer-based-control design, however for nonlinear systems the theory is not complete, nor completely successful. Nowadays, nonlinear observer design is the subject of research for many groups, several estimation techniques have been developed and the application to biological systems is increasing [5–10]. A first classification of state observers could be based on the full/partial knowledge of the model structure [2]. In the first case, a drawback is present; the uncertainty in the model parameters can generate possibly large bias in the estimation of the unmeasured states. The second case, the observers are named asymptotic observers, these are based on the hypothesis that the uncertainty in the model system lies within the kinetic reaction structures, so that the observers are designed employing the mass and energy balances, not necessarily needing the kinetic information [11, 12].

A second classification for the designed observers is based on the robustness of the estimator algorithm against disturbances, noise output or dynamic uncertainties commonly present in biological systems. High gain and sliding mode observers satisfied some of the above criteria. The high gain observer [13] robustly estimates the unmeasured states against unmodelled dynamics while asymptotically attenuating disturbances with the drawback of noise amplification.
Some bacteria such as Desulfovibrio alaskensis 6SR conduct a process through its own observer gain and peaking phenomenon [1, 14]. The sliding mode observer [15, 16] has the objective of maintaining stability and performance in the presence of discrepancies between the plant and its corresponding model. Generally speaking, the sliding mode observer, instead of feeding back the output error between the observer and the system linearly (linear innovative term), the output error is fed back via a discontinuous switched signal ($\text{sgn}$ function term) [7, 10, 17]. This has the advantage of robustness to disturbances, insensitivity to unknown inputs and a finite time convergence, but with the disadvantage of chattering, increasing the relative degree of the system and in some cases destabilize the closed loop system [7, 18]. In order to diminish the chattering problem and improve the corresponding performance of the observed, the higher order sliding mode (HOSM) observers were developed in the nineties [19] and are still being researched [18, 20–22], however, the chattering phenomenon is still present (for a complete state of the art see [23]).

As mentioned above state observers have great potential for application in biological systems, where it is often difficult or impossible to monitor online the concentrations of the reacting species.

The aim of this work is to propose a smooth bounded nonlinear observer applied to a class of batch bioreactor model in order to estimate the unmeasured but observable mass concentrations under model uncertainties. The bio-kinetic model used was experimentally corroborated; where additive modeling uncertainties were considered. Some numerical simulations are presented in order to illustrate the main results of this research.

**MATERIAL AND METHODS**

**Data Analysis and Mathematical Model**

The sulfate reducing (SR) process conducted by some bacteria such as Desulfovibrio alaskensis 6SR [24] (taken as study case) is important due to the pollution in water caused by sulfate ions, these are produced and discharged by mining and mineral processing. It affects negatively on the population of fish and plant, and moreover it’s toxic for humans. There are some physicochemical treatments for the sulfate ion removal, but the biological approach has taken special attention for being environmental friendly, not expensive, lowers the sulfate levels to minimal quantities and when metabolized sulfur is produced. Following the sulfate-reducing metabolism of Desulfovibrio alaskensis 6SR in a batch culture was possible by monitoring three response variables: biomass, sulfate, and sulfide concentrations by dry weight method, turbidimetric method based on barium precipitation and colorimetric assay, respectively as is reported in [25]. For the model construction, three data series were generated and analysed, an average value of each measurement point was calculated. The biosystem presents product inhibition kinetic behaviour as is reported in [24] indicated in the transition of the 3 state variables through time, where a decrease in the biomass growth is found pointed in the transition of the 3 state variables through time, where a decrease in the biomass growth is found.

The estimation of the SR-model parameters was made employing numerical software, POLYMATH 6.0 Professional™ using forward finite differences algorithm Eq. (2) and a nonlinear polynomial regression (as Levenberg–Marquardt routine). Three set of experimental data (biomass, sulfate and sulfide concentrations) were analysed. The value of the kinetic parameters are showed in table.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu_{\text{max}}$</td>
<td>7.00 $\text{h}^{-1}$</td>
</tr>
<tr>
<td>$K_{S}$</td>
<td>2.227 $\text{kg S m}^{-3}$</td>
</tr>
<tr>
<td>$K_{I}$</td>
<td>0.56553 $\text{kg S}^{2} \text{m}^{-2}$</td>
</tr>
<tr>
<td>$K_{P}$</td>
<td>0.55712 $\text{kg P m}^{-3}$</td>
</tr>
<tr>
<td>$m$</td>
<td>0.10</td>
</tr>
<tr>
<td>$Y_{S}$</td>
<td>14.13 $\text{kg S Kg X}^{-1}$</td>
</tr>
<tr>
<td>$Y_{P}$</td>
<td>2.14 $\text{kg P kg X}^{-1}$</td>
</tr>
</tbody>
</table>

The kinetic parameters obtained by nonlinear regression for Desulfovibrio alaskensis 6SR bioprocess model

### Estimation of the Kinetic Parameters

The estimation of the SR-model parameters was made employing numerical software, POLYMATH 6.0 Professional™ using forward finite differences algorithm Eq. (2) and a nonlinear polynomial regression (as Levenberg–Marquardt routine). Three set of experimental data (biomass, sulfate and sulfide concentrations) were analysed. The value of the kinetic model parameters are showed in table.

$$\frac{dX}{dt} \approx \left( \frac{\Delta X}{\Delta t} \right) = \left( \frac{X_{t+1} - X_{t}}{t_{t+1} - t_{t}} \right).$$

To validate the model, a comparison between the experimental and predicted data transformed to a linearized form was obtained also an overall correlation coefficient ($R^{2}$) was calculated (Fig. 1).