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Super-twisting estimation of a virtual output for extremum-seeking output feedback control of bioreactors

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ABSTRACT

In biotechnological processes such as fed-batch reactors the lack of reliable and robust on-line sensors and the limited number of actuators make the task of operating at optimal conditions very difficult. We present a feedback controller that aims at regulating the substrate concentration at an optimum value such that biomass production is enhanced while by-product formation is not favored. We use a virtual output that is estimated using a bank of weighted super-twisting observers to drive an output-feedback extremum-seeking controller. The only online measurements needed are the biomass concentration and the oxygen and carbon dioxide mass transfer rates. Simulations on a fed-batch bioreactor model show its applicability.

1. Introduction

In biotechnological applications it is common to optimize the operation of fed-batch bioreactors to attain a desired performance by manipulating the feed rate. A particular case is the maximization of the final biomass while minimizing an undesired by-product.

The fed-batch growth of certain strains of *Escherichia coli* presents overflow metabolism [1]: its catabolism has a limited energy production for cell growth and division because of a limited capacity to oxidize the main substrate, usually glucose. Thus, under excess of this nutrient, it can follow another metabolic pathway more commonly known as fermentation, producing a by-product which is generally a growth inhibitor, e.g. acetate.

The mathematical model of this process has already been described [2,3] and it involves three reactions: substrate oxidation, substrate fermentation, and by-product oxidation. The first two reactions occur only when the substrate is in excess, i.e. when its concentration is above a critical value, whereas the first and last reactions are active when this concentration is below the critical level. The state variables are the biomass (X), the substrate (S), the by-product (P), the dissolved oxygen (O) and the CO_2 (C) concentrations, as well as the current volume in the reactor (V). It has a main control input which is the dilution rate $u = Q_{in}/V$, where Q_{in} is the volumetric inflow rate. Other inputs to the system are the substrate inflow concentration (S_{in}) and the supplied oxygen through agitation or a sparger, influencing the mass transfer coefficient ($k_L a$).

We consider in this contribution a simplified model of the system, where it is assumed that no by-product (acetate) is formed nor consumed. Then we can write the system as

$$\dot{\xi} = K\rho X - \xi u + f, \quad \xi(0) = \xi_0, \tag{1a}$$

$$\dot{V} = u \quad V(0) = V_0, \tag{1b}$$

where V is the volume, $\xi = [X, O, C, S]^T$ is the state vector, $K \in \mathbb{R}^{4\times 2}$ contains the pseudo-stoichiometric coefficients, u is the dilution rate, and $f = [0, f_{OTR}, -f_{CTR}, S_{in}u]^T$ is the vector of gas and mass flow rates in and out of the reactor; f_{OTR} and f_{CTR} are the oxygen and CO_2 transfer rates. The specific reaction rate vector is $\rho = [r_1, r_2]^T$, where r_1 is the respiration rate and r_2 is the fermentation rate, which depend on a critical rate r_S^*:

$$r_1 = \min(r_S, r_S^*), \quad r_2 = \max(0, r_S - r_S^*). \tag{2}$$

Substrate (glucose) is consumed with rate r_S, which follows a Monod model,

$$r_S = \mu_S \left(\frac{S}{S + K_S} \right). \tag{3}$$

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The rate r_S^* defines a critical substrate concentration S^*, such that respirative regime occurs when $S(t) < S^*$ and respiro-fermentative regime occurs when $S(t) > S^*$. Although it is not modeled by (1), acetate is produced in respiro-fermentative regime, but only slowly consumed in respirative regime [3]. This by-product (P) is inhibitory for biomass growth, as its accumulation decreases the critical consumption rate r_S^* as follows:

$$r_S^* = \mu_S^* \left(\frac{O}{O+K_O}\right)\left(\frac{K_{iP}}{K_{iP}+P}\right), \tag{4}$$

where μ_S^*, K_O, and K_{iP} are constants.

The best strategy for enhancing biomass production without accumulating acetate is thus to operate in the boundary between regimes, i.e. maintaining $S(t)$ at the critical value S^*, where $r_S(S^*) = r_S^*$. This way, no acetate is produced and thus the critical r_S^* remains at a maximum, leading to maximum biomass growth. However, S^* is not known *a priori* and furthermore it may decrease slowly during the fed-batch cultivation if acetate accumulates.

For this reason real-time optimization (RTO) schemes have been proposed [3–5]. They use a virtual output that is a linear combination of the two main reaction rates in the process:

$$y = \nu(S) = r_1(S) - r_2(S) = \gamma^T \rho(S) \quad \gamma = [1, -1]^T. \tag{5}$$

As a function of S, $y(S)$ has a maximum whenever $S = S^*$ and thus $y = r_S^*$. The proposed controllers manipulate the dilution rate $u(t)$ to keep $y(t)$ near its optimum value at r_S^*. For example, Dewasme et al. [3] propose the use of an extremum-seeking strategy that provides an estimate of S^* to regulate $S(t)$ at this value; it assumes on-line measurement of S. In contrast, Vargas et al. [5] propose the use of a modified PI-controller to regulate $y(t)$ at its maximum value y^* without the need to measure S.

A problem with these controller proposals is that this output cannot be measured directly. This is why we call it a *virtual output*. Dewasme et al. [3] propose an algebraic approach to estimate it under the assumption of quasi-steady-state, perfect knowledge of the matrix K, and online measurement of all the signals in $f(t)$. However, it has the disadvantage of being very sensitive to the exactness of the matrix K of pseudo-stoichiometric coefficients and it only estimates the quantity $(r_1 - r_2)X$, so it also becomes sensitive to the noise present in X.

In a recent contribution we proposed the use of a bank of super-twisting observers to estimate the virtual output [6]. The approach uses only the on-line measurements of X, O, and C (using probes), as well as f_{OTR} and f_{CTR} (using a gas analyzer). Measurement of S is not needed, nor the knowledge of S_{in}. Knowledge of the matrix K is assumed, but if this is not possible, a methodology is proposed to build an estimate of its underlying structure, given gathered data from a previous batch operation.

In this contribution we now explain further the estimation procedure for the virtual output using the bank of observers and combine the use of the observer with a simple discrete two-level extremum-seeking controller. This leads to an output-feedback controller that is able to bring substrate trajectories close to the optimum value $S^*(t)$ and thus enhance the biomass growth.

The next section presents first the weighted super-twisting observer (WSTO) and discusses some of its useful properties. This observer is used in Section 3 to propose a bank of WSTO's for estimating the virtual output. This is followed by a section devoted to the choice of a crucial transformation matrix and how to estimate it with recorded data. Section 5 presents the (virtual) output-feedback two-level controller. Then, the simulation results with the bioreactor case study are presented and discussed, and finally some conclusions are drawn.

2. A weighted super-twisting observer

Consider the class of second-order systems

$$\dot{x}_1 = f_1(x_1, u) + b(t)x_2 + \delta_1(t, x, u), \tag{6a}$$

$$\dot{x}_2 = f_2(x_1, x_2, u) + \delta_2(t, x, u, w), \tag{6b}$$

$$y = x_1, \tag{6c}$$

where $x_1 \in \mathbb{R}$, $x_2 \in \mathbb{R}$ are the states, $u \in \mathbb{R}^m$ is a known input, $w \in \mathbb{R}^r$ represents an unknown input and $y \in \mathbb{R}$ is the measured output; f_1 is a known continuous function and f_2 corresponds to a known possibly discontinuous or multivalued function; δ_1 and δ_2 represent uncertain terms. The measured variables are x_1 and the known input u. The signal $b(t)$ is a *known* positive function that acts as a weight on x_2, which is lower and upper bounded,[1] i.e.

$$0 \le b_m \le b(t) \le b_M. \tag{7}$$

It is assumed that system (6) has solutions in the sense of Filippov [7].

When $\delta_1(t, x, u) \equiv 0$ the observability map $\mathcal{O} : [x_1, x_2]^T \mapsto [y, \dot{y}]^T$ is globally invertible for every u and w, so it is possible to determine the unmeasured state x_2 from the measurement of x_1. In the absence of w, the system (6) is *uniformly observable for every input* [8] and if w is present, then it is only *strongly observable* [9,10]. However, if $\delta_1(t, x, u) \neq 0$, then observability is lost and it is impossible to determine exactly the state x_2. This happens usually when there is noise in the measurements of x_1.

The proposed weighted super-twisting observer (WSTO) is:

$$\dot{\hat{x}}_1 = -\ell_1\phi_1(e_1) + f_1(\hat{x}_1, u) + b(t)\hat{x}_2, \tag{8a}$$

$$\dot{\hat{x}}_2 = -\ell_2\phi_2(e_1) + f_2(\hat{x}_1, \hat{x}_2, u), \tag{8b}$$

where $e_1 = \hat{x}_1 - x_1$, and $e_2 = \hat{x}_2 - x_2$ are the state estimation errors. The *constant* observer gains ℓ_1 and ℓ_2 are selected to ensure the convergence of e_1 and e_2 to zero. The injection nonlinearities ϕ_1 and ϕ_2 are monotone increasing functions of e_1 and are given by:

$$\phi_1(e_1) = \mu_1|e_1|^{(1/2)}\mathrm{sign}(e_1) + \mu_2|e_1|^q\mathrm{sign}(e_1), \tag{9a}$$

$$\phi_2(e_1) = \frac{\mu_1^2}{2}\mathrm{sign}(e_1) + \mu_1\mu_2\left(q + \frac{1}{2}\right)|e_1|^{q-(1/2)}\mathrm{sign}(e_1) + \mu_2^2 q|e_1|^{2q-1}\mathrm{sign}(e_1), \tag{9b}$$

where $\mu_1 \ge 0$ and $\mu_2 \ge 0$ are non negative constants, not both zero, and $q \ge 1$ is a real number. Note that $\phi_2(e_1) = \phi_1'(e_1)\phi_1(e_1)$; ϕ_1 is continuous while ϕ_2 is discontinuous at $e_1 = 0$. Solutions of the observer (8) are understood in the sense of Filippov [7]. The dynamics of the state estimation errors $e_1 = \hat{x}_1 - x_1$ and $e_2 = \hat{x}_2 - x_2$ (i.e. the estimation error vector $e = [e_1, e_2]^T$) is described by

$$\dot{e}_1 = -\ell_1\phi_1(e_1) + b(t)e_2 + \varrho_1(t, e, x, u), \tag{10a}$$

$$\dot{e}_2 = -\ell_2\phi_2(e_1) + \varrho_2(t, e, x, u, w), \tag{10b}$$

where

$$\varrho_1(t, e_1, x, u) = f_1(x_1 + e_1, u) - f_1(x_1, u) - \delta_1(t, x, u), \tag{11a}$$

$$\varrho_2(t, e, x, u, w) = f_2(x_1 + e_1, x_2 + e_2, u) - f_2(x_1, x_2, u) - \delta_2(t, x, u, w). \tag{11b}$$

[1] The case where $b(t, u, y)$ is always strictly negative can be treated similarly.