A geometric approach for adaptive estimation of unknown growth kinetics in bioreactors

Ehsan Moshksar, Martin Guay[*]

Department of Chemical Engineering, Queen's University, Kingston, ON, Canada

ABSTRACT

This paper proposes a new approach for the estimation of unknown and time-varying specific growth rate in fed-batch bioprocess. A novel adaptive estimation technique based on the concept of invariant manifold is proposed as an effective approach to estimate growth kinetic parameters. An asymptotic nonlinear observer is used to provide simultaneous on-line estimation of biomass concentration and growth kinetic. The method is easy to implement and requires only one tuning parameter. The effectiveness of the proposed algorithm is illustrated with representative bioreactor simulation examples.

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1. Introduction

Bioprocesses are now commonplace in a wide range of industries [13]. Despite significant advances, the study of bioprocess dynamics and control still faces considerable challenges in the development of effective and reliable techniques. Bioprocesses display some particular features that often require tailored approaches. These systems typically display a high degree of nonlinearity and their dynamics are often subject to significant sources of uncertainties. These uncertainties originate, in part, from the limited knowledge of the growth kinetics [7]. In most applications, the description of growth kinetics is limited to simple analytical expressions for the growth rate functions which have been shown to achieve some success both empirically and/or experimentally. Several studies have been published on the estimation of unknown parameters for bioprocesses governed by popular growth kinetics model structures such as Haldane and Monod models (see, e.g., [11,23,6,10]). Due to their empirical nature, such growth rate kinetic models can often be unreliable in practice. Growth kinetics can often be subject to changes related to changes operating conditions and cell metabolism that cannot be captured by simple models. As a result, it is necessary to develop algorithms for precise on-line estimation growth rate in bioprocesses.

Direct estimation of the growth rate has been the subject of many studies. The extended Kalman filter has been used for growth rate estimation in [20]. Although the extended Kalman filter is easy to implement, it has some major disadvantages. First, its stability and convergence properties are inherently local and there is no guarantee for acceptable performance over wide ranges of operating conditions. Second, exponential convergence of the filter relies on the assumption that the linearized model is observable in a neighbourhood of an equilibrium point. As noted in [17], this assumption may prove to be limiting in practical situations.

Adaptive estimation approaches have also been proposed to estimate the unknown and time-varying specific growth rate function. Under the assumption that the states of the system are available for measurement [9], the stability property of adaptive estimation techniques for systems with unknown kinetic models has been investigated in [2]. In most instances, these approaches can deliver acceptable performance. However, most existing designs require the tuning of a significant number of design parameters that must be assigned in the absence of any specific tuning rules. This problem was partially solved in [5] by using high-gain approaches, and in [16] by relating the stability conditions to the choice of design parameters.

In many practical situations, only part of the state variables of the bioprocess are available for measurement. As a result, state observers must be developed for these systems in order to overcome the limited set of measurements. Asymptotic observers are the most common techniques for this problem since they provide state estimates without requiring the knowledge of process kinetics [4]. The combination of state and parameter estimations for bioprocesses have been considered in the literature (e.g. see [2,22,21] and the references therein).

Due to the popularity of geometric invariance in nonlinear control theory [1], this concept has also emerged in bioprocesses mainly via sliding mode-based techniques. The main purpose is to increase the robustness of algorithms with respect to uncertainties in the process dynamics [19]. This nonlinear technique can be used in the observer structure to estimate the unknown growth kinetics. In [18], sliding mode observers have been applied to a bioprocess for finite time estimation of the specific growth rate and substrate concentration. However, for substrate estimation, it is assumed that the growth rate function has a close approximation to the Monod model, which may not be practical for all range of operating conditions. The modification of this algorithm has been considered in [3] to provide improvements in convergence time for fault detection applications. Also, it has been shown that the chattering phenomena of conventional sliding mode algorithms is significantly reduced. Recently, second-order sliding mode observers have been used for multiple kinetic rates estimation with no requirement of additional dynamics [15].

In this work, an alternative approach based on the concept of invariant manifolds is proposed for specific growth rate estimation. The idea of an invariant manifold is similar to one exploited in sliding mode-based technique. Instead of a sliding surface, an almost invariant manifold is constructed using high gain estimators and filters. This approach allows one to construct implicit functions that relate known variables and unknown variables. A parameter update law is assigned using the almost invariant manifold. The proposed technique guarantees the exponentially convergence of the estimated parameter to a small region of its true values. Also, an asymptotic observer is considered for state estimation, and convergence conditions are established. In contrast, the combination of state and parameter estimation has not been fully addressed in sliding mode observers.

The paper is organized as follows. The problem description is given in Section 2. In Section 3, the proposed invariant manifold design and parameter estimation technique are presented. The extension of the algorithm to the joint estimation of unknown parameters and state variables is presented in Section 4. This is followed by simulation examples in Section 5 and brief conclusions in Section 6.

2. Problem description

Consider the following microbial growth process

$$\dot{x} = \mu(s)x - ux \tag{1}$$

$$\dot{s} = -\frac{1}{Y}\mu(s)x + (s_0 - s)u \tag{2}$$

where $x \in [0, \infty)$ and $s \in [0, \infty)$ denote biomass and substrate concentrations, respectively, $u > 0$ is the dilution rate, s_0 denotes the concentration of the substrate in the feed, and $Y > 0$ is the yield coefficient. The inlet substrate is fed into the tank with a constant concentration s_0. It is assumed that the inlet flow rate and the output flow rate are same values, so the overall volume V of the tank is kept constant. Also, the solution in the mixing tank is assumed to be well-mixed. A simple schematic representation of the bioreactor is given in Fig. 1.

The variables x and s are state variables and u is the input variable for state space model (1) and (2). The nonlinear function $\mu(s)$ is the growth rate of the process. Many different choices of $\mu(s)$ have been used in the literature to describe large classes of biochemical processes [23]. In general, the development of suitable analytic expressions can be difficult due to the inherent complexity of the $\mu(s)$ models [5].

In this work, we treat the growth rate model as an unknown time-varying parameter $\mu(t)$, to be estimated. For this purpose, the
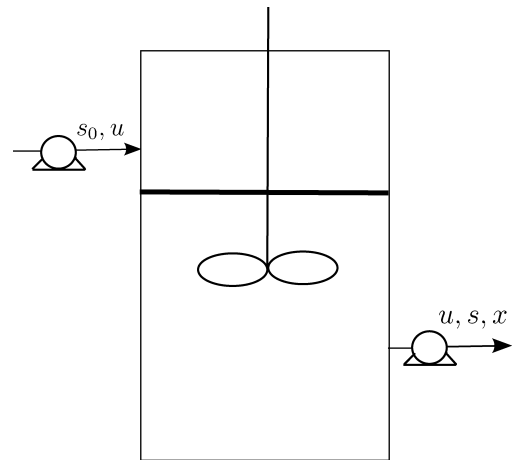

Fig. 1. A simple schematic representation of the bioreactor.

concepts of invariant manifold and adaptive parameter update law are used for estimation of $\mu(t)$.

Two different cases are considered in this paper. First, it is assumed that both x and s can be measured on-line. In the second case, we assume that the biomass concentration, x, is not available for measurement. A nonlinear observer is proposed to estimate the biomass concentration.

The following assumptions are required.

Assumption 1. The state trajectories $y = [x, s]^T$ evolve on a known compact subset of $\mathbb{Y} \in \mathbb{R}^2$.

Assumption 2. The physical nature of the problem is such that the growth rate $\mu(s)$ and its first order derivative with respect to time are inherently bounded. It is assumed that $|\dot{\mu}(t)| \leq \gamma$, $\forall t \geq t_0$. Also, γ is a known positive constant.

Assumption 3. The known input dilution rate is such that $u \geq u_0$ with known lower bound $u_0 > 0$.

3. Manifold-based adaptive estimation

We first consider the adaptive estimation design for plant (1) and (2) when all states of the system are available for measurement.

3.1. Invariant manifold design

The idea is to find a mapping from known variables to the unknown variables that has an almost invariance property for sufficiently large value of the design gain. This implicit mapping can be used to estimate the unknown parameters [14].

Let $y = [x, s]^T$, $f = [-ux, (s_0 - s)u]^T$, and $g = [x, -\frac{1}{Y}x]^T$. The estimator model for (1) and (2) is defined as

$$\dot{\hat{y}} = -k^2(\hat{y} - y), \quad k > 0 \tag{3}$$

with accompanying filters given by:

$$\dot{\psi} = -k^2(\psi - f(y, u))$$
$$\dot{\phi} = -k^2(\phi - g(y, u)). \tag{4}$$

Assumption 4. The vector-valued function $\phi(t)$ is bounded with a known bound as $\|\phi\| \leq \lambda$, $\forall t \geq t_0 \geq 0$.

Remark 1. The assumption implies that the norm of the vector $g(y, u)$ is bounded. This can be achieved by continuity of $g(y, u)$, the boundedness of y and u $\forall t \geq 0$. Also the constant value λ can be achieved along with the Assumption 1.