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A pseudo-Port-Hamiltonian Representation and Control of a Continuous Bioreactor

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Abstract:

Port-Hamiltonian (PH) systems are energy-rooted representations of dynamical systems which allow, through energy shaping, to design controller based on physical considerations. Since, bioreactions kinetics are based on data fitting, the obtention of a passive or a PH representation of a continuous bioreactor is not straightforward. Its is shown that an adequate change of coordinates and the use of appropriate energy functions allow for a pseudo-PH formulation of the dynamics of continuous fermenters. Different candidate energy functions are being tested and an adaptive controller is designed to cope with uncertainties on the specific growth rate. Simulations show the relevance of the approach.

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1. INTRODUCTION

Power-based representations of dynamical systems such as Bond-Graphs or Port-Hamiltonian (PH) systems allow for scalability and physical interpretation. The subsequent use of passivity theory allows to design stable power-based output-feedback controllers embedding real-world model parameters (Ortega et al. (2002)). Whereas these tools are well known for electro-mechanical systems, their straightforward extension to chemical or enzymatic reactions is impossible due to internal irreversible transformations. The first attempts in such modeling used to only propose an analogy with mechanical or electrical systems Hangos et al. (2001). However, it is possible to propose quasi-Porthamiltonian representations using different energy functions and subsequent controllers (entropy, enthalpy, Gibbs free energy etc., see e.g. Hoang et al. (2011a), Makkar and Dieulot (2013), Makkar and Dieulot (2014)). When it comes to bioreactions, a true energetic representation becomes impossible, since the kinetics is very complex and involves many reactions. In practice, the kinetics is simplified and based on empirical data fitting and not chemical-based considerations, as for the popular Monod equation (Bastin and Dochain (1990)). The kinetics can be interpreted a posteriori as modelling a number of phenomena such as substrate or product inhibition, etc. However, some attempts have been made to derive pseudo-Port-Hamiltonian representations of continuous bioreactors. Selişteanu et al. (2010) have tried to represent a Bond-Graph (BG) model for bioreactors and wastewater treatment, although deriving no controller directly from the model. Couenne et al. (2006) and Zhang et al. (2006) also tried to express energetic behavior through BG models of closed reactors. Ito (2004) designed a controller for a

wastewater plant based on the passivity theory, Dorfler et al. (2009) and Liu et al. (2010) have proposed pseudo Port-Hamiltonian models, but these do not meet the real Port-Hamiltonian structure, that is, do not exhibit skewsymmetric interconnection and symmetric dissipation matrices. In Ramirez et al. (2013), the authors also went through thermodynamic phase space of a chemical reaction, which does not actually reveal the conservation of energy and irreversible entropy creation. In Hoang et al. (2011b) and Hoang et al. (2012), the authors derived Port-Hamiltonian representation from Brayton-Moser formulation using ectropy (-entropy) and a quadratic-like function Fossas et al. (2004). However, the Energy function given in these forms and the PH model given by a generic decomposition of the nonlinear model was lacking the physical insight i.e. pseudo.

Since the kinetics of bioreactions are often derived of curve fitting from batch experiments, there exist substantial parameters uncertainties. Hence, the design of adaptive control around optimal or non-optimal productivity set-points is a key issue, leading to different kinds of algorithms whether extremum-seeking is sought or not (e.g. Cougnon et al. (2011), Dieulot (2012), Dimitrova and Krastanov (2011)). However, there exists little literature on adaptive Port-Hamiltonian systems, let alone the works of Wang et al. (2007) and Dirksz and Scherpen (2012). In the latter paper, the uncertainties are embedded into an augmented state-space representation which turns out to be under the port-Hamiltonian form, hence allowing subsequent outputfeedback controllers design. This paper proposes, via a change of variable and a few manipulations, a pseudo port-Hamiltonian representation of a continuous bioreactor. It will be shown that the output is a simple function of the biomass concentration, and that new control laws can

easily be derived from the model. Eventually, a tailored application of the adaptive scheme for port-Hamiltonian systems described in Dirksz and Scherpen (2012) will be shown to cope with parameter uncertainties.

2. PORT HAMILTONIAN MODELS AND CONTROLLERS

Passivity is a fundamental property of physical systems which are able to transform and dissipate energy. For such systems, passivity balances the energy of a system quantifying the external input and generated output. Under mild conditions, a passive system implies stability at the equilibrium point.

Definition 1: A dynamical system with collocated input and output u and y with a storage function H can be said to be passive if it holds the following inequality: $\frac{dH}{dt} \leq u^T y$. Passivity leads to the definition to an energy-based representation called Port-Hamiltonian systems.

Definition 2: Ortega et al. (2002) A dynamical Port-Hamiltonian system is described:

$$\dot{x} = (J(x) - R(x))\frac{\partial H}{\partial x} + gu, \tag{1}$$

$$y = g^T \frac{\partial H}{\partial x},\tag{2}$$

where x is the energy variable and H(x) accounts for the total stored energy. u, y are collocated port power variables which are called conjugate variables, as their duality product defines the power flows exchanged.

The interconnection matrices consist of the skew-symmetric structure matrix J(x), and the symmetric dissipation matrix R(x). It has been proven that if R(x) > 0 then the system is strictly passive Ortega et al. (2002). An adequate modification of the storage function and matrices allows for the design of the following Interconnection and damping assignment passivity-based control (IDA PBC).

Proposition 1: Ortega et al. (2002) Consider the PH system in (1) and a desired equilibrium point x_d . Assume there are matrices $J_d = -J_d^T$, $R_d = R_d^T \geq 0$ and a smooth energy function $H_d: H_d \geq 0$, then the Port Controlled Hamiltonian (PCH) system with dissipation verifies the matching equation:

$$(J(x) - R(x))\frac{\partial H}{\partial x} + gu = (J_d - R_d)\frac{\partial H_d}{\partial x}.$$
 (3)

Then the closed loop system with control $u = \beta(x)$

$$\beta(x) = \left(g^T g\right)^{-1} g^T \left((J_d - R_d) \frac{\partial H_d}{\partial x} - (J - R) \frac{\partial H}{\partial x} \right) \tag{4}$$

is asymptotically stable.

Proof: Substituting the value of $u = \beta(x)$ given in (4) in equation (1), yields (3).

 H_d is the desired Hamiltonian which is assumed to have a strict (local) minimum at the new equilibrium point x_d . J_d , R_d are specified interconnection (skew-symmetric) and damping (symmetric) matrices respectively. (3) is the general IDA-PBC matching equation and its main objective is to find a control u by an adequate choice of the desired

Hamiltonian and assignment of interconnection and damping matrices such that the system becomes asymptotically stable.

3. A PSEUDO PORT-HAMILTONIAN REPRESENTATION OF BIOREACTORS

Consider a well mixed bioreactor where a microbial reaction $S \longrightarrow X$ takes place. The tank is continuously fed with substrate at the concentration s_0 . The dilution rate $u = \frac{Q}{V}$, that is the ratio of the volumetric flow over the volume of the reactor, is considered as the sole control input.

The growth equations are:

$$\begin{cases} \dot{x} = \mu(s)x - ux, \\ \dot{s} = \frac{-\mu(s)x}{Y} + u(s_0 - s), \end{cases}$$
 (5)

where $x \in [0, +\infty[$ and $s \in [0, s_0]$ are respectively the biomass and substrate concentrations, and Y is a constant yield coefficient. The specific growth rate $\mu(s)$ is assumed to depend only on substrate s.

Consider a change of variable $w = s_0 - s - \frac{x}{V}$, and take $u = v + \hat{\mu}$ where $\hat{\mu}$ is an estimate of the specific growth rate μ . One has the following representation:

$$\begin{cases} \dot{w} = -\hat{\mu}w - vw + w(\hat{\mu} - \mu), \\ \dot{s} = \mu w + v(s_0 - s) + (s_0 - s)(\hat{\mu} - \mu), \end{cases}$$
(6)

Remark

Passivity can be shown for this model at (w, s, v) = (0, 0, 0)(which corresponds to near-batch operating conditions) using such a very simple energy function such as a sum of quadratic terms $H = w^2 + s^2$ and taking y = s as a possible output.

Nevertheless, in this case, one will not have the nice symmetry properties given for PH systems in (1), which need an appropriate energy function to be shown. Note that, since $u \ge 0$, and $\dot{w} = -uw$, w will always converge towards 0. This change of variable, which can be extended further to any continuous with only one input stream, is indeed a specific case of the General Dynamical Model of bioreactors which is presented in Bastin and Dochain (1990).

Proposition 2: The system in equation (6) with $\hat{\mu} = \mu$, and $\mu = f(s)s$, where f is non-singular at s = 0, can be written in a PH form with an energy function H such that $\delta H = \frac{\partial H}{\partial s} = \frac{\partial H}{\partial w}$, where $\lim_{x\to 0} \frac{s}{\delta H} \neq 0$. Assuming that the system is zero-state detectable, then a simple output feedback v = -ky, where k > 0, stabilizes asymptotically the system at the equilibrium point y = 0.

Proof: Note $H_{(.)} = \frac{\partial H}{\partial (.)}$. From (6) one has the pseudo-PH form:

$$\begin{pmatrix} \dot{w} \\ \dot{s} \end{pmatrix} = \begin{pmatrix} 0 & -\frac{\mu(s)w}{\delta H} \\ \frac{\mu(s)w}{\delta H} & 0 \end{pmatrix} \begin{pmatrix} H_w \\ H_s \end{pmatrix} + \begin{pmatrix} -w \\ s_0 - s \end{pmatrix} v \qquad (7)$$

$$y = \begin{pmatrix} -w \\ s_0 - s \end{pmatrix}^T \begin{pmatrix} H_w \\ H_s \end{pmatrix} \tag{8}$$

The output feedback property is inherent to PH systems (Ortega et al. (2002)).

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