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Parameter Estimation of a Microbial Fuel Cell Process Control-Oriented Model

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Abstract— Microbial fuel cells (MFCs) are novel devices capable of producing electricity while cleaning wastewater. Yet, MFC monitoring and control strategies are at very early stages of the development and therefore, dynamic mathematical models represent a crucial tool for the future design of software sensors and model-based control strategies. To this end, this work considers a MFC process control-oriented model obtained by combining fundamental equations based on mass and electron balances with equations describing an equivalent electrical circuit. Such model accounts for the experimentally observed double layer capacitance effect and complex nonlinear dynamics. Additionally, this work benefits from a previous online estimation procedure developed to estimate key electrical parameters of the model. Initially, sensitivity analysis was used to select identifiable model parameters. Then, parameter estimation results showed the importance of internal resistance for fitting the voltage generated by the MFC and the effluent carbon source concentration at long-term operation (hours to days). Meanwhile, capacitance was crucial when the MFC was operated at high frequencies (up to 100 Hz). Finally, simulations of a centralized nonlinear model predictive controller (NMPC) are shown. The goal of the controller is to maximize the electrical power produced while keeping the output substrate concentration at its nominal value under disturbances of the input substrate concentration.

I. INTRODUCTION

MFCs are devices consisting of two electrodes connected by an external circuit. The main difference with respect to conventional fuel cells, is that the anode houses a biofilm formed by exoelectricigenic bacteria able to externally re-lease electrons and protons from the oxidation of organic matter. The presence of an electrical potential difference makes the resulting electrons to be transferred to the anode surface from where they flow through the external circuit to the cathode. Simultaneously, protons migrate to the cathode crossing the electrolyte and reaching the electrons at the cathode surface where both are used to reduce oxygen and form water [1].

Such novel technology perfectly fits future scenarios of renewable energy supply, where forecasts indicate an increase of more than 33% in the world energy demand and a rise of 85% in water consumption by 2035 [2]. The need of cleaning wastewater while being able to recover electrical energy, instead of consuming it, foretells a very good application opportunity for MFCs [3]. Nevertheless, monitoring and control strategies of MFC operation are at very early stages of

development. Consequently, dynamic mathematical models represent a useful tool, not only in portraying unsteady-state behavior and understanding fundamental properties of MFCs, but also for the development of software sensors and the design of model-based process control strategies [4].

Recently developed models are able to adequately describe long-term behavior (hours to days) of MFCs operated with a fixed external resistance [5]. Some models consider a single microbial population without biofilm formation [6], [7], [8], others consider several microbial populations while assuming biofilm formation [9], others directly describe MFCs as a one-dimensional conductive matrix [10] and, finally, the more complex simulation models are able to describe the evolution in time and in space of important variables, such as current, charge, voltage, power and consumption of substrates (carbon sources) for several microbial populations [11], adapted to microbial populations present during the degradation of wastewater [12] or even including pH calculations [13]. These models, however, do not account for the double layer capacitance effect and complex non-linear dynamics observed in most recent experiments, in particular tests involving pulse-width modulated connection of the external resistance (electrical load) [14], [15], [16]. Furthermore, the higher the complexity of the models, the more unsuitable they become for process control and parameter estimation.

II. MODEL FORMULATION AND STRUCTURE

This work considers a MFC model obtained by merging fundamental equations based on mass and electron balances with equations describing an equivalent electrical circuit representing the double layer capacitance effect. Thus, the substrate in the reactor (1) is consumed by two microbial populations (electricigenic (2) and methanogenic (3)) with kinetics governed by double and simple Monod terms (6)-(9). Anodic biofilm formation and retention is accounted for by limiting the maximum attainable concentration of the microorganisms (10). Direct contact, nanowires or a mediator-based electron transfer mechanism from the carbon source (acetate) are assumed and the electron transfer by the electricigenic bacteria is considered to involve the oxidized and reduced forms of an intracellular mediator, e.g. NADH/NAD⁺ (4) & (11). The dilution rate is defined as in (12). Concerning the cathode, a non-limiting reaction rate is assumed.

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