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# Cellular non-linear network model of microbial fuel cell

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ABSTRACT

A cellular non-linear network (CNN) is a uniform regular array of locally connected continuous-state machines, or nodes, which update their states simultaneously in discrete time. A microbial fuel cell (MFC) is an electro-chemical reactor using the metabolism of bacteria to drive an electrical current. In a CNN model of the MFC, each node takes a vector of states which represent geometrical characteristics of the cell, like the electrodes or impermeable borders, and quantify measurable properties like bacterial population, charges produced and hydrogen ion concentrations. The model allows the study of integral reaction of the MFC, including temporal outputs, to spatial disturbances of the bacterial population and supply of nutrients. The model can also be used to evaluate inhomogeneous configurations of bacterial populations attached on the electrode biofilms.



## 1. Introduction

Microbial fuel cells are renewable bioelectrochemical transducers that convert biochemical energy into electricity. MFCs empower simultaneous treatment of wastewater and energy extraction from mixed organic media via the usage of microbial consortia as bio-catalysts. In addition to treating anthropogenic waste and wastewater, whilst producing rather than consuming electrical energy, MFCs have the ability of degrading toxic pollutants and the advantage of not burdening further the carbon cycle in the way fossil fuels do (Ieropoulos et al., 2013). They bear some resemblance to conventional fuel cells, given that they comprised two compartments, the anode and the cathode, divided by a Proton Exchange Membrane (PEM), where oxidation and reduction reactions occur. A major difference is that MFCs use abundant, renewable fuels, such as organic substrates, that are metabolised by bacteria, whereas chemical fuel cells are fuelled by pure compounds (which could be toxic as methanol or explosive as hydrogen) oxidised by precious metals. As a result, their inexpensive functionality and maintenance designate MFCs as a viable solution for producing energy in isolated areas.

Despite the fact that MFCs were proposed more than a century ago (Potter, 1911), it is still a subject of rigorous research, due to the increased power densities that have been achieved in the last decade. In addition, since they operate in ambient conditions (ambient environment temperature, atmospheric pressure, neutral pH) and given the aforementioned advantages, they can efficiently support systems for applications like remotely deployed sensors and robotics (Taghavi et al., 2016). Nonetheless, their analysis in copious conducted experiments reveal significant limitations on their performance due to low microbial activity (low growth rate or metabolic rate, due to non-optimal growth conditions or unsuitable microcosm — insufficient anodophiles), ohmic losses, mass transfer limitations on the electrode surfaces, non-optimised electrode architectures and transfer potential through the PEM. The process of defining the factors that limit the performance of MFCs can lead to more efficient designing methods. Although some techniques used in the conventional chemical fuel cells could be adopted, they cannot be expected to provide the same results due to the fundamental differences of the systems particularly due to the biological nature.

MFCs are complicated devices that contain bio-electrochemical reactions, mass and charge balance principles, biotic or abiotic transformation processes. As a result, their analysis and design process require a multidisciplinary approach with background in electrochemistry, microbiology, physics and engineering. On top of that, there are numerous differentiations in the MFCs studied which range from their configurations (having two chambers separated by a PEM or a membrane-less single-chamber MFCs) to the type of their incorporated mechanism of donating electrons to the anode electrode (mediated or mediator-less MFCs).

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Given the complexity of these systems, the number of parameters that affect their outputs and the costs in time and money needed to perform laboratory experiments, the development of computerised mathematical models simulating these systems is of great importance. The implementation of modelling techniques can contribute to the investigation of the principles covering their operation and affecting their performance, producing better arrangement designs of MFCs and working circumstances.

To address spatial dynamics of biophysical processes in a MFC we designed a cellular non-linear network (CNN) model. A CNN is a uniform regular array of locally connected continuous-state machines, or nodes, which update their states simultaneously in discrete time (Chua and Roska, 1993; Chua, 1998). Essentially, CNN is a finite-difference scheme with time step one. A CNN is a subset of cellular automata (CA). A CA is the same as CNN but states of nodes are discrete. CA and CNN are often mixed, many researchers do not differentiate these two types of machines. What is imitated in CA can be imitated in CNN and both offer powerful modelling capability as well. There are several studies published on CNN/CA or hybrid models of reaction-diffusion (Dab and Boon, 1989; Berryman and Franceschetti, 1989; Chopard and Droz, 1991; Chopard et al., 1994; Chopard, 1995; Droz, 1997; Bandman, 1999; Weimar, 2002; Matsubara et al., 2004; Suzuki et al., 2005) and prototyping of chemical computers (Adamatzky et al., 2006a,b, 2005, 2008; Marchese, 2002; Adamatzky, 2012) and molecular computers (Hiratsuka et al., 2001), spatial dynamics of bacterial colonies (Picioreanu, 1996; Krawczyk et al., 2003; Vitvitsky, 2016; Odagiri and Takatsuka, 2009; Margenstern and Takatsuka, 2013). Other approaches relevant to CNN modelling of MFCs are CA models of fuel loading patterns in nuclear reactors (Fadaei and Setayeshi, 2009), dynamics of nuclear reactors (Boroushaki et al., 2005; Hadad and Piroozmand, 2007; Pirouzmand and Nabavi, 2016; Akishina et al., 2005), neutron transport (Hadad et al., 2008), wastewater treatment by aerobic granules (Benzhai et al., 2014), sequencing batch reactor (Zhang et al., 2006), fluid flow in a porous medium (Bandman, 2011).

The proposed CNN-based model simulates biochemical and electrochemical reactions in a MFC based on synthetic redox mediators. To the best of the authors' knowledge this is the first attempt to simulate the outputs of a MFC with a CNN model. Despite the fact that the application of CNNs has been widely used to simulate several biological, chemical and physical processes as indicted previously, the novelty of this study can be pinpointed in the fact that all the processes and, thus, the behaviour of a batch-fed MFC has not been previously presented in a single CNN lattice with a local state comprised of all the critical quantities (several chemical species concentrations, biomass concentrations and current produced). Such a model will allow for a detailed analysis of integral outcomes of spatial processes inside MFCs, including a possible uneven distribution of nutrients in the MFC chamber, patterns of bacterial population in biofilms covering electrodes and distributions of diffusing metabolites. Nonetheless, the use of CNN as the mathematical basis for the model allows the employment of the inherent fully parallel nature of synchronised locally interconnected simple unities. The subject device is a two chamber MFC with the presence of electroactive microbes in suspension in the bulk liquid and forming biofilms on the surface of a planar anode electrode and assuming electron transfer from the microbes to the electrode with the use of an externally added diffusible chemical mediator. That mechanism can be differentiated to emulate various types of MFCs, that will be the aim of future works. Nonetheless, the present study can lead towards exploiting the parallelism of the simulating tools and, as a result, intensively accelerating the simulation of MFCs, by the implementation of the CNN-based algorithm on parallel hardware, as illustrated in Dourvas et al. (2015) and Tsompanas et al. (2016).

## 2. Previous work

Despite the intense investigation in the laboratory experimental field to optimise the performance of MFCs, results from computational models are not derived with the same rate. Moreover, the few models developed are targeting specific MFC configurations each and are so strictly specified that they become impractical for implementation on different configurations. The first model presented (Zhang and Halme, 1995), investigated a single population using an external mediator as receptor of electrons. That model analysed the correlation of the concentration of the external mediator with the higher possible power output.

The authors of Picioreanu et al. (2007) introduced the simulation of a MFC with an added mediator and several populations of suspended and attached biofilm microorganisms. The model was developed on two or three dimensions providing the resultant current produced by homogeneous or not biofilms. The results were derived by taking into account several parameters, like the content of different microbial species, the amount of suspended microbes compared with ones attached, the potential of the mediator, the initial concentrations of the mediator and the substrate and many more. The results provided were compared with experimental data from a batch MFC fed with acetate and inoculated with *Proteus* and found in a good agreement.

The model presented in Picioreanu et al. (2007) was updated in Picioreanu et al. (2008) with the incorporation of International Water Association (IWA's) anaerobic digestion model (ADM1) (Batstone et al., 2002). The coexistence of several types of methanogenic and electroactive bacteria is simulated, taking into account whether they are suspended or attached to the anode electrode. A batch MFC was simulated to test the effects of the electrical circuit on the population of the microorganisms and the results were compared with laboratory data. The model is also based on a one, two or three dimensions partial differential equations system to represent the spatial distribution of solutes in the biofilm.

In Picioreanu et al. (2009), a model simulating a MFC with only suspended microorganisms and externally inserted mediator was studied. In this model the conservation of mass for the dissolved ingredients has a basic role. The biomass growth is not studied in that model while a batch mode MFC which was periodically fed was simulated. The results were compared with laboratory data from MFCs inhabited with suspended *Proteus* cells and incorporating thionine as a mediator, proving accurate representation of the system. The model introduces the ideas of endogenous metabolism or intracellular substrate storage to justify a small amount of current present between the feeding pulses. As the conditions and concentrations in the anode were considered uniform, a one dimensional solution of the algorithm's equations was presented. Some key parameters of the equations used were extracted from fitting the outputs to the experimental data, while some others were estimated.

Another study (Picioreanu et al., 2010) proposing a mathematical model for MFCs, was based on two dimensional macroscale mass balance equations and microscale biofilm evolution. The model contains hydrodynamic calculations and mass and charge balances through diffusion, convection and electromigration to simulate the current output, species concentrations and pH distributions throughout the anode. Nonetheless, the possibility of depicting on two or three dimensions irregular biofilm and electrodes configurations and simulate the effects on the MFC operation and outputs was provided. The model was used to reproduce the system's outputs such as its pH distributions, the effect of multiple communities of electroactive, methanogenic and fermentative bacteria existing in the anode biofilm and the effect of the flow over or through complex electrodes.