



Simulation of the current generation of a microbial fuel cell in a laboratory wastewater treatment plant



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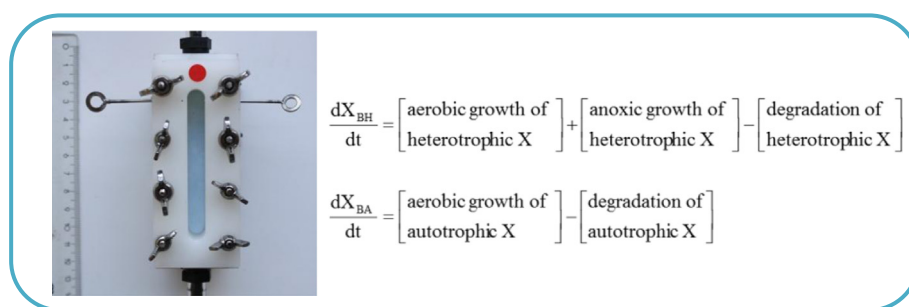
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HIGHLIGHTS

- ASM 1 was applied to describe effluent parameters of a lab scale treatment plant.
- Simulated parameters for active biomass correlate with the measured current flow.
- Model parameter X_{BH} and X_{BA} can be used to describe the current output of a MFC.
- The simulation connects data from wastewater treatment to MFC performance.
- ASM1 based simulation can be used to find ideal operation points of MFCs.

GRAPHICAL ABSTRACT



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ABSTRACT

Microbial fuel cells (MFCs) are devices generating electrical current from a wide range of organic substrates by using bacterial metabolism. Integrations of MFCs into wastewater treatment plants seem to be the most likely application of this technology. Due to the fact that the current flow in a MFC is fundamentally produced by the metabolic activity of microorganisms, it would be desirable to elucidate the capacity of the microbial systems to optimize the energy extraction processes in MFCs. In this study, the correlation between the parameters X_{BH} (active heterotrophic biomass) and X_{BA} (active autotrophic biomass) from the established activated sludge model number 1 (ASM1) and the measured current flow in MFCs was investigated for the first time. The simulation protocol based on ASM1 shows a good congruence between measured and simulated effluent values for the wastewater treatment plant. Comparisons between the measured current densities and the simulated concentrations of active biomass showed linear correlations at substrate pulses and at different residence times of the substrate. Therefore, it can be concluded that the model parameter X_{BH} and X_{BA} of the ASM1 can be used to estimate the current output of a MFC in wastewater treatment plants. The identified correlations can be used to optimize operating conditions and to generate high current outputs of the MFCs based on simulations.

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1. Introduction

Different bacteria have evolved strategies to transfer electrons to a solid abiotic electron acceptor far beyond the cell surface to

survive in ecological niches, which lack other electron acceptors for respiration, e.g. oxygen. If an electrode can be used for the electron transfer by these organisms, instead of the natural redox partner, the organisms are considered as electroactive bacteria (EAB) and can be used in bioelectrochemical systems (BES) [1]. Combining the advantages of biological components (e.g. reaction specificity, self-replication) and electrochemical techniques in BESs

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offers the opportunity to develop novel efficient and sustainable processes for the production of a number of valuable products, if the microorganisms can take up electrons from a cathode, or for the conversion of chemical energy into electrical energy, if microorganisms degrade organic matter and transfer electrons to an anode [2]. Therefore, the application of BESs is of great significance for several industrially relevant fields such as synthesis of fine and bulk chemicals, energy conversion and storage, and remediation processes.

Energy issues and energy management gained increasing interest during the recent years. However, even in energy intense processes, like in the chemical industry, energy management and optimization is often put in second place [3]. Wastewater treatment is considered also as an energy intense process. Therefore, energy management needs to be improved to ensure a sustainable and cost effective operation of the wastewater treatment plants [4,5]. Recent publications discuss the net energy production potential of wastewater treatment plants, since large amounts of energy remain unused within the organic matter in wastewater [6]. During the process, the highest amount of energy is consumed by pumps and aeration of the wastewater. Energy can be gained by anaerobic digestion of the remaining sludge. Microbial fuel cells (MFCs) could increase the energy output of wastewater treatment. Generally, MFCs are devices that utilize microorganisms to break down (mainly) organic substrates to generate electricity (Fig. 1).

MFCs have a bigger potential to generate energy than anaerobic digestion, since the electrical energy produced by MFC is considered as a “cleaner” energy compared to CH_4 or H_2 produced by anaerobic digestion. The electrical current could be used directly to provide the process energy for pumps and aeration [7]. Recently, several studies showed the applicability of microbial fuel cells in wastewater treatment plants [8–11].

During the recent years, a lot of publications dealing with the design [12,13] as well as the optimization of several components [14–19] of MFCs have been published (the progress is revised in [2]). In order to improve the knowledge of MFC performance, several groups started to develop mathematical models as a tool to gain insight into the complex bioelectrochemical interactions. To

our best knowledge there is no model published, which connects data from wastewater treatment plants (WWTPs) to MFC performance. This is a major gap in order to predict and evaluate MFC performance. Modeling and simulation at all levels of the processes within MFCs is crucial for a rational process design. The more knowledge gained about the process, the more accurate models can be developed, thereby improving predictions for further optimization of MFCs. The modeling can be performed at several process levels (e.g. the electrochemical behavior and components [20,21], interaction between electrodes and conductive biofilms [22–25], reactor type [26] and microbial level [27]). Several modeling approaches have been recently reviewed [28].

An immediate change from established wastewater treatment systems to MFC technologies is not feasible. Therefore, an integration of MFCs into classical WWTPs may enable a sustainable decentralized wastewater treatment of medium and low strength wastewater in future [7,8]. Therefore, a mathematical description of the degradation of organic matter (usually expressed via the chemical oxygen demand, COD) in wastewater and the resulting current of the MFC is needed for a knowledge based design of suitable processes. Wastewater treatment includes highly complex reaction networks, which can however be described by fairly simplified models. The biochemical processes occurring within WWTP can be modeled using the activated sludge model number 1 (ASM1) developed by Henze et al. [29]. This model (and the refined models ASM2 and ASM2d) is an internationally accepted standard for modeling WWTPs. ASM1 is based on the mathematical model of Monod, which describes the growth of microorganisms. Changes of the different organic fractions and nitrogen are described under aerobic and anoxic conditions, while transport processes are neglected. Henze et al. described typical dimensions of the desired model parameters [29]. However, the absolute values of the parameters are not part of ASM1 and need to be evaluated experimentally (see Table 2). The core of the model is a system of coupled differential equations. The ASM1 model characterises wastewater and activated sludge, considering seven soluble and six particular substances (Table 1).

These 13 substances are influenced by a total of eight processes; the interrelations are shown in Fig. 2. In ASM1 the organic ingredients are described by using the chemical oxygen demand (COD). The process velocities are described by 14 parameters in kinetic expressions and five stoichiometric parameters (see Table 2).

The following equations of ASM1 show the mathematical descriptions, which are used to calculate changes in concentrations of active heterotrophic (X_{BH}) and active autotrophic biomass (X_{BA}), respectively.

$$\frac{dX_{\text{BH}}}{dt} = \left[\text{aerobic growth of heterotrophic X} \right] + \left[\text{anoxic growth of heterotrophic X} \right] - \left[\text{degradation of heterotrophic X} \right]$$

Table 1
Substances and substance groups of ASM1.

Substance group	Symbol	Unit
Biological inert, soluble organic substances	S_I	gCOD m^{-3}
Biological fast degradable, soluble organic substances	S_S	gCOD m^{-3}
Biological inert, organic particles	X_I	gCOD m^{-3}
Biological slow degradable, soluble organic substances	X_S	gCOD m^{-3}
Active heterotrophic biomass	X_{BH}	gCOD m^{-3}
Active autotrophic biomass	X_{BA}	gCOD m^{-3}
Particular decay products of the biomass	X_P	gCOD m^{-3}
Solved oxygen	S_O	g m^{-3}
Oxygen from nitrate and nitrite	S_{NO}	gN m^{-3}
Nitrogen from ammonia and ammonium	S_{NH}	gN m^{-3}
Biological degradable, soluble organic bound nitrogen	S_{ND}	gN m^{-3}
Particular organic nitrogen compounds	X_{ND}	gN m^{-3}
Alkalinity	S_{ALK}	mol m^{-3}

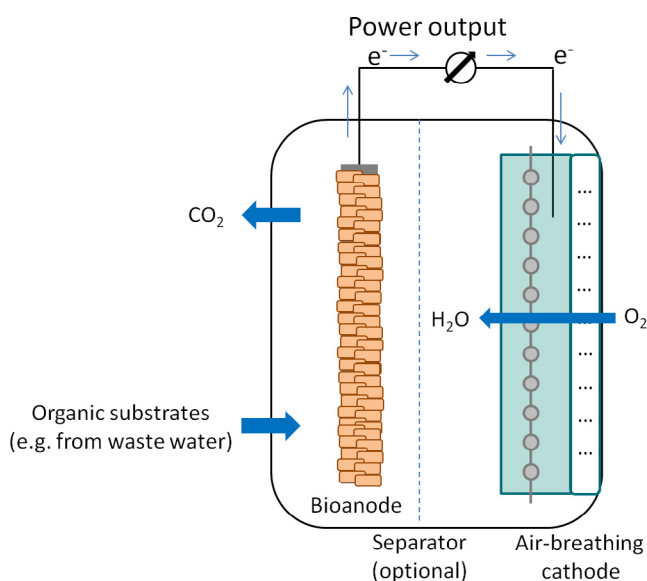


Fig. 1. Principle of a microbial fuel cell: organic substrates (usually from wastewater) are oxidized to carbon dioxide by electroactive bacteria. These bacteria respire with an anode and the electrons are transferred to a cathode (e.g. a gas diffusion electrode) to reduce oxygen to water; chemical energy is converted to electrical energy.

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