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Short communication

# Computational investigation of the flow field contribution to improve electricity generation in granular activated carbon-assisted microbial fuel cells

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## H I G H L I G H T S

- CFD-multi order Butler Volmer reaction model is used to study porous anode.
- The addition of GAC improves the mixing by creating a uniform flow field.
- Such a flow field increases current by enhancing the convective substrate transfer.
- Improved flow field contributes to at least 17% of the current enhancement.
- New findings are instructive to MFC optimization on both design and operations.

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## A B S T R A C T

Microbial fuel cells (MFCs) offer an alternative approach to treat wastewater with less energy input and direct electricity generation. To optimize MFC anodic performance, adding granular activated carbon (GAC) has been proved to be an effective way, most likely due to the enlarged electrode surface for biomass attachment and improved mixing of the flow field. The impact of a flow field on the current enhancement within a porous anode medium (e.g., GAC) has not been well understood before, and thus is investigated in this study by using mathematical modeling of the multi-order Butler-Volmer equation with computational fluid dynamics (CFD) techniques. By comparing three different CFD cases (without GAC, with GAC as a nonreactive porous medium, and with GAC as a reactive porous medium), it is demonstrated that adding GAC contributes to a uniform flow field and a total current enhancement of 17%, a factor that cannot be neglected in MFC design. However, in an actual MFC operation, this percentage could be even higher because of the microbial competition and energy loss issues within a porous medium. The results of the present study are expected to help with formulating strategies to optimize MFC with a better flow pattern design.

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## 1. Introduction

Microbial fuel cells (MFCs) have been considered as a next-generation technology to recover electrical energy from wastewater, due to its advantages such as reduced energy consumption, minimal sludge production, and direct electricity generation [1]. In an MFC, organics are degraded by microbial consortia within an

anodic compartment, and the produced electrons are transferred to a cathodic compartment via an external circuit [2]. Because of the complex interaction between microbial, electrochemical and engineering factors, a good understanding of the anodic performance is key to MFC design and optimization [3]. The anode electrode plays an important role in electricity generation, and a large surface of the anode electrode is preferred for biofilm attachment. Several strategies have been employed to increase the electrode surface, such as modifying an anode electrode with nano-materials [4], using a pre-fabricated carbon brush [5], or adding granular activated carbon (GAC) [6]. Among those, GAC may be the most cost-effective approach because the material is inexpensive. GAC not

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only provides a large surface area for bacteria adhesion, but also increases the affinity for anodic substrates, resulting in better kinetic performance versus other electrode materials [7]. Packing GAC in an anode compartment also affects substrate distribution and liquid flow pattern, which has not been well understood before.

Computational fluid dynamics (CFD) can be used to simulate and predict fluid flow and species transport by solving the governing advection-diffusion equations. In the past decade, researchers have attempted to use CFD techniques to assess proton accumulation and substrate distribution by analyzing the hydrodynamics within the anodic compartment [8–11]. These studies proved that varying flow conditions is indeed a key factor to improve electricity generation due to the effects of convection on diluting accumulated protons and enhancing substrate distribution within the anodic compartment. However, none of these studies have attempted to examine the correlation between the varied hydrodynamic conditions and electrical generation within a porous anode.

To further understand improvement of electricity generation using GAC and quantify the contribution of flow field to the improvement, an established and validated multi-order Butler-Volmer equation [12] was applied to analyze the complex hydrodynamics and bioelectrochemical process in an anodic compartment packed with GAC. Comparing to other MFC models that usually integrate conventional Monod and Butler-Volmer equations [13], the multi-order Butler-Volmer equation is expected to provide a simple but realistic simulation. It is assumed that the addition of GAC can provide enough surface area for microbial adhesion and also change the flow pattern of the substrate and microbes within the bulk liquid. The present study aims to gain a deeper insight into the interactions among anode chamber configuration, fluid flow and MFC performance, and provide instructional advice on optimizing the design and operation of MFCs.

## 2. Materials and methods

### 2.1. MFC setup and operation

The MFC was constructed as a tubular reactor (32 cm tall and 3.8 cm inner diameter) made of anion exchange membrane (AEM-Ultrex AMI 7001, Membrane International, Inc, Glen Rock, New

Jersey, USA), resulting in a total anodic liquid volume of 350 mL (Fig. 1). Carbon cloth (Zoltek Corporation, St. Louis, MO, USA) was used as the material for both the anode and cathode electrodes. Before use, the carbon cloth was soaked in acetone solvent overnight and then heated for 30 min at 450 °C. The finished anode electrode (with effective surface dimensions of 22 cm-long and 2.9 cm-diameter) was installed along the inner surface of the AEM tube and supported by a plastic mesh. A total mass of 132 g of  $4 \times 10$  GAC (Calgon Carbon Corp, Pittsburgh, PA, USA) was used as an additional electrode inside the AEM tube, resulting in a net liquid volume of 217 mL. The cathode electrode (23 cm  $\times$  12 cm) was coated with Pt/C powder (Etek, Somerrest, NJ, USA) at a loading rate  $0.3 \text{ mg Pt cm}^{-2}$ , and wrapped the AEM tube. The anode and cathode electrodes were connected to a  $10 \Omega$  resistor.

The MFC was operated at room temperature. Its anodic compartment was inoculated with anaerobic sludge from the Peppers Ferry Wastewater Treatment Plant (Radford, VA, USA) and fed with a synthetic solution containing (per L of tap water): sodium acetate 0.5 g;  $\text{NH}_4\text{Cl}$  0.15 g;  $\text{NaCl}$  0.5 g;  $\text{MgSO}_4$  0.015 g;  $\text{CaCl}_2$  0.02 g;  $\text{KH}_2\text{PO}_4$  0.53 g;  $\text{K}_2\text{HPO}_4$  1.07 g; and 1 mL trace elements [14]. No recirculation was applied to the anolyte, but the catholyte (50 mM phosphorus buffer solution) was recirculated at  $5 \text{ mL min}^{-1}$ . The flowrate of the anolyte was controlled by a peristaltic pump to achieve the desired hydraulic retention time (HRT) of 10 h.

### 2.2. Measurements and analysis

The MFC voltage was recorded every 5 min by a digital multimeter (2700, Keithley Instruments, Cleveland, OH). The pH was measured using a benchtop pH meter (Oakton Instruments, Vernon Hills, IL, USA). The concentration of chemical oxygen demand (COD) was measured by using a colorimeter according to the manufacturer's procedure (Hach DR/890, Hach Company, Loveland, CO, USA).

### 2.3. Computational model development

A steady, laminar, incompressible flow was assumed since the Reynolds number is 0.42 based on the inlet velocity of  $1.44 \times 10^{-5} \text{ m s}^{-1}$ . The conservation equations for mass and

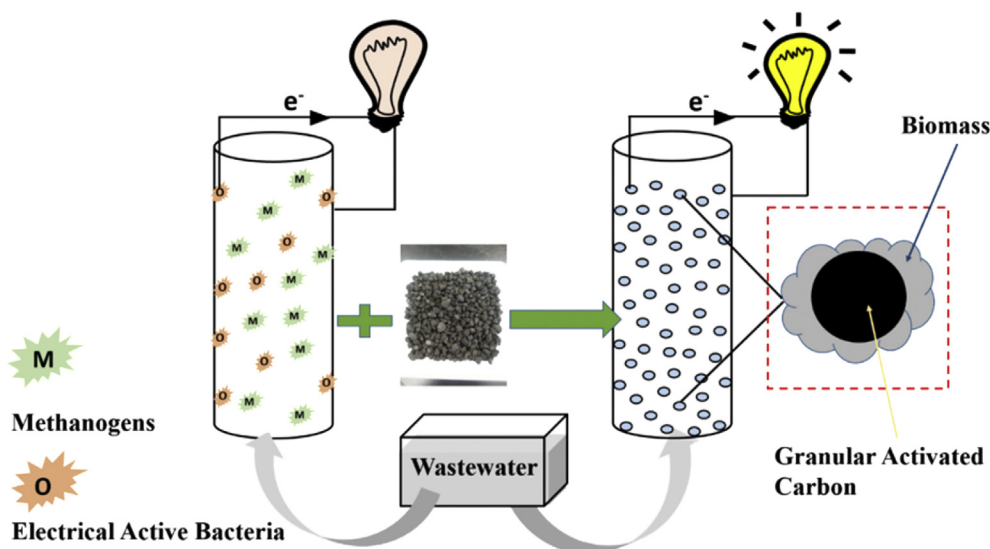


Fig. 1. A schematic of a tubular GAC-MFC operated with low-strength organic stream.

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