243w The Dynamic Modeling Framework for the Microbial Fuel Cell with Metabolic Flux Analysis and the Electrochemical Pemfc Model

Wonjun Park, Hyun Uk Kim, and Il Moon

This paper suggests the integrative modeling framework for the microbial fuel cell. The metabolism for the microbial was investigated to optimize the electrochemical performance with *in silico* model. The dynamic modeling is constructed with metabolic pathway analysis and the integrative methodology for the electrochemical fuel cell model of PEMFC without catalyst layer analyzes the substrate conversion rate of microbial with the optimal pathway under axenic culture condition.

The microbial fuel cells (MFCs) have the microorganisms as catalysts. Microbial used in the MFC converts protons and electrons from the substrate with metabolism. This has been recognized as a potential device to solve the environmental problem as well as energy with lower costs due to absence of catalyst. To realize the practical process with this, the systematic approach for the analysis of microbial behaviors and responses from the external condition. The selection of suitable bacterial consortia is considered for the optimal condition as a preliminary screening. *Escherichia coli* was chosen as a target microorganism owing to its characteristics favorable for the performance of MFC. First of all, it is known to be a good strain for the MFC performer generating the relatively high amount of electricity, compared to other bacterial species. Also, systems approach is eligible for evaluating its metabolism due to its rich genomic information. It has been recognized that *E. coli* particularly performs well under the fermentative condition. Consequently, its anaerobic metabolic pathways leading to the production of hydrogen and/or proton were retrieved from the publicly available databases in order to estimate its electrochemical performance. Then, metabolic flux analysis (MFA) was performed to gain better understanding of the optimal pathways that lead to the maximal production of proton. A particular emphasis was put on its central carbon and energy metabolism since they are deeply associated with the generation of proton, an essential source for the electricity generation. Moreover, dynamic modeling was constructed based on the resultant MFA.

This metabolic modeling is combined with the electrochemical modeling of PEMFC with streaming of proton. The mediate layer and boundary are considered to realize the transportation of proton between microbial and anode. The conventional PEMFC without catalyst layer is used to calculate the performance of fuel cell. The fuel cell layer has lumped and empirical equations for the whole systems. The consideration of mass transfer has been taken to check the dynamic performance. The dynamic modeling in metabolic pathway and electrochemical performance shows that the conversion rate of lactates is analyzed. The parameter estimations are performed with the range of constraints which is arranged with MFA. The rigorous pathway with metabolite flux is derived because metabolic and kinetic data for the *E. coli* are enough to estimate the parameters in the microbial pathway.

The microbial performance such as substrate conversion rate and overpotentials at the anode due to the proton maximized pathway. Dynamic electrochemical performance is analyzed with the integrated *in silico* modeling. This modeling suggests the integrative methodology as a emerging technology. This paper concentrates on the usage of optimal metabolic pathway to evaluate the performance. The dynamic modeling realizes the dynamic performance of the microbial fuel cell. The systematic analysis for the microbial fuel cell is performed and it suggests the fundamental modeling structure to apply another potential microbial.