ASEAN Engineering Journal

Full Paper

OPTIMIZATION OF MATHEMATICAL MODELING OF MICROBIAL ELECTROLYSIS CELL FOR THE PRODUCTION OF HYDROGEN FROM SAGO WASTEWATER SUBSTRATE

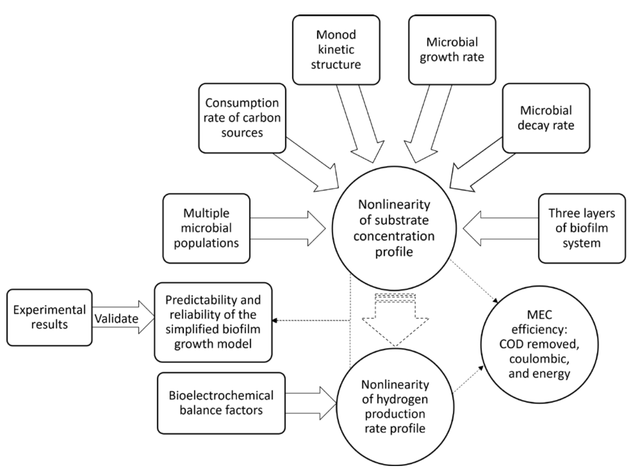
Mohamad Afiq Mohd Asrul[a], Mohd Farid Atan[a,b,c,d], Hafizah Abdul Halim Yun[a,e*], Noraziah Abdul Wahab[a,b,c,d], Hu Hin Hung[a], Josephine Chang Hui Lai [a,b], Ivy Ai Wei Tan[a]

[a]Department of Chemical Engineering and Energy Sustainability, Faculty of Engineering, Universiti Malaysia Sarawak, 94300, Kota Samarahan, Sarawak, Malaysia.
[b]Institute of Sustainable and Renewable Energy (ISuRE), Universiti Malaysia Sarawak, 94300, Kota Samarahan, Sarawak, Malaysia.
[c]Institute of Social Informatics and Technological Innovations (ISITI), Universiti Malaysia Sarawak, 94300, Kota Samarahan, Sarawak, Malaysia.
[d]University Sustainability Centre, Universiti Malaysia Sarawak, 94300, Kota Samarahan, Sarawak, Malaysia.
[e]Centre for Applied Learning and Multimedia, Universiti Malaysia Sarawak, 94300, Kota Samarahan, Sarawak, Malaysia.

Article history
Received
18 May 2023
Received in revised form
30 October 2023
Accepted
07 November 2023
Published online
31 May 2024

*Corresponding author
ahyhafizah@unimas.my

Graphical abstract



Abstract

The experimental runs of a 4-L double-chamber microbial electrolysis cell (MEC) produce hydrogen from sago wastewater within the retention time of 16 days. The simulation of the simplified microbial biofilm growth model provides the results to validate the experimental data. However, the comparable profiles have a nonlinear phenomenon, such as the data deviation in substrate concentration and hydrogen production rate. The stoichiometric reaction and kinetics affect the behavior of the substrate concentration profile. In addition, the bioelectrochemical factors also affect the hydrogen production rate profile. The artificial neural network (ANN) predicts the experimental hydrogen production rate according to the input of pH of the catholyte at controlled applied potential of 0.8 V and current density of 0.632 $A \cdot m^{-2}$. The convex method assists the model in finding the optimal input values that lead to the minimum mean square error (MSE) between modelling and experimental data. Evaluation of the COD removal efficiency, coulombic efficiency, and energy efficiency determines the process limit of the model MEC. At an optimum applied potential of 0.45 V, anode surface area of 0.06 m^2, anodic chamber volume of 5.2 L, and initial substrate concentration of 2,476.14 $mg \cdot L^{-1}$, the MEC model reached maximum steady-state percentage at 100.0% of COD removal efficiency, 50.0% of Coulombic efficiency, and 7.8% of energy efficiency.

Keywords: Biohydrogen, microbial electrolysis cell, biofilm growth, artificial neural network, mathematical model, optimization

1.0 INTRODUCTION

A microbial electrolysis cell (MEC) is an integrated fermentation redox reactor for the production of hydrogen from a variety of organic wastewaters with very low energy input [1–6]. However, current performance has not yet reached the point where it can be realized on a large scale [7]. The anaerobic environment of the anodic chamber could prevent the MEC from producing oxygen gas and electricity to ensure that hydrogen gas is the final product in the cathodic chamber [1, 2, 6]. Adopting a dual-chamber configuration could effectively minimize the tendency for methane emissions during the microbial reaction [8]. The excellent energy efficiency of sago wastewater as a substrate in MEC processes has been scientifically demonstrated [9], which is due to its typical composition with high sugar content. Otherwise, direct discharge without proper treatment may negatively affect the aquatic ecosystem of the river, especially by changing the pH of the water and groundwater quality [10–13].

The bioelectrochemical reaction of hydrogen from fermentation of wastewater, also known as substrate in MEC [2], is subject to nonlinearity, and the interactions for several variables are complex [14]. All these complexities could be related to the fact that the variation of dynamic bacterial activity causes the nonlinear effect of biohydrogen production [3]. The modeling technique seems promising to overcome the existing limitations of experimental analysis [3, 4, 15].

The dynamic phenomena of the bioelectrochemical process in the MEC have been critically analyzed in many studies using a simplified model of microbial biofilm growth based on the assumptions of Pinto et al. [16]. Statistical analysis of MEC processing of sago mill wastewater substrate to hydrogen gas using response surface methodology (RSM) has been reported previously [17]. However, nonlinearity occurred in laboratory runs of batch MEC fed sago wastewater in 16 retention days. This was related to the significant deviation between the experimental data and the comparable results from the simulated mathematical model. Substrate concentration was measured by the COD of the anolyte. The hydrogen production rate was indicated by the pH drop of the catholyte.

The variation of the input values of the stochiometric reaction and kinetics parameters and the changes in the initial values of the state variables had a significant effect on the substrate concentration profile [6, 18], and these uncertainty parameters could not be adjusted or controlled in the experiment. On the other hand, the perturbation value of the applied potential has a direct effects on the hydrogen production rate [14]. The underestimation of the hydrogen production profile in certain process time intervals is indirectly influenced by the stochiometric reaction and kinetic factors that affect the MEC current with respect to the microbial equilibrium concentrations [19]. As far as the authors are aware, no optimization of the model has been performed in the literature to minimize the data variance of substrate concentration and hydrogen production rate due to the aforementioned nonlinear interactions of the various input factors.

Unlike the substrate concentration data, the hydrogen production rate data were measured in pH values that require unit conversion. The relationship between catholyte pH and hydrogen production rate with multivariate effects of current density and applied potential [20] was complex to correlate, but it is possible to do so with the application of artificial intelligence algorithms capable of deriving a mathematical equation from artificial neural networks (ANN) data learning.

The main objective of the research is to improve the validity and reliability of the simplified biofilm growth model for the purpose of optimizing the laboratory MEC process for biohydrogen production from sago wastewater. MATLAB (R2022a software license number: 40774331) was accessed to achieve the following sub-objectives: (i) to validate the mathematical modeling results of the substrate concentration profile and hydrogen production rate profile using the data from the MEC experiment on biohydrogen production from sago wastewater substrate, and (ii) to determine the process limit of MEC by maximizing the reactor efficiency using convex nonlinear optimization as the objective function for the validated mathematical model.

The stoichiometric reaction and kinetics parameters in the simplified biofilm growth model [16] that are considered in the optimization include the maximum consumption rates, half-rate Monod kinetic constants, maximum growth rates, and decay rates. Microorganisms such as fermentative bacteria, acetoclastic methanogenic bacteria, electroactive bacteria, and hydrogenotrophic methanogenic bacteria are assumed to be present in the biofilm system. The maximum attainable biomass concentration on the biofilm was defined for the outer anodic layer, the inner anodic layer, and the cathodic layer.

The bioelectrochemical balance parameters considered in the optimization included current density, applied potential, counter electromotive force for the MEC, maximum resistance, minimum resistance, curve steepness constant, cathode efficiency, and yield rate for the hydrogenotrophic methanogenic bacteria.

Levenberg-Marquardt (LM) is a preferred training algorithm, although it requires more memory than the other options, as reported in the previous ANN modeling study of the biohydrogen fermentation process [21, 22]. Therefore, the LM algorithm was used in the iterative ANN data training to identify the optimal nodes for the single hidden layer. The topology consists of three input nodes (catholyte pH, current density, and applied potential) and one output node (hydrogen production rate).

The use of experimental data is focused on validating the simulation results of the simplified microbial biofilm growth model. The process domains of MEC considered in this study are as follows: (i) a double chamber reactor configuration with a proton exchange membrane as the hydrogen-proton junction; (ii) using as substrate a wastewater sample from a local sago processing mill in Mukah, Sarawak, Malaysia; and (iii) the applied potential ($E_{applied}$) in the range of 0.1 to 0.8 V [1, 23, 24]. The bioelectrochemical efficiencies such as COD removal efficiency, coulombic efficiency, and energy efficiency [25] were used to evaluate the process limit of the model MEC.

2.0 METHODOLOGY

2.1 Source of Experimental Data

In the mathematical modeling study, the experimental data are needed to improve the reliability and validity of the results before they can be used to optimize the MEC process. The data were obtained from the results of a MEC experiment. Briefly, a laboratory-scale dual-chamber MEC was developed consisting of a proton exchange membrane made of pretreated ALDRICH