Journal of Bioscience and Bioengineering
VOL. xx No. xx, 1–8, 2018
www.elsevier.com/locate/jbiosc

Predictive modelling of chromium removal using multiple linear and nonlinear regression with special emphasis on operating parameters of bioelectrochemical reactor

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Received 5 December 2017; accepted 18 February 2018
Available online xxx

Bioelectrochemical system (BES) is a novel, self-sustaining metal removal technology functioning on the utilization of chemical energy of organic matter with the help of microorganisms. Experimental trials of two chambered BES reactor were conducted with varying substrate concentration using sodium acetate (500 mg/L to 2000 mg/L COD) and different initial chromium concentration (Cr_i) (10–100 mg/L) at different cathode pH (1–7). In the current study mathematical models based on Multiple linear regression (MLR) and Non-linear regression (NLR) approach were developed using laboratory experimental data for determining Chromium removal efficiency (CRE) in the cathode chamber of BES. Substrate concentration, rate of substrate consumption, Cr_i, pH, temperature (temp.) and Hydraulic retention time (HRT) were the operating process parameters of the reactor considered for development of the proposed models. MLR showed a better correlation coefficient (0.972) as compared to NLR (0.952). Validation of the models using t-test analysis revealed unbiasedness of both the models, with t critical value (2.04) greater than t-calculated values for MLR (−0.708) and NLR (−0.86). The root-mean-square error (RMSE) for MLR and NLR were 5.06 % and 7.45 %, respectively. Comparison between both models suggested MLR to be best suited model for predicting the chromium removal behavior using the BES technology to specify a set of operating conditions for BES. Modelling the behavior of CRE will be helpful for scale up of BES technology at industrial level.

[**Key words:** Bioelectrochemical system; Mathematical model; Chromium removal efficiency; Multiple linear regression; Non-linear regression]

Globally, scientists and researchers are working on different methods of metal removal from wastewater due to the growing concern of water usage and water pollution caused by industrial discharge. Henceforth, treatment of wastewater is of prime importance to avoid environmental and economic loss. Chromium contamination in the water and wastewater is found to be toxic for flora and fauna and can cause mutagenic changes in humans and led to teratogenicity in infants (1–3). Considering the widespread application of chromium and its booming economics, it is of industrial importance. To reduce environmental toxicity and utilize economic advantages of chromium, its removal from industrial wastewater is of major significance. Industrial practices of chromium removal from wastewater majorly include chemical precipitation and membrane technologies with rare use of phytoremediation and adsorption (4–8). Unfortunately, conventional metal removal technologies deal with constraints on the use of high energy, chemical consumption, generation and disposal of hazardous wastes.

In recent times, researchers are interested in BESs such as microbial fuel cells (MFCs) and microbial electrolysis cells (MECs) for chromium removal. MFC is used for hexavalent chromium removal from electroplating wastewater along with electricity generation (9,10). Plant-microbial fuel cell (PMFC) is an another variant of BES being developed for electricity generation and chromium remediation from wastewater or soil using biodegradation of plant root exudates, rhizodeposits and other organic matter (11). Use of biocathodes for Cr (VI) removal using *Shewanella oneidensis* MR-1 microbial culture in the cathode chamber and lactate as substrate in the anode chamber have increased the flexibility of MFC applications (12). Studies for improved efficiency of chromium removal and bioelectricity production are being carried, considering the effect of carbon-based materials with graphite fibers, graphite felt and graphite granules equipped with tubular MFCs (13).

BES is a combination of biological, physico-chemical and electrochemical processes which overcomes the drawbacks of existing metal removal technologies (14–22). The technology functions on the energy produced due to degradation of substrate by the catalytic breakdown of organic matter with the help of microorganisms to produce electrons in the anode chamber. BES converts chemical energy stored in organic matter to electrical energy via a cascade of redox reactions mediated by microbial metabolism in the anode chamber. This electrical energy produced using oxidation of organic matter is the driving force of BES working. The system utilizes this energy to drive the electrochemical process. The produced electrons in the anode chamber generate a potential difference

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https://doi.org/10.1016/j.jbiosc.2018.02.013

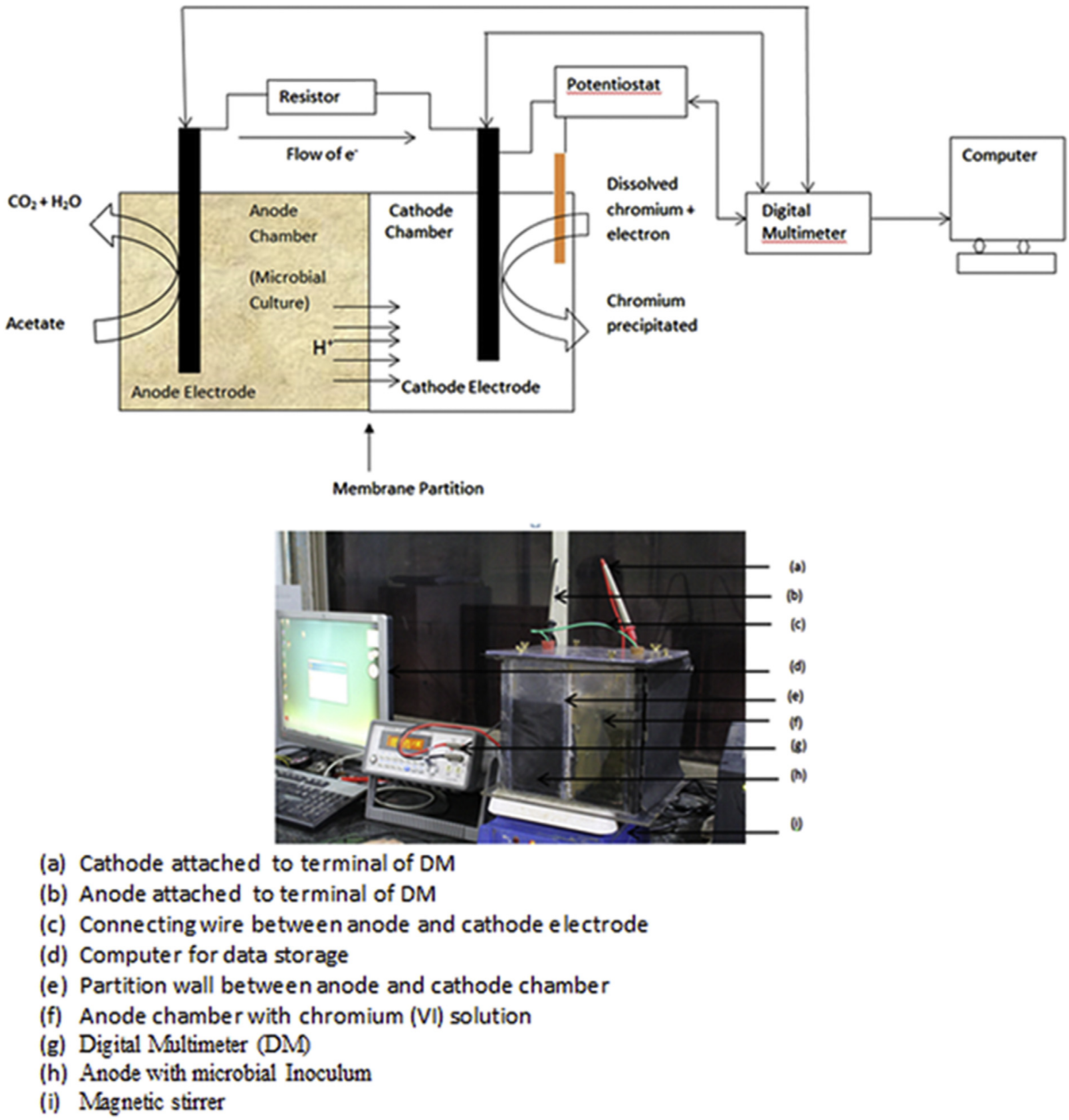

FIG. 1. Schematic diagram and experimental setup of BES.

between the two electrodes. This potential difference is the motivating power required for removal of metal ions in BES. The metal ions in the cathode chamber serve as a terminal electron acceptor (TEA) (23–27). The produced electrons in the anode chamber are responsible for the reduction of metal ions in the cathode chamber of BES reactor. The major factor responsible for faster reduction of metal ions is dependent on strong electron acceptor condition (i.e., High redox potential). The higher redox potential of metal ions than the redox potential of standard hydrogen potential is a favourable thermodynamic condition for metal reduction. The BES is made up of two chambers, the anode and the cathode chamber with electrodes in the respective chambers. The added substrate is degraded by microorganisms in the anode chamber as given in Eq. (1), which describes the breakdown of acetate and production of electrons. These electrons are transferred to cathode chamber and the chromium ions are precipitated into chromium hydroxide as shown in Eqs. (2,3).

$$CH_3COO^- + 4H_2O \rightarrow 2HCO_3^- + 9H^+ + 8e^- \quad \text{At Anode} \qquad (1)$$

$$Cr_2O_7^{2-} + 14H^+ + 6e^- \rightarrow 2Cr^{3+} + 7H_2O \quad \text{At cathode} \qquad (2)$$

$$2Cr^{3+} + 7H_2O \rightarrow 2Cr(OH)_{3(s)} + 6H^+ + H_2O \quad \text{pH Range} = 6.5 \text{ to } 10 \qquad (3)$$

Operational parameters of BES study include a substrate, its type and concentration, the consumption rate of organic matter, metal concentration, HRT, pH and temperature of the reactor. It is observed that substrate, its type and concentration, determine the amount of electrons that are generated (28–30). Temperatures below 25°C and above 40°C range have a detrimental effect on growth of microorganism and thus decrease microbial efficiency in