Modeling Bioelectrochemical Systems for Waste Water Treatment and Bioenergy Recovery with COMSOL Multiphysics®

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Abstract

Background and Relevance

Most conventional wastewater treatment processes are quite energy intensive. The global wastewater production is increasing due to an increase in population, industrialization, and urbanization. Thus, there is an urgent need to develop energy-efficient wastewater treatment technologies. Moreover, waste streams (industrial and domestic) have drawn renewed interests as resource for water, energy, and product recovery.

Bioelectrochemical systems (BES) are based on the typical electrochemical systems (which convert chemical to electrical energy or vice versa) with the inclusion of microbes, serving as catalysts in transferring electrons to/from external electron acceptors (electrodes).

They present a unique potential to utilize waste streams to treat wastewater and produce energy, as well as to provide a renewable source for many important chemicals.

However, we are still a long way from commercial implementations of BES. A key challenge is the poor understanding of the complex phenomena involved.

The focus of this work is to perform a model-based technical evaluation of the different BES scenarios for (waste)water treatment as well as to enhance the understanding of the basic chemical, biological, and physical phenomena (especially the mechanisms of extracellular electron transfer and the ecology of the microbial communities) that are critical for the performance of BES using COMSOL Multiphysics®.

Use of COMSOL Multiphysics: Figure 1 illustrates the COMSOL-based framework that will be used for this study.

First, the model structure is defined in Excel® and the microbial characteristics are coded in MATLAB®. Then, the model structure validation and parameter calibration are performed in COMSOL using the electrochemistry module (and experimental data from literature). The model structure is modified until an acceptable form is obtained. Different configurations and reactor

designs of BES for wastewater treatment, chemical, and energy production can then be evaluated.

Results: This study will produce a generalized model that:
a. Elucidates non-trivial interactions between the physical, chemical, and biological variables involved.
b. Provides a systematic and reproducible framework for parameter identification for BES.
c. Suitable for control design studies, scale-up strategies, and biorefinery applications.

Figure 2 shows one of the expected results. It represents a snapshot of a microbial electrosynthesis cell in which multiple bio-catalyzed reactions are occurring. Butyrate and acetate are reduced to ethanol and butanol in the cathode. Such figures would be helpful in selecting the optimum operating electrode voltages.

Conclusions: This work will be very important step towards the commercialization of BES for different applications. The model structure produced can be used to perform technical evaluations of BES applications including wastewater treatment, industrial chemical production (using microbes), water desalination, and bioremediation.

Figures used in the abstract

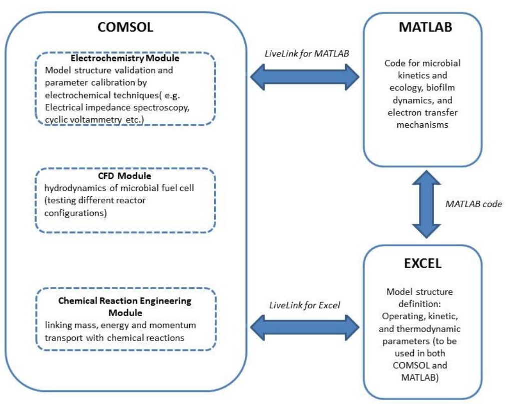

Figure 1: Framework for investigating bioelectrochemical systems using COMSOL Multiphysics.

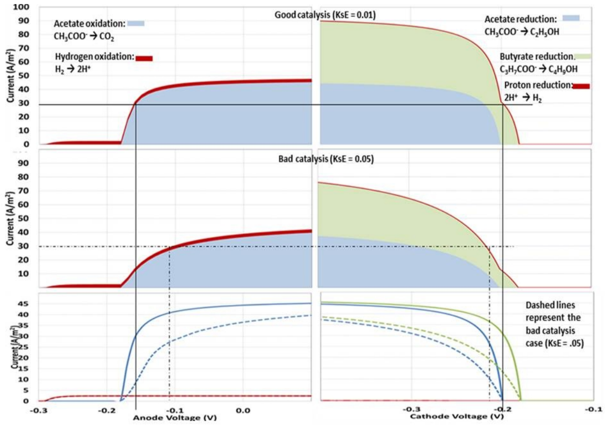

Figure 2: Comparison of potentials and individual current contributions for the simultaneous oxidations of acetate and hydrogen (anode) and reductions of butyrate, acetate and protons (cathode) at two different electrode catalysis efficiencies (KsE = 0.01 and 0.05). Arbitrary fixed cathode and anode bulk liquid concentrations of 0.1M of butyrate and acetate; 0.3mM for dissolved hydrogen and pH 5 are used.