



Constructing COMSOL Models of a Bacteriological Fuel Cell

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Introduction

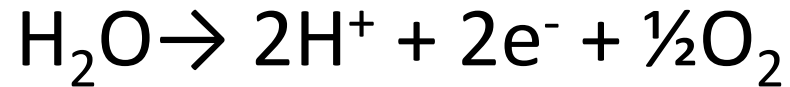
- NASA is pioneering new approaches for future human missions beyond Earth orbit.
- All spacecraft systems must be minimized with respect to mass, power, and volume.
- Space Synthetic Biology (SSB) seeks cutting-edge Synthetic Biology (SB) tools to redefine tradespaces.
- Here, we show very initial work on a specific bioelectrochemical system (BES), a bacteriologically driven 'fuel cell' (BFS), that is intended to process waste products, such as CO₂ and brine.
 - Processing is the priority, not power generation
 - Really a Microbial Electrolysis Cell (MEC)

Space Bacteriological Fuel Cell

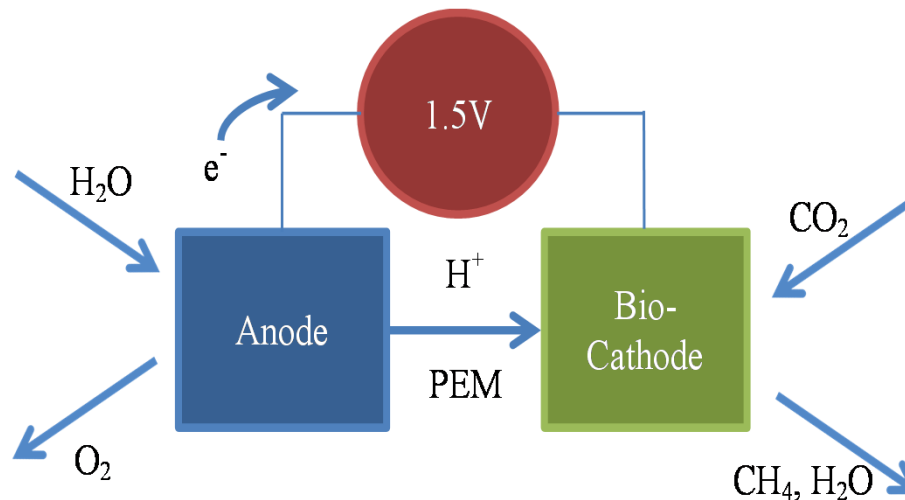
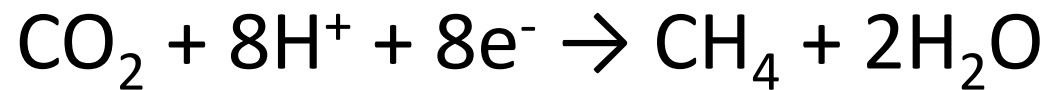
- High reaction rates with low-energy substrates
- Increased efficiency
- No costly precious metal catalysts
- Mild operating temperature and pressure
- Flexibility in reactants
- Need to add nutrients
- Need to minimize hydrogen peroxide
- Need to maximize contact of low-solubility gases in liquid compartments without gravity

Notional Reactants

- Anode: water oxidation



- Cathode: carbon dioxide reduction to methane



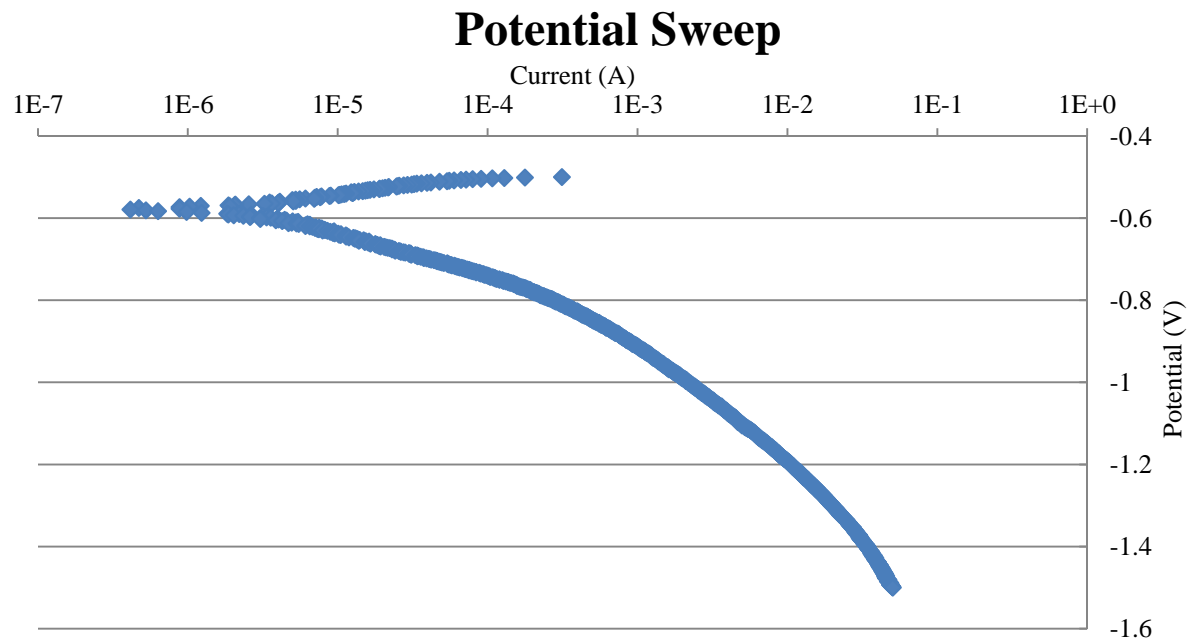
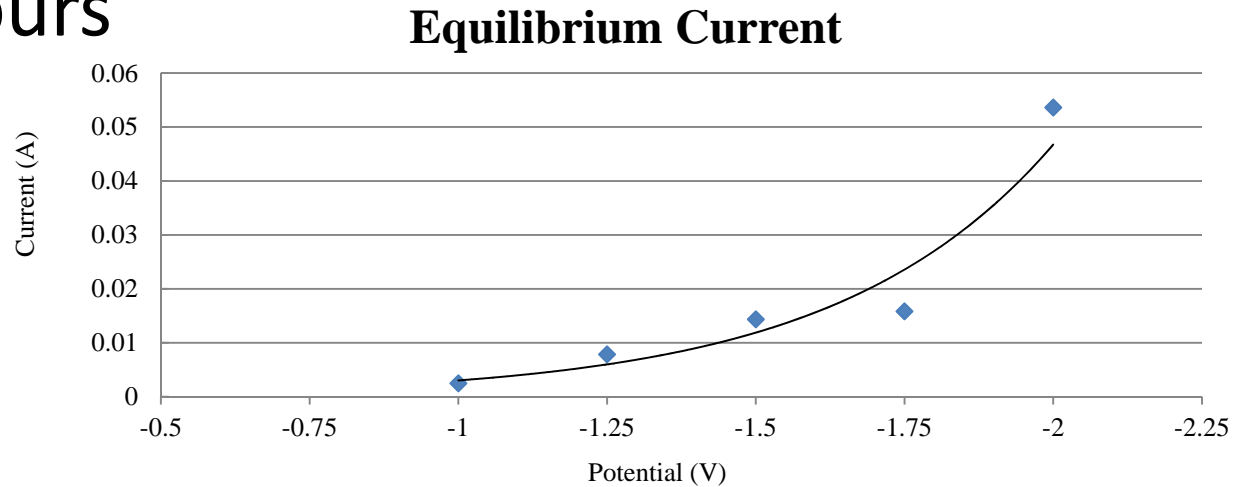
Initial Experimental Setup

- Abiotic testing first
- Nafion PEM separating flasks
- Appropriate salts
- Graphite rod (A)
carbon paper (C)
- pH buffered



First Results

- Runs are 4 hours
- Current generated by hydrogen
- Cathode potential sweep shows production behavior over large voltage ranges

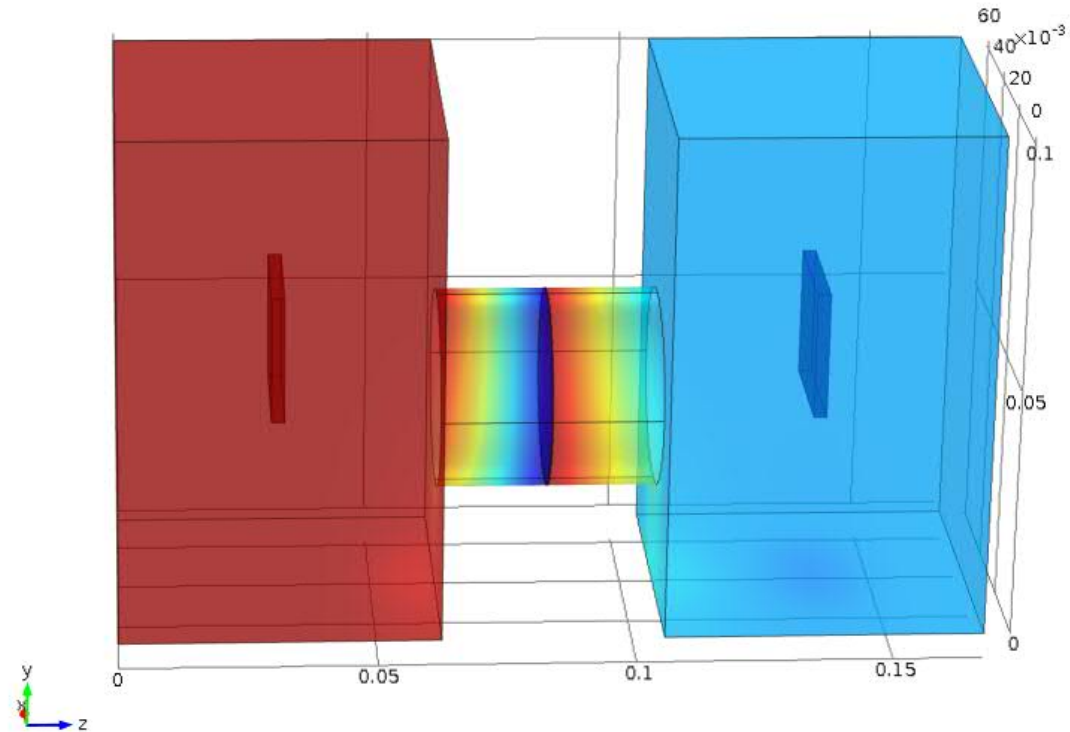


Comsol Model Description

- Physics nodes
 - Secondary Current Distribution
 - Two electrolyte-electrode boundary interfaces with reactions
 - Transport of Diluted Species
 - Convection, diffusion, and migration
 - Two electrode-electrolyte interface couplings
 - Flux boundary across PEM (set by SIEC)
- Simplified Geometry
- Just Hydrolysis for now
- Problem: need to track pH

Comsol Model Description

- The devil is in the details:
 - BCs
 - Signs
 - Low concentrations
 - Initial conditions



Summary

- *Just* starting to use Comsol for SynBio problems
- Variety of numerical stability issues
- Need to understand how Comsol does currents and reactions