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A DYNAMIC 2D MATHEMATICAL MODEL FOR TUBULAR-AIR CATHODE MICROBIAL FUEL CELLS USING CONDUCTION-BASED APPROACH FOR ELECTRONS TRANSFER TO THE BIOFILM AND VOLATILE FATTY ACIDS AS SUBSTRATE

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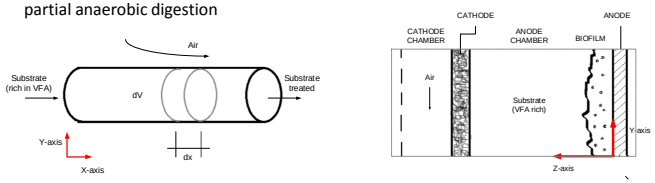
MOTIVATION

- The MFC to be modelled is a spirally wound MFC, which is similar to a single chamber tubular air-cathode cell. No practical models for tubular MFCs morphology - > Need of a new model
- The substrate considered for the MFC is a Volatile Fatty Acids mixture coming from a partial anaerobic digestion



Schematic section of the modelled MFC; Figure 6b schematic representation of the MFC as a plug flow reactor.

- **OBJECTIVE: Calculate the electrical current and voltage generated under different operational conditions considering spatial variations within the biofilm layer and across the tubular MFC**

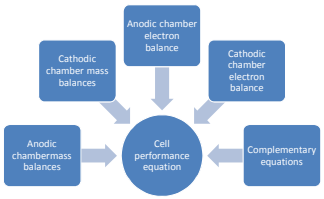
MAIN ASSUMPTIONS

- The MFC feedstock will flow along the x-axis. Components variations along y-axis will be considered as negligible. The biofilm grows along the z-axis perpendicular to the anode surface
- No added mediator to the anolyte => the **electrons transfer mechanism is conduction**
- The **anodic chamber of the MFC will be modelled as a plug flow reactor**
- For the **cathodic chamber**, oxygen concentration gradients in the air-side of the MFC will be considered negligible, thus **a CSTR approach will be followed**
- Part of the biomass will suffer an inactivation process (cells death, decomposition...) and will stop consuming substrate. As for the active biomass, a mixed microbial population, including methanogenic and anodophilic organisms will be considered. The MB will be able to transform acetate into methane and the EAB will produce electrons by reducing the feedstock carbon source. Both communities will produce electrons through respiration. Hence, the **biofilm will be a wild type mixed culture including bacteria competing for the resources**. No hydrolytic, acidogenic bacteria and acetogenic bacteria will be considered
- As for the VFA, the following composition is expected: acetate, propionate, butyrate, valerate and caproicate, but only **acetate, propionate and butyrate will be considered as substrate**, i.e. carbon source according to literature

THEORETICAL MODEL

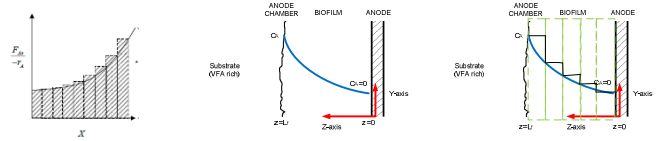
- Biofilm matrix is a conductor characterized by the **biofilm conductivity, k_{bio}** (mS cm^{-1}).
- Use of **volumetric coefficient** ($ø_i$, inactive biomass volumetric coefficient, dimensionless; $ø_a$, active biomass volumetric coefficient, dimensionless).)
- Use of a parameter (σ_i where i= EAB_A (acetate), EAB_P (propionate) and/or EAB_B (butyrate), dimensionless) aimed to implement the **selectivity of the biomass culture** as for the different VFAs

PROCESSES			
j	Description	Reaction	Place
1	Acetate oxidation by EAB	$CH_3COO^- + 4H_2O \rightarrow 2HCO_3^- + 9H^+ + 8e^-$	Anode
2	Propionate oxidation by EAB	$CH_3CH_2COO^- + 7H_2O \rightarrow 3HCO_3^- + 16H^+ + 14e^-$	Anode
3	Butyrate oxidation by EAB	$CH_3CH_2CH_2COO^- + 10H_2O \rightarrow 4HCO_3^- + 28H^+ + 20e^-$	Anode
4	EAB Inactivation process	---	Anode
5	EAB Respiration process	---	Anode
6	Acetate consumption by MB	$CH_3COO^- + H_2O \rightarrow CH_4 + HCO_3^-$	Anode
7	MB Inactivation process	---	Anode
8	MB Respiration process	---	Anode
9	Oxygen reduction	$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$	Cathode
10	Biofilm formation and retention of EAB	---	Anode
11	Biofilm formation and retention of MB	---	Anode
12	Biofilm erosion of EAB	---	Anode
13	Biofilm erosion of MB	---	Anode



MODEL IMPLEMENTATION

- **Matlab implementation -> Simplification needed -> Model discretisation** -> Change to a dimensionless and time-discreet model
- **Space variables discretisation: Finite Volume Method** i.e. the plug flow approach can be implemented as multiple CSTR (both for the anodic chamber and the biofilm)
- **Time discretisation: Zero Order Hold Approach**



Reactor volumes for multiple CSTRs in series and comparison with Plug flow approach for the anodic chamber and the biofilm layer.

- Model being currently validated with experimental data coming from an air-cathode MFC operation using as substrate a VFA misture coming from partial anaerobic digestión of wastewater sludge

FUTURE STEPS AND RESEARCH LINES

- Final model validation with more experimental data and sensitivity analysis
- Use of substrate in an elementary basis (C, H, O, N composition) in line with ADM1 approach

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