Supplementary Information

Performance Evaluation of a Continuous-flow Bioanode Microbial Electrolysis Cell Fed with Furanic and Phenolic Compounds

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Text: S1– S2

Figures: S1 – S2

Pages: 5

Text S1. Calculations

1. Coulombic Efficiency

The Coulombic efficiency (CE) was calculated as follows:

$$CE = \frac{\frac{I}{F}}{\frac{V_a}{HRT}\frac{(sCOD_{inf} - sCOD_{eff})}{8}} \quad (S1)$$

where I is the steady-state current (mA) and F is the Faraday constant (96485 C/mol). V_a is the anode liquid volume (0.2 L) and HRT is the hydraulic retention time (h). $sCOD_{inf}$ and $sCOD_{eff}$ are the influent and effluent soluble COD concentrations during stable operation (mg/L). The factor of 8 is for the conversion from g COD to mol e^-.

2. Energy Efficiency

(1) Electrical energy efficiency (η_e) is defined as follows:

$$\eta_e = \frac{W_{H_2}}{W_e} \quad (S2)$$

where W_{H_2} is the H_2 energy recovery rate (J/s),

$$W_{H_2} = -\Delta H Q_{H_2} \quad (S3)$$

where ΔH is the higher heating value of H_2, -285.8 kJ/mol,[1] and Q_{H_2} is the H_2 production rate during stable operation (mmol/d).

W_e is the electrical energy input rate (J/s),

$$W_e = IU \quad (S4)$$

where I is the steady-state current (mA) and U is the applied voltage (V).

(2) Overall energy efficiency (η_{e+s}) is defined as follows:

$$\eta_{e+s} = \frac{W_{H_2}}{W_e + W_s} \quad (S5)$$

where W_{H_2} and W_e are calculated as described above, and W_s is substrate energy input rate (J/s) defined as follows:

$$W_s = \frac{V_a}{HRT}\left(sCOD_{inf} - sCOD_{eff}\right)\Delta H_s \quad (S6)$$

where V_a, HRT, $sCOD_{inf}$ and $sCOD_{eff}$ are as defined above, ΔH_s is estimated heat of combustion of COD (14.7 kJ/g COD).[2]

3. Biomass Yield Coefficient

The observed yield coefficient (Y_{obs}) is defined as follows:

$$Y_{obs} = \frac{\Delta X_{total}}{\Delta sCOD} \quad (S7)$$

where ΔX_{total} is the total biomass COD (g/L), and $\Delta sCOD$ is soluble COD removed (g/L)

ΔX_{total} is calculated from the protein concentration as follows:

$$\Delta X_{total} = 1.42 \frac{\Delta P_{biofilm} + \Delta P_{planktonic}}{0.55} \quad (S8)$$

where 0.55 is the mass fraction of protein in *E.coli* cell , and 1.42 is the COD equivalent of biomass based on the empirical formula of $C_5H_7O_2N$.[3] $\Delta P_{biofilm}$ and $\Delta P_{planktonic}$ are biofilm protein accumulation and planktonic protein collected in the effluent, respectively, over a period of stable operation (d), calculated as follows :

$$\Delta P_{biofilm} = P_{biofilm,t} - P_{biofilm,t_0} \quad (S9)$$

$$\Delta P_{planktonic} = \frac{P_{planktonic,t}}{HRT}(t - t_0) \quad (S10)$$

where $P_{biofilm,t}$ the biofilm protein concentration (mg/L) measured at time t, and $P_{biofilm,t_0}$ is the biofilm protein concentration measured at a previous time t_0. $P_{planktonic,t}$ is planktonic protein concentration measured at time t, and ($t - t_0$) is the operational duration (d). All protein concentrations are normalized to the anode liquid volume.

$\Delta sCOD$ is cumulative COD removed during the operational period (d), calculated as follows:

$$\Delta sCOD = \frac{sCOD_{inf} - sCOD_{eff}}{HRT}(t - t_0) \quad (S11)$$

where $sCOD_{inf}$ and $sCOD_{eff}$ are the influent and effluent soluble COD concentrations (mg/L).

Text S2. Fate of the parent compounds in abiotic control assays

In the abiotic assays at both 0.6 and 1.0 V, on average, 13% and 22% of 5-hydroxymethyl furfural and furfural, respectively, diffused to the catholyte through the ion exchange membrane in 7 days. Another 20% and 40% of HMF and FF, respectively, was transformed presumably through electrochemical reactions. The detected products were 2,5-bis(hydroxymethyl)furan and furoic acid, consistent with our previous study.[4] In comparison, the phenolic compounds were more stable, with more than 74% of syringic acid and 95% of vanillic and 4-hydroxybenzoic acid remaining in the anolyte at both 0.6 and 1.0 V. None of the five compounds was detected in the catholyte with an active bioanode even at open circuit (Fig. S2). The transformation rate of the five parent compounds was also considerably faster in the bioanode with an open circuit (i.e., fermentative condition) than in the abiotic anode with a closed circuit. Thus, the observed increase in current production with the bioactive MEC was not associated with any abiotic electrochemical reactions triggered by the increase of voltage from 0.6 to 1.0 V.

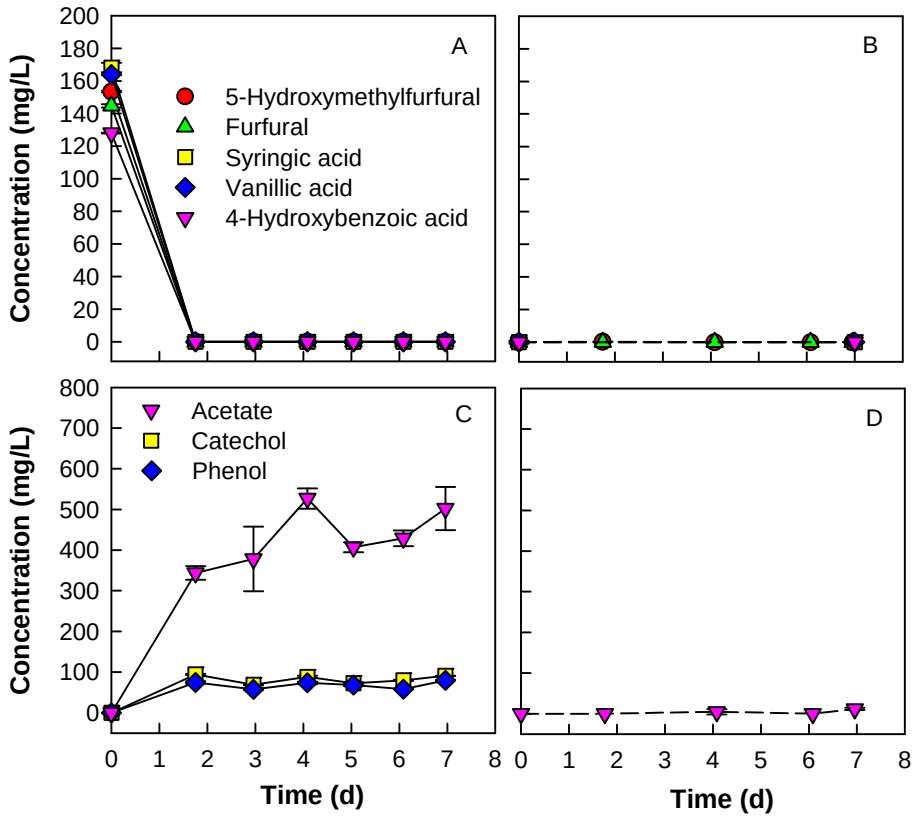

Fig. S1. Concentration of the five parent compounds (A, anode; B, cathode) and detected metabolites (C, anode; D, cathode) during an open circuit batch assay. Error bars represent mean values ± one standard deviation, $n = 2$.

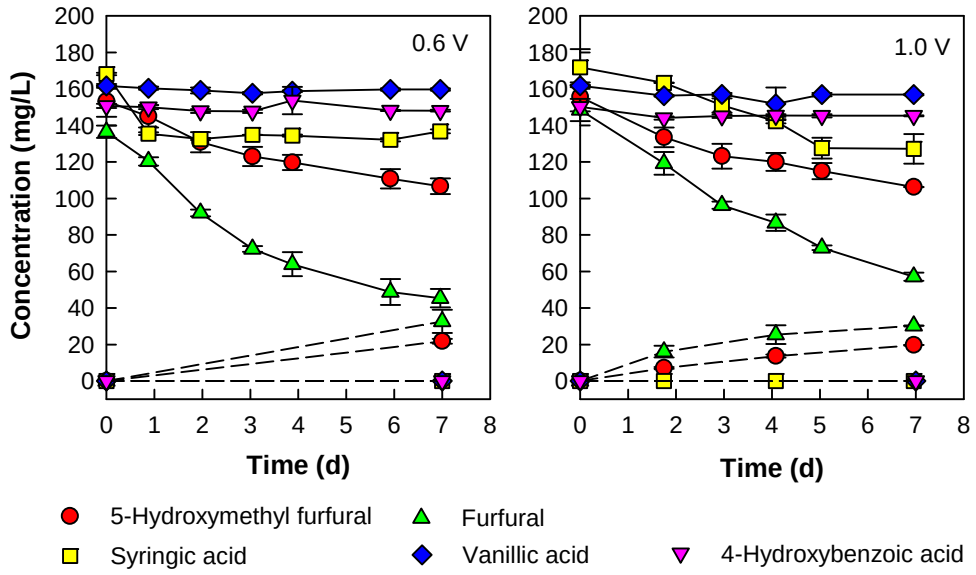

Fig. S2. Concentration of the furanic and phenolic compounds in anode (solid lines) and cathode (dashed lines) during the abiotic batch assays conducted at 0.6 V and 1.0 V. Error bars represent mean values ± one standard deviation, $n = 2$.

References

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