Supplementary Information

Powering lignocellulose biorefineries with solar energy – A critical review with furfural as a case study

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Kinetics contribution calculations

The relation between applied potential and current in an electrochemical redox reaction can be described by the Butler-Volmer equation:

$$j = j_0 \cdot [exp\left(\frac{\alpha nF}{RT}(E - E_{eq})\right) - exp\left(- \frac{(1 - \alpha)nF}{RT}(E - E_{eq})\right)]$$

Where j is the current density (A.m^{-2}), j_0 is the exchange current density (A.m^{-2}), α is the charge transfer coefficient, n the number of electrons exchanged during the reaction, F the faraday constant, R the gas constant (J.K^{-1}.mol^{-1}), T temperature (K), E the applied potential (V) and E_{eq} the equilibrium potential (V).

When the applied potential is sufficiently far away from the equilibrium potential, the equation can be simplified by its anodic or anodic contribution (depending on the direction of the potential shift):

$$j_{an} = j_0 \cdot \exp\left(\frac{\alpha nF}{RT}\eta\right)$$

$$j_{cath} = j_0 \cdot exp(\frac{(1 - \alpha)nF}{RT}\eta)$$

where $\eta = |E - E_{eq}|$

This simplified equation, once rearranged, is analogous in form to the Tafel equation[1]:

$$\eta = \frac{RT}{n\alpha F}\ln\left(\frac{j}{j_0}\right)$$

Ohmic losses η_Ω (V) are associated with internal resistance (comprising the membrane) on a surface of 1 cm² and calculated using the following formula:

$$\eta_\Omega = R_{int} \cdot j$$

With R_{int} the internal resistance (Ω) and j the current density (A.cm^{-2}).

Reactor cost contribution to Levelized Cost of Conversion estimation

1- In Viar *et al.*[2], their liquid-phase process for furfuryl alcohol (FOH) synthesis from furfural costs an Equivalent Annual Operating Cost (EAOC) of 25 572 853 $.yr^{-1}. The resulting Minimum Selling Price (MSP) is 1347 $.t$_{FOH}^{-1}$.
CAPEX costs once annualized represent 2 860 317 $.yr^{-1}. Costs associated to the "reaction section" account for 38% of the total, so they weigh 1 086 920 $.yr^{-1}. Costs associated to the reactor are thus $\frac{1\ 086\ 920}{25\ 572\ 853} = 4.25\%$ of the MSP so $1347 * \frac{4.25}{100} = 57.25\ \$.t_{FOH}^{-1}$.

2- Li *et al.* showed in their study of a conceptual plant producing tetrahydrofurfuryl alcohol by furfural hydrogenation[3]. Tetrahydrofurfuryl alcohol was deemed as a close enough molecule to FOH to use this study in our estimate. The reactor cost represents 17.32% of the CAPEX. Once annualized, CAPEX represents 11.08% of the annual costs. The Levelized Production Cost being 1855.85 $.t$_{THFA}^{-1}$, the reactor cost represents $0.1732 * 0.1108 * 1855.85 = 35.61\ \$.t_{THFA}^{-1}$

We chose the mean value of those two studies for our calculations and assumed reactor costs for 2MF were similar to those for FOH synthesis: $\frac{57.25 + 35.61}{2} = 46.5\ \$.t_{FOH/2MF}^{-1}$

Table S1. Parameters of the kinetic model

Parameter	Description	Units	Value	Reference
E°(H_2O/O_2)	Standard potential for OER	V vs SHE	1.23	
E°(FF/FOH)	Standard potential for furfural to furfuryl alcohol reduction	V vs SHE	0.19	[4]
E°(FF/2MF)	Standard potential for furfural to 2-methylfuran reduction	V vs SHE	0.13	[4]
n_{FOH}	Number of exchanged electrons for FOH synthesis	/	2	
n_{2MF}	Number of exchanged electrons for 2MF synthesis	/	4	
n_{OER}	Number of exchanged electrons during OER	/	4	
$j_{0,FOH}$	Exchange current density	$A.cm^{-2}$	3.50e-11	[5]
$j_{0,2MF}$	Exchange current density	$A.cm^{-2}$	4.76e-14	[5]
$j_{0,OER}$	Exchange current density	$A.cm^{-2}$	1.88e-11	[6]
α	Transfer coefficient	/	0.5	[7]
R_{int}	Electrolyser internal resistance	Ω	0.5	[7]
R	Gas constant	$J.K^{-1}.mol^{-1}$	8.314	
T	Reaction temperature	K	298	
F	Faraday constant	$C.mol^{-1}$	96500	

Table S2. Parameters of the economic analysis (low & high estimates)

Parameters	Unit	Case 1 (PV)	Case 2 (PV+grid)	Case 3 (grid)	Reference
CAPEX electrolyser	\$/kW	1000-2000	1000-2000	1000-2000	[8]
LCOE	\$/MWh	31-46	31 (PV)/60-80 (grid)	60-80 (grid)	[9] (PV)
r (capital rate)	%	6	6	6	
n (project lifetime)	Years	20	20	20	
OPEX rate	% of CAPEX	5	5	5	
E, PV annual energy production used by electrolyser	kWh/kW_{el}	2775	2135	0	[10] (Case 2)
E, annual grid energy used by the electrolyser	kWh/kW_{el}	0	5963	7884	
Curtailment rate	%	25	0	0	
Conversion energy	$GJ/t_{FOH/2MF}$	4.38/12	4.38/12	4.38/12	

Parameters for electrolyser cost come from Shafiee and Schrag[8], PV annual production rate originates from NREL (2024 v2 Annual Technology Baseline Workbook 7-19-2024)[9], and PV LCOE from Lawrence Berkeley National Laboratory[10]. Base case is set as PV mean LCOE (46\$/MWh) while optimistic case includes tax returns (31\$/MWh).

SI references

1 T. Shinagawa, A. T. Garcia-Esparza and K. Takanabe, *Sci. Rep.*, 2015, **5**, 13801.

2 N. Viar, I. Agirre and I. Gandarias, *Chem. Eng. J.*, 2024, **480**, 147873.

3 Q. Li, T. U. Rao, Y. Uehara, H. Machida, Z. Huo and K. Norinaga, *ACS Sustain. Resour. Manag.*, 2024, **1**, 316–327.

4 S. K. Green, J. Lee, H. J. Kim, G. A. Tompsett, W. B. Kim and G. W. Huber, *Green Chem.*, 2013, **15**, 1869.

5 A. S. May, S. M. Watt and E. J. Biddinger, *React. Chem. Eng.*, 2021, **6**, 2075–2086.

6 Y. Lu, W. Wang and F. Xie, *J. Electroanal. Chem.*, 2020, **871**, 114281.

7 C. Rozain and P. Millet, *Electrochimica Acta*, 2014, **131**, 160–167.

8 R. T. Shafiee and D. P. Schrag, *Joule*, 2024, S2542435124004215.

9 Lawrence Berkeley National Laboratory Energy Markets and Policy Department, Utility-Scale Solar, 2024 Edition, 2024.

10 NREL, Electricity Annual Technology Baseline (ATB) Data Download, https://atb.nrel.gov/electricity/2024/data, (accessed 27th February 2025).