Version of Record at: https://doi.org/10.1021/acs.accounts.3c00098

Supporting Information

Turning Carbon Dioxide into Sustainable Food and Chemicals: How Electrosynthesized Acetate Is Paving the Way for Fermentation Innovation

Author list

Bradie S. Crandall[1], Sean Overa[1], Haeun Shin[1], Feng Jiao[1*]

Affiliations

[1]Center for Catalytic Science & Technology, Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE 19716, USA

[*]Corresponding author: jiao@udel.edu

Supplementary Discussion 1: Electrochemical acetate production model

The techno-economic simulation of electrochemical CO_2 reduction to acetate was performed using our previously published models.[1–4] To better capture the true cost of electrolysis, a few adjustments were made to the previous input parameters (Table S2). A numerical evaluation of the product price needed for a net present value of 0 at the end of the plant life was used to identify the electrochemical production cost of acetic acid. The modeled performance parameters and materials were based upon that which was experimentally demonstrated in our previous work (Table S3). The downstream separations which included distillation, acetate protonation, and electrolyte recovery were modeled in ASPEN Plus software with the Economic Analyzer plugin as described in our previous work.[3] The cost of the CO feed was based upon state-of-the-art high-temperature solid-oxide electrolyzer cell (SOEC) technology. The Topsoe SOEC for CO production was modeled at scale by incorporating published information on the system into our model for CO_2 electrolysis (Table S4). Once the entire model was completed including the high-temperature solid oxide CO_2 electrolysis, low-temperature CO electrolysis, and separation steps, the annualized return on investment (ROI) was determined across a spectrum of production costs and market prices (Equation S1):

$$Annualized\ ROI = \frac{Total\ Profit\ Generated\ Over\ Plant\ Lifespan}{Capital\ Cost\ Investment \times Plant\ Lifespan} \times 100\% \qquad \text{(Eq S1)}$$

Supplementary Discussion 2: Techno-economic assessment of electrochemical acetate as a fermentation carbon-source

Based upon the acetic acid production model, it was determined that electrochemical acetic acid can be produced at a cost of 0.32 USD kg^{-1}. The price of fermentation-grade glucose for use in

Version of Record at: https://doi.org/10.1021/acs.accounts.3c00098

industrial processes has been previously modeled at 0.40 USD kg^{-1}.[5] The cost per mol of carbon contained in a molecule of glucose and acetate could then be calculated operating under the assumption that a similar yield could be achieved with both carbon sources during fermentation. Based on this analysis, the cost per mol of carbon was determined to be 20% cheaper from acetate than glucose. The fraction of the total cost made up by the carbon source in industrial scale fermentation processes has been shown to be 77.8%.[6] Thus, it was determined that the use of acetate as a carbon source instead of glucose can yield a 15.6% lower production cost (Equation S2):

$$\frac{Cost\ of\ Carbon\ Source}{Total\ Process\ Cost} \times \frac{(Glucose\ Cost/mol\ C) - (Acetate\ Cost/mol\ C)}{Glucose\ Cost/mol\ C} \times 100\% = 15.56\% \qquad \text{(Eq S2)}$$

Table S1. Global market size and market price for example target chemicals produced via fermentation.

Chemical	Market Price (USD kg^{-1})	Source	Global Market Size (B USD)	Source
Sorbitol	0.8	7	1.25	8
Erythritol	3.0	9	0.20	10
Xylitol	3.0	11	0.36	12
Glycerol	3.0	13	2.6	14
2,3-Butanediol	2.5	15	0.07	16
Citric acid	4.0	17	1.75	18
Itaconic acid	1.8	19	0.12	20
Succininc Acid	2.5	15	0.13	21
Propionic Acid	1.8	22	1.6	23
Gluconic Acid	1.4	24	0.06	25
2-Phenylethanol	4.3	26	0.26	27
Cobalamin	30	28	0.31	29
Acetoin	40	15	0.25	30
Malic Acid	2.0	15	0.18	31
Fumaric Acid	1.5	15	0.67	32

Table S2. Input parameters for electrolyzer techno-economic assessment.

Parameter	Value	Source
Plant Production Scale	50,000 kg day^{-1}	[2]
Plant Lifetime	20 years	[2]
Income Tax Rate	38.9%	[2]
Nominal Interest Rate	3.7%	[33]
Balance of Plant	61% of electrolyzer capital cost	[2]
Maintenance Cost	2.5% of electrolyzer capital cost	[34]
Material Replacement Costs	40% of electrolyzer capital cost	[34]

Table S3. Performance parameters and material usage based upon state-of-the-art CO electrolysis.

Parameter	Value	Source
Cell Voltage	2.1 V	[3]
Faradaic Efficiency	65%	[3]
Current Density	300 mA cm^{-2}	[3]
Cathode Catalyst	500 mg Cu cm^{-2}	[3]
Anode Catalyst	2 mg Ni cm^{-2} / 1 mg Fe cm^{-2}	[3]
Copper Cost*	1.18 USD kg^{-1}	[35]
Nickel Cost*	2.49 USD kg^{-1}	[36]
Iron Cost*	0.07 USD kg^{-1}	[37]

*Bulk metal costs were determined by taking a 5-year average from 2015-2019.

Table S4. Topsoe SOEC techno-economic parameters.

Parameter	Value	Source
Energy Usage	6 kWh Nm^{-3}_{CO}	[38]
Power Usage	13 kW m^{-2}	[39]
CAPEX	1,250 USD kW^{-1}	[39]
Current Density	850 mA cm^{-2}	[39]
Cell Voltage	1.5 V	[39]
CO_2 Cost	35 USD ton^{-1}	[40]

References

(1) Jouny, M.; Luc, W.; Jiao, F. General Techno-Economic Analysis of CO_2 Electrolysis Systems. *Ind. Eng. Chem. Res.* **2018**, *57* (6), 2165–2177.

(2) Shin, H.; Hansen, K. U.; Jiao, F. Techno-Economic Assessment of Low-Temperature Carbon Dioxide Electrolysis. *Nat. Sustain.* **2021**, 1–10.

(3) Overa, S.; Crandall, B. S.; Shrimant, B.; Tian, D.; Ko, B. H.; Shin, H.; Bae, C.; Jiao, F. Enhancing Acetate Selectivity by Coupling Anodic Oxidation to Carbon Monoxide Electroreduction. *Nat. Catal.* **2022**, *5* (8), 738–745.

(4) Crandall, B. S.; Brix, T.; Weber, R. S.; Jiao, F. Techno-Economic Assessment of Green H_2 Carrier Supply Chains. *Energy and Fuels* **2022**.

(5) *Techno-Economic Analysis of New Fermentation Processes*, EuroBioRef Summer School, 2011, http://www.eurobioref.org/Summer_School/Lectures_Slides/day4/L09_T.Grotkjaer.pdf accessed 2023-02-07).

(6) Kwiatkowski, J. R.; McAloon, A. J.; Taylor, F.; Johnston, D. B. Modeling the Process and Costs of Fuel Ethanol Production by the Corn Dry-Grind Process. *Ind. Crops Prod.* **2006**, *23* (3), 288–296.

(7) *Sorbitol Prices*. Intratec, https://www.intratec.us/chemical-markets/sorbitol-price (accessed 2023-02-14).

(8) *Sorbitol Market Size, Share an Global Trend by Type (Liquid/Syrupy and Powder/Crystal), Application (Food & Beverages, Personal Care & Cosmetics, Pharmaceuticals, and Others), and Geography Forecast 2019-2026, Fortune Business Insights*, https://www.fortunebusinessinsights.com/industry-reports/sorbitol-market-100206 (accessed 2023-02-14).

(9) *Erythritol China Domestic Price*. Echemi, https://www.echemi.com/productsInformation/temppid160705007778-erythritol.html (accessed 2023-02-14).

(10) *Erythritol Market Size By Form (Powder, Granular), Application (Beverage, Bakery, Confectionery & Dairy Products, Personal Care, Pharamaceutical, Regional Outlook, Application Potential, Price Trends, Competitive Market Share & Forecase, 2020-2026*, Global Market Insights, https://www.gminsights.com/industry-analysis/erythritol-market (accessed 2023-02-14).

(11) *Xylitol China Domestic Price*, Echemi, https://www.echemi.com/productsInformation/temppid160705012013-xylitol.html (accessed 2023-02-14).

(12) *Xylitol Market Growth Analysis comes up with Highest CAGR Value Forecast 2023-2027*, Market Watch, https://www.marketwatch.com/press-release/xylitol-market-growth-analysis-comes-up-with-highest-cagr-value-forecast-2023-2027-92-pages-report-2022-12-12#:~:text=The%20global%20Xylitol%20market%20was,3.7%25%20during%202021%2D2026 (accessed 2023-02-14).

(13) *US Glycerol Prices*, Selina Wamucii, https://www.selinawamucii.com/insights/prices/united-states-of-america/glycerol/

(accessed 2023-02-14).
(14) *Glycerol Market Analysis By Source, By Type, By End Use, By Region And Segment Forecasts From 2020 To 2027*, Million Insights, https://www.millioninsights.com/industry-reports/glycerol-market (accessed 2023-02-14).
(15) Bruni, G. O.; Terrell, E. A Review on the Production of C4 Platform Chemicals from Biochemical Conversion of Sugar Crop Processing Products and By-Products. *Fermentation* **2022**, *8* (5).
(16) *Global 2,3-Butanediol Market Insights*, Forecast to 2025, Market Research, https://www.marketresearch.com/QYResearch-Group-v3531/Global-Butanediol-Insights-Forecast-12781642/ (acessed 2023-02-14).
(17) *U.S. - Citric Acid And Its Salts And Esters - Market Analysis, Forecast, Size, Trends And Insights*, Index Box, https://www.indexbox.io/blog/citric-acid-price-per-ton-august-2022/#:~:text=Citric%20Acid%20Price%20in%20America%20Averages%20%244%2C077%20per%20Ton,-U.S.%20Citric%20Acid (accessed 2023-02-14).
(18) *Global Citric Acid Market Size Analysis 2023 Profoundly determine New Revenue Generation Techniques, Strategies and Forecast 2027*, Market Watch, https://www.marketwatch.com/press-release/global-citric-acid-market-size-analysis-2023-profoundly-determine-new-revenue-generation-techniques-strategies-and-forecast-2027-2022-12-09#:~:text=The%20global%20Citric%20Acid%20market%20was%20valued%20at%20USD%201744.5,1.2%25%20during%202021%2D2026 (accessed 2023-02-14).
(19) De Carvalho, J. C.; Magalhães, A. I.; Soccol, C. R. Biobased Itaconic Acid Market and Research Trends-Is It Really a Promising Chemical? *Chim. Oggi/Chemistry Today* **2018**, *36* (4), 56–58.
(20) *Itaconic Acid Market Size And Forecast*, Verified Market Research, https://www.verifiedmarketresearch.com/product/itaconic-acid-market/#:~:text=Itaconic%20Acid%20Market%20was%20valued,3.79%25%20from%202019%20to%202026 (accessed 2023-02-14).
(21) *Succinic Acid Market by Type (Bio-Based Succinic Acid, Petro-Based Succinic Acid), End-Use Industry (Industrial, Food & Beverage, Coatings, Pharmaceutical), and Region (APAC, Europe, North America, South America, Middle East & Africa) – Forecast to 2023*, Markets and Markets, https://www.marketsandmarkets.com/Market-Reports/succinic-acid-market-402.html (accessed 2023-02-14).
(22) *Propionic Acid Price Trend and Forecast*, Chem Analyst, https://www.chemanalyst.com/Pricing-data/propionic-acid-1184 (accessed 2023-02-14).
(23) *Market value of propionic acid worldwide from 2015 to 2021, with a forecast for 2022 to 2029*, Statista, https://www.statista.com/statistics/1244417/global-market-value-propionic-acid/ (accessed 2023-02-14).
(24) *D-Gluconic Acid*, Pharma Compass, https://www.pharmacompass.com/price/d-gluconic-acid (accessed 2023-02-14).
(25) *Gluconic Acid Market Size By Application (Industrial [Agrochemical & fertilizers, Metal surface treatment, Textile], Beverages, Food [Confectionary, Dairy, Flavors, Instant food, Meat, Sauces & Dressings], Pharmaceutical, Personal care, Cleaners & Detergents), By*

Downstream Potential (Sodium Gluconate, Calcium Gluconate, Potassium Gluconate, Glucono Delta-Lactone, Industry Analysis Report, Regional Outlook, Application Potential, Price Trend, Competitive Market Share & Forecast, 2018 – 2024, Global Market Insights, https://www.gminsights.com/industry-analysis/gluconic-acid-market (accessed 2023-02-14).

(26) Mitri, S.; Koubaa, M.; Maroun, R. G.; Rossignol, T.; Nicaud, J. M.; Louka, N. Bioproduction of 2-Phenylethanol through Yeast Fermentation on Synthetic Media and on Agro-Industrial Waste and By-Products: A Review. *Foods* **2022**, *11* (1).

(27) *2-Phenylethanol Market Size By Product (Synthetic, Natural), By Application (Cosmetics & Personal Care, Laundry & Home Care, Food & Beverages, Pharmaceuticals), Industry Analysis Report, Regional Outlook, Application Development Potential, Price Trend, Covid-19 Impact Analysis, Competitive Market Share & Forecast, 2022 – 2028*, Global Market Insights, https://www.gminsights.com/industry-analysis/2-phenylethanol-market (accessed 2023-02-14).

(28) *Vitamin Monthly Report*, Vega, 2021. https://www.vegapharma.com/uploads/20210630/Vitamin%20Market%20Report%20June%202021-VEGA.pdf

(29) *Global Vitamin B12 (Cobalamin, Cyanocobalamin) Market Size is expected to reach a value of USD 400 Million by 2028*, Digital Journal, https://www.digitaljournal.com/pr/global-vitamin-b12-cobalamin-cyanocobalamin-market-size-is-expected-to-reach-a-value-of-usd-400-million-by-2028-cagr-3-1 (accessed 2023-02-14).

(30) Petrov, K.; Petrova, P. Current Advances in Microbial Production of Acetoin and 2,3-Butanediol by Bacillus Spp. *Fermentation* **2021**, *7* (4), 1–24.

(31) *Malic Acid Market Size, Share & Trends Analysis Report By End Use (Beverages, Confectionery & Food, Personal Care & Cosmetics), By Region, And Segment Forecasts, 2019 – 2025*, Grand View Research, https://www.grandviewresearch.com/industry-analysis/malic-acid-market#:~:text=The%20global%20malic%20acid%20market,5.0%25%20over%20the%20forecast%20period (accessed 2024-02-14).

(32) *Fumaric Acid Market By Extraction Type, By Application (Food Additive, Rosin Paper Sizes, Unsaturated Polyester Resins (UPR), Alkyd Resins, Animal Feed, Others), And By End Use Industry, Forecasts To 2027*, Reports and Data, https://www.reportsanddata.com/report-detail/fumaric-acid-market (accessed 2023-02-14).

(33) *H2A: Hydrogen Analysis Production Models*, *Current Central Hydrogen Production from Polymer Electrolyte Membrane (PEM) Electrolysis (2019) version Nov 2020,* National Renewable Energy Laboratory, https://www.nrel.gov/hydrogen/h2a-production-models.html (accessed 2023-02-14).

(34) Sa, B. J.; Sa, W. C.; Sa, J. M.; Nrel, G. S. PEM Electrolysis H2A Production Case Study Documentation By : Authors ' Contact Information. **2013**, No. December, 1–27.

(35) *Copper*, Mining, https://www.mining.com/markets/commodity/copper/ (accessed 2023-02-14).

(36) *Nickel*, Mining, https://www.mining.com/markets/commodity/nickel/ (acccessed 2023-02-14).

(37) *Iron Ore Price Worldwide from September 2016 to December 2022*, Statista, https://www.statista.com/statistics/300419/monthly-iron-ore-prices/#:~:text=In%20November%202022%2C%20iron%20ore,month%20of%20the%20previous%20year (accessed 2023-02-14).
(38) *Produce Your Own Carbon Monoxide*, Topsoe, https://www.topsoe.com/processes/carbon-monoxide (accessed 2023-02-14).
(39) Ramdin, M.; De Mot, B.; Morrison, A. R. T.; Breugelmans, T.; Van Den Broeke, L. J. P.; Trusler, J. P. M.; Kortlever, R.; De Jong, W.; Moultos, O. A.; Xiao, P.; Webley, P. A.; Vlugt, T. J. H. Electroreduction of CO_2/CO to C2 Products: Process Modeling, Downstream Separation, System Integration, and Economic Analysis. *Ind. Eng. Chem. Res.* **2021**, *60* (49), 17862–17880.
(40) *Levelized Cost of CO_2 Capture by Sector and Initial CO_2 Concentration*, Internationalk Energy Agency, 2019, https://www.iea.org/data-and-statistics/charts/levelised-cost-of-co2-capture-by-sector-and-initial-co2-concentration-2019 (accessed 2023-02-14).