Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supplementary Information

Technical, economic, and environmental potential for glycerol hydrogenolysis: A roadmap towards sustainable green chemistry future

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Appendix 1:

The following is a description of the process flow of the work based on Figure 2:

a) Step 1: Collecting data based on our experimental work and previous studies, including catalyst preparation, experimental methodology, Aspen Plus configuration, battery limit of the work, and life-cycle function unit.

b) Step 2: Developing the process flow diagram for the proposed conceptual design based on the data obtained in Step 1.

c) Step 3: Performing techno-economic analysis to examine the economic feasibility of the plant.

d) Step 4: Conducting environmental analysis to examine the environmental factors of the plant.

e) Step 5: Validating the entire conceptual plant design through collaboration with industrial key partners from Asia and Oceania, such as senior process engineers and energy consultants.

f) Step 6: Benchmarking the conceptual plant design with other potential products from glycerol valorization to provide future outlooks for glycerol biorefinery.

Table S1. Parameters used for the development of the PSA model

Parameters	Remarks
Bed materials	Zeolite and activated carbon
Bed volume ratio (zeolite: activated carbon)	3:7
Total length of bed	4.8 m
Adsorption time	180 s
Interstitial velocity	0.45 m/s
Inlet temperature	298 K
Inlet pressure	6.5 bar

Table S2: Key parameters for the techno-economic assessment.

Economic parameter	Basis
Cost year for analysis	2021 (CEPCI 708)
Plant life	20 years
Operating hours (factor)	0.904 (7920 hours per year)
Plant schedule	One-year design, One-year construction, start production afterwards
Distribution of permanent investment (capital)	Construction year 50% 1st, 2nd production year 25% each
Plant decommissioning cost	$ 0
Depreciation rate	12%
Sales Tax	25%
Loan rate	6%
Inflation rate	1%
Capital cost (total permanent investment)	Lang factor: 3.63 Land: 3.80 of Total Depreciable Capital Plant start-up:10% Total Depreciable Capital Site preparation: 5% Total bare module cost Service facilities: 5% Total bare module cost Utility plants and related facilities: $300,000 Contingencies and Contractor fees: 20.0% of Direct Permanent Investment
Bare module factors	3.21% purchase equipment cost
Operating cost: Operations	Operators per shift: 24 operators with 3 shifts per day Direct wages and benefits: $40 /operator hour Direct salaries and benefits: 15% Direct wages and benefits
Operating cost: Maintenance	Wages and benefits: 4.5% of Total Depreciable Capital Salaries and benefits: 25.0% of maintenance wages and benefits (MWB) Materials and Services: 100.0% of maintenance wages

	and benefits Maintenance Overhead: 5.0% of maintenance wages and benefits
Operating cost: overhead	General plant overhead: 7.10% of maintenance and operations wages and benefits Mechanical department services: 2.40% of maintenance and operations wages and benefits Employee Relations Department: 5.90% of maintenance and operations wages and benefits Business services: 7.40% of maintenance and operations wages and benefits
Operating cost: Property taxes and insurance	2.0% of Total Depreciable Capital
Variable cost	Transfer expenses: 3.0% of Sales Direct research: 4.8% of Sales Allocated research: 0.5% of Sales Administrative expense: 2.0% of Sales Management Incentive Compensation: 1.3% of Sales

Table S3: Equipment cost for the proposed conceptual design.

Equipment unit	Cost (USD)
Reformer (R1)[a]	800,000
Reformer (R2)[a]	4,800,000
Hydrogenation reactor (R3)[a]	5,600,000
Heater (H1)	22,800
Heater (H2)	42,200
Heater (H3)	22,800
Mixer (M1)	8,300
Mixer (M2)	7,800
Mixer (M3)	8,100
Pressure swing adsorption (P1)[b]	3,300,000
Flash drum (F1)	21,000
Flash drum (F2)	21,000
Compressor (B1)	24,200
Compressor (B2)	28,500
Cooler (C1)	14,300
Cooler (C2)	10,500
Distillation column (D1)	1,723,000
Distillation column (D2)	1,723,000
Distillation column (D3)	1,723,000
Total cost	19,892,000

[a]Calculated based on the assumption of downward reformer using the basis of sixth-tenth rule output power, higher heating value, and flowrate of product

[b]Assuming the single bed PSA with length of 4.8m. The cost of PSA also includes

installation of vacuum pump