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Supporting information

Techno-Economic and Life Cycle Analyses of the Synthesis of a Platinum-Strontium Titanate Catalyst

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Section 1: Scaled-up production analysis

Table S1. Equipment list for the design process

Equipment type	Material of construction	Quantity	Specifications	Capacity (unit)	Purchased price/unit (USD)	Reference
Reactor (jacketed, agitated)	stainless steel	1	Volume	1.5 m^3	$162,405	CatCost[1]
Reactor (jacketed, agitated)	stainless steel	1	Volume	12 m^3	$455,836	CatCost[1]
Muffle Furnace	stainless steel	4	Duty	18 kW	$20,562	Across International[2]
Vacuum Oven	stainless steel	1	Internal volume	47.2 L	$19,473	Cascade TEK[3]
Solid-liquid Separator	stainless steel	1	Bowl volume	23 L	$275,968	Vendor[4]
Ozone Generator	carbon steel	1	Duty	25 kW	$275,000	Vendor[5]

Table S2. Materials used for 0.99 kg strontium titanate (STO) production

Reactant	Amount (kg)
Strontium hydroxide octahydrate	1.98
Acetic acid	2.33
Titanium tetrachloride	1.34
Ethanol	12.27
Sodium hydroxide	4.04
Nitrogen	7.47
Process water	44.67

Table S3. Materials used for 1 kg Pt/STO catalyst production

Reactant	Amount (kg)
Strontium titanate (STO)	0.99
Pentane	2.48
Toluene	10.30
Dodecane	2.97
Trimethyl(methyl-cyclopentadienyl) Platinum (IV)	0.01
Hydrogen gas	0.01
Nitrogen gas	1.27

Table S4. Utility consumption for the design process

Utility	Consumption (/kg catalyst)	Units
Process water	0.79	m^3
Electricity	26.73	kWh
Natural gas	29.19	MJ

Table S5. Raw materials, chemical, and utilities price list for the design process

Item	Unit	*Cost	Source
Strontium hydroxide octahydrate	$/kg	2.01	BLD pharm [6]
Acetic acid	$/kg	0.54	CatCost [1]
Titanium tetrachloride	$/kg	2.53	ChemAnalyst[7]
Ethanol	$/kg	1.10	Davis et al. [8]
Sodium hydroxide	$/kg	0.75	Davis et al. [9]
Process water	$/kg	0.0006	Davis et al. [8]
Toluene	$/kg	1.02	Davis et al. [8]
Dodecane	$/kg	3.81	BLD Pharm [6]
Pentane	$/kg	8.28	BVV [10]
Trimethyl(methylcyclopentadienyl)platinum(IV)	$/kg	70,000	Umicore [11]
Hydrogen gas	$/kg	2.26	Davis et al. [8]
Nitrogen gas	$/kg	0.02	Airgas [12]
Natural gas	$/MMBtu	4.39	U.S. EIA [13]
Electricity	$/kWh	0.085	U.S. EIA [14]

*Cost adjusted for the analysis basis year 2023.

Section 2: Techno-economic analysis methods

Table S6. TEA analysis factored capital expenditures

Item	Cost item	Cost factor [1]
1. Direct capital	• Purchased equipment (PE)	100% of PE
	• Installation	60% of PE
	• Instrumentation and controls	26% of PE
	• piping	31% of PE
	• Electrical	10% of PE
	• Buildings	29% of PE
	• Yard improvements	12% of PE
	• Service facilities	55% of PE
	• Waste treatment	5% of PE
	• Land	6% of PE
2. Indirect capital	• Engineering and supervision	32% of PE
	• Construction expenses	34% of PE
	• Legal expenses	4% of PE
	• Contractor’s fee	19% of PE
	• Contingency	37% of PE
3. Total fixed capital investment (FCI)	Direct capital cost + indirect capital cost	
Total capital investment (TCI)	FCI+ working capital (75% of PE)	

Table S7. TEA analysis factored operating expenditures

Item	Cost item	Cost factors [1]
1. Direct labor cost (DL)	• Direct labor operators	3 operators
	• Direct labor hours per year	26,280 hr/year
	• Direct labor rate	48 $/hr
2. Direct operating costs (LSM)	• Supervisory & clerical labor(L)	18% of DL
	• Laboratory charges	15% of DL
	• Maintenance & repair (M &R)	5% of FCI
	• Operating supplies (S)	15% of M&R
3. Fixed/ Indirect operating cost	• Local taxes	2.5% of FCI
	• Insurance	0.8% of FCI
	• Rent	10% of land value
	• Plant overhead	60% of LSM
General expenses	• Administration	20% of LSM
	• Distribution and marketing	10% of op. costs
	• Research and development	5% of op. costs

Table S8. Assumptions to estimate the spent catalyst value ($/kg)

Inputs	Base [1]
Metal to recover	Platinum (Pt)
Pt losses during use	4%
STO losses during use	2%
Metal losses during refining	2%

* % By default, the value from reference 1.

Section 3: Life-cycle analysis methods.

Table S9. Characteristics of the different electricity sources [15]

Source	U.S. average grid mix	California (CA) grid mix	Nuclear power	Wind energy
Residual oil	0.3%	-	-	-
Natural gas	38.5%	42.8%	-	-
Coal	20.6%	3.4%	-	-
Biomass	0.3%	0.9%	-	-
Nuclear	18.9%	8.3%	100%	-
Hydroelectric	6.8%	12.5%	-	-
Geothermal	0.4%	3.8%	-	-
Wind	10.7%	7.4%	-	100%
Solar PV	3.3%	20.3%	-	-
Other	0.4%	0.7%	-	-
GHG emissions	0.440	0.010	0.002	0.000

(kg CO_2e/kWh)

Section 4: Supplementary results for techno-economic analysis

Table S10. Estimation of the catalyst cost

Item		Cost ($/kg catalyst)
(Capital Costs (20-year plant life)	Fixed capital investment (FCI)	11.69
	Working capital	1.91
Total capital investment		**13.60**
2. Total operating costs		
	Raw materials	800.69
	Process utilities	2.90
	Labor, Supplies, Maintenance, Lab	80.55
	Taxes, Insurances Rent, Overhead	56.35
	General expenses	110.16
Total operating cost		**1,050.65**
3. Selling margin		67.99
Catalyst purchase cost		1,132.24
Spent catalyst cost (SCV)		290.45
Net catalyst cost		**842**

Solvent conditions	Catalyst cost ($/kg)	% Change from the baseline

Baseline (No recycling)	842	
Recycling (25%)	822	-2%
Recycling (50%)	803	-5%
Recycling (75%)	784	-7%

Table S11. Solvent recycling effect on the catalyst cost

Section 5: Supplementary results for life-cycle analysis

Table S12. Tabulated GHG emissions results from Figure 6 (kg CO_2e/kg catalyst)

Materials and energy sources	Baseline	Solvent recycling			Clean energy sources			Combined strategies
		25%	50%	75%	CA grid	Nuclear power	Wind energy	
Natural gas	2.0	2.3	2.6	3.0	2.0	2.0	2.0	2.6
Electricity	11.7	11.7	11.7	11.7	7.2	0.1	0.0	0.0
Sodium hydroxide	8.3	8.3	8.3	8.3	6.7	4.3	4.3	4.3
Platinum	1.3	1.3	1.3	1.3	1.3	1.3	1.3	1.3
Nitrogen	1.6	1.6	1.6	1.6	1.0	0.0	0.0	0.0
Hydrogen	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Strontium hydroxide octahydrate	3.7	3.7	3.7	3.7	3.5	3.1	3.1	3.1
Titanium tetrachloride	2.3	2.3	2.3	2.3	2.0	1.5	1.5	1.5
Acetic acid	1.3	1.3	1.3	1.3	1.2	1.0	1.0	1.0
Ethanol	18.0	13.5	9.0	4.5	17.4	16.5	16.5	8.2
Pentane	2.0	1.5	1.0	0.5	2.0	1.8	1.8	0.9
Toluene	10.7	8.0	5.4	2.7	10.7	10.6	10.6	5.3
Dodecane	2.4	1.8	1.2	0.6	2.3	2.2	2.2	1.1
Total	65.6	57.5	49.5	41.6	57.4	44.4	44.3	29.3

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