

Reconciling the Sustainable Manufacturing of Commodity Chemicals with Feasible Technoeconomic Outcomes: Supplementary Information

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Table S1: Typical calculation for calculation of required oxygen mass transfer coefficient (k_{LA}) based on Aspen HYSYS mass and energy balance.

Parameter	Value	Unit	Comments
Bioreactor Outlet oxygen concentration, $C_{g,off-gas}$	3.35	% (mol/mol)	
Design oxygen uptake rate, OUR	230	mmol O ₂ l ⁻¹ h ⁻¹	
Bioreactor headspace back-pressure, P_b	4	bara	
Loop reactor downcomer hydrostatic pressure, P_h	2.02	bar	Assumes a working volume of 80% (v/v) and a gas hold-up of 25% (v/v).
Inlet oxygen concentration, $C_{g,air}$	21	% (mol/mol)	
Inlet oxygen saturation in aqueous phase, $C_{L,air}$	1.00	mmol O ₂ l ⁻¹	Estimated using the Lee Kesler Plocker equation of state.
Outlet oxygen concentration, $C_{g,off-gas}$	3.35	% (mol/mol)	
Outlet oxygen saturation in aqueous phase, $C_{L,off-gas}$	0.26	mmol O ₂ l ⁻¹	Estimated using the Lee Kesler Plocker equation of state.
Broth dissolved oxygen concentration, DO	0	mmol O ₂ l ⁻¹	Micro-aerobic conditions.
Log mean concentration difference, $LMCD$	0.552	mmol O ₂ l ⁻¹	$\frac{(C_{L,air} - DO) - (C_{L,off-gas} - DO)}{\ln \frac{(C_{L,air} - DO)}{(C_{L,off-gas} - DO)}}$
Required oxygen mass transfer coefficient, k_{LA}	415	h ⁻¹	$\frac{OUR}{LMCD}$
Total ungasged broth volume, V	298	m ³	
Air Volumetric Flow Rate, Q	2927	m ³ h ⁻¹	Actual temperature and pressure.
Air superficial gas velocity, u_g	0.075	m s ⁻¹	
Power input to achieve required, k_{LA} (1)	450	kW	$\left(\frac{V}{1000}\right) \left(\frac{k_{LA}}{103 \cdot u_g^{0.824}}\right)^{\frac{1}{0.482}}$

Table S2: Capital cost estimation for the solvent plant using the NREL method.

Plant section	Major ISBL equipment item	Quantity	Purchase cost US\$	ISBL installed Cost Cran factor	Installed cost (2006) US\$	CE cost index adjustment to 2019 US\$	Location factor	Total installed cost US\$	Total plant section US\$	
Feedstock pre-treatment	SCWG thermal cycle									
	High pressure pump	1	86,721	2.30	199,459	242,342	0.51	123,369	21,548,182	
	Heat pump condenser	1	618,283	2.20	1,360,223	1,652,671		841,325		
	Heat pump compressor	1	1,566,961	1.60	2,507,138	3,046,173		1,550,715		
	SCWG recovery HE	1	602,795	2.20	1,326,148	1,611,270		820,249		
	SCWG plug flow reactor	1	417,687	1.50	626,531	761,235		387,522		
	Vapour heater	1	235,313	2.20	517,689	628,993		320,201		
	Heat pump recovery HE	1	272,464	2.20	599,420	728,296		370,754		
	Combustion heater	1	33,243	2.20	73,135	88,859		45,235		
	Supercritical heater	1	75,606	2.20	166,334	202,096		102,881		
	Turbo-expander	1	3,717,523	1.80	6,691,541	7,737,174		3,938,764		
	Air compression after cooler	1	7,281	2.20	16,018	19,462		9,908		
	H ₂ bioreactor cooler	1	241,164	2.20	530,561	644,631		328,163		
	Combustion									
	H ₂ combustion feed heater	1	26,928	2.20	59,242	71,979	36,643	0.51		
	Bioreactor off-gas combustion feed heater	1	22,629	2.20	49,783	60,487	30,792			
	Combustion chamber	1	2,072,893	1.80	3,731,208	4,533,418	2,307,827			
	Combustion turbine	1	9,281,863	1.80	16,707,353	20,299,434	10,333,834			
	Fermentation	Seed fermenters								
Seed fermenters		1	186,818	2.00	373,637	453,969	0.51	231,102		6,109,348
Seed fermenter recirculation pumps		1	24,809	2.30	57,060	69,328		35,293		
Seed fermenter HE		1	26,767	2.20	58,887	71,548		36,423		
Production fermenters										
Production fermenters		4	2,578,892	2.00	5,157,784	6,266,707	0.51	3,190,193		
Production fermenter recirculation pumps		4	516,321	2.30	1,187,539	1,442,860		734,517		
Production fermenter HE		4	788,587	2.20	1,734,891	2,107,892		1,073,065		
Centrifuge	4	817,228	1.60	1,307,565	1,588,692	808,755				
Product recovery from bioreactor aqueous and vapour	Absorption									
	Acetone stripper tower	1	125,436	2.40	301,047	365,772	0.51	186,204	1,853,509	
	Water stripper tower	1	106,657	2.40	255,977	311,012		158,327		
	Isopropanol pre-flash distillation tower									
	Pre-flash bottoms recovery heater	1	58,797	2.20	129,354	157,166	0.51	80,008		
	Pre-flash condensate recovery heater	1	8,196	2.20	18,031	21,908		11,153		
	Tower	1	206,398	2.40	495,355	601,857		306,387		
	Reboiler	1	12,468	2.20	27,429	33,326		16,965		
	Condenser	1	8,196	2.20	18,031	21,908		11,153		
	Isopropanol and acetone concentration distillation									
	Column feed heater	1	11,033	2.20	24,273	29,492	0.51	15,013		
	Tower	1	700,026	2.40	1,680,062	2,041,275		1,039,152		
	Reboiler	1	9,476	2.20	20,848	25,330		12,895		
Condenser	1	11,413	2.20	24,866	30,213	15,530				
Acetone product distillation										
Tower	1	180,458	2.40	433,099	526,216	0.51	267,881	685,795		
Reboiler	1	9,772	2.20	21,498	26,120		13,297			
Condenser	1	7,177	2.20	15,790	19,185		9,767			
Solvent distillation										
Pre-heater	1	7,180	2.20	15,797	19,193	0.51	9,771			
Tower	1	245,120	2.40	588,287	714,769		363,868			
Reboiler	1	7,225	2.20	15,895	19,313		9,832			
Condenser	1	8,364	2.20	18,400	22,356		11,381			
Low pressure swing distillation										
Feed condenser	1	7,901	2.20	17,383	21,120	0.51	10,752		1,539,261	
Tower	1	539,856	2.40	1,295,655	1,574,221		801,389			
Reboiler	1	7,179	2.20	15,794	19,190		9,769			
Condenser	1	11,597	2.20	25,513	30,998		15,780			
High pressure swing distillation										
First pre-heater	1	7,917	2.20	17,417	21,162	0.51	10,773			
Second pre-heater	1	7,400	2.20	16,280	19,780		10,070			
Tower	1	447,603	2.40	1,074,247	1,305,211		664,444			
Reboiler	1	11,968	2.20	26,329	31,990		16,285			
Steam and water management	Steam and water management									
	CO ₂ flash drum steam heater	1	33,438	2.20	73,564	89,380	0.51	45,501		785,217
	Steam mechanical vapour compressors	1	706,707	1.60	1,130,732	1,373,839		699,380		
	Water recycle to fermentation cooler	1	11,040	2.20	24,287	29,509		15,022		
	Water recycle to SCWG gasification	1	11,227	2.20	24,700	30,011		15,278		
	IPA cooler to absorber	1	7,376	2.20	16,227	19,716		10,037		

Table S3: Additional capital cost for the solvent plant associated with the NREL method.

Additional costs for determining Total Capital Investment (TCI)				
Item	Description	Unit (basis)	Annual cost US\$ year ⁻¹	Comments
Additional direct costs				
Warehouse	4	% of installed cost of ISBL equipment	1,300,852	On-site storage of equipment and supplies.
Site development	9	% of installed cost of ISBL equipment	2,926,918	Includes fencing, curbing, parking lot, roads, well drainage, rail system, soil borings, and general paving. This factor allows for minimum site development assuming a clear site with no unusual problems such as right-of-way, difficult land clearing, or unusual environmental problems.
Additional piping	5	% of installed cost of ISBL equipment	1,463,459	To connect ISBL equipment to storage and utilities outside the battery limits.
Indirect costs				
Pro-rateable costs	10	% of TDC	3,821,254	This includes fringe benefits, burdens, and insurance of the construction contractor.
Field expenses	10	% of TDC	3,821,254	Consumables, small tool and equipment rental, field services, temporary construction facilities, and field construction supervision.
Home office and construction	20	% of TDC	7,642,508	Engineering plus incidentals, purchasing, and construction.
Project contingency	10	% of TDC	3,821,254	Extra cash on hand for unforeseen issues during construction.
Other costs	10	% of TDC	3,821,254	Start-up and commissioning costs. Land, rights-of-way, permits, surveys, and fees. Piling, soil compaction/dewatering, unusual foundations. Sales, use, and other taxes. Freight, insurance in transit, and import duties on equipment, piping, steel, instrumentation, etc. Overtime pay during construction. Field insurance. Project team. Transportation equipment, bulk shipping containers, plant vehicles, etc.
TOTAL ADDITIONAL COSTS			28,618,754	

Table S4: Capital cost estimation for the solvent plant using the TS method.

Plant section	Major ISBL equipment item	Quantity	Purchase cost US\$	ISBL installed cost lang factor	Installed cost (2006) US\$	CE cost index adjustment to 2019 US\$	Location factor	Total installed cost US\$	Total plant section US\$				
SCWG thermal cycle													
Feedstock pre-treatment	High pressure pump	1	86,721	3.3	286,180	347,709	0.51	177,008	38,484,617				
	Heat pump condenser	1	618,283		2,040,334	2,479,006		1,261,988					
	Heat pump compressor	1	1,566,961		5,170,973	6,282,732		3,198,351					
	SCWG recovery HE	1	602,795		1,989,222	2,416,905		1,230,374					
	SCWG plug flow reactor	1	417,687		1,378,368	1,674,717		852,548					
	Vapour heater	1	235,313		776,534	943,489		480,302					
	Heat pump recovery HE	1	272,464		899,131	1,092,444		556,130					
	Combustion heater	1	33,243		109,703	133,289		67,853					
	Supercritical heater	1	75,606		249,501	303,144		154,321					
	Turbo-expander	1	3,717,523		12,267,826	14,184,819		7,221,067					
	Air compression after cooler	1	7,281		24,027	29,193		14,861					
	H ₂ bioreactor cooler	1	241,164		795,841	966,947		492,244					
	Combustion												
	H ₂ combustion feed heater	1	26,928		88,863	107,969		54,964					
Bioreactor off-gas combustion feed heater	1	22,629	74,675	90,730	46,188								
Combustion chamber	1	2,072,893	6,840,548	7,329,158	3,731,055								
Combustion turbine	1	9,281,863	30,630,148	37,215,629	18,945,362								
Seed fermenters													
Fermentation	Seed fermenters	1	186,818	3.3	616,501	749,048	0.51	381,318	10,081,936				
	Seed fermenter recirculation pumps	1	24,809		81,869	99,471		50,638					
	Seed fermenter HE	1	26,767		88,331	107,322		54,635					
	Production fermenters												
	Production fermenters	4	2,578,892		3.3	8,510,344		10,340,067		0.51	5,263,819		
	Production fermenter recirculation pumps	4	516,321			1,703,860		2,070,190			1,053,872		
Production fermenter HE	4	788,587	2,602,336	3,161,838		1,609,597							
Centrifuge	4	817,228	2,696,853	3,276,677		1,668,058							
Absorption													
Product recovery from bioreactor aqueous and vapour	Acetone stripper tower	1	125,909	3.3	415,498	504,830	0.51	256,994	2,568,914				
	Water stripper tower	1	106,671		352,014	427,697		217,728					
	Isopropanol pre-flash distillation tower												
	Pre-flash bottoms recovery heater	1	58,797	3.3	194,032	235,748	0.51	120,012					
	Pre-flash condensate recovery heater	1	8,196		27,047	32,862		16,729					
	Tower	1	206,398		681,113	827,553		421,282					
	Reboiler	1	12,468		41,144	49,990		25,448					
	Condenser	1	8,196		27,047	32,862		16,729					
	Isopropanol and acetone concentration distillation												
	Column feed heater	1	11,033	3.3	36,409	44,237	0.51	22,520					
	Tower	1	700,026		2,310,085	2,806,753		1,428,834					
	Reboiler	1	9,476		31,272	37,995		19,342					
	Condenser	1	11,413		37,663	45,760		23,295					
	Acetone product distillation												
Solvent recovery	Tower	1	180,458	3.3	595,512	723,546	0.51	368,336	949,723				
	Reboiler	1	9,772		32,247	39,180		19,945					
	Condenser	1	7,177		23,686	28,778		14,650					
	Solvent distillation												
	Pre-heater	1	7,180	3.3	23,695	28,789	0.51	14,656					
	Tower	1	245,120		808,895	982,807		500,318					
	Reboiler	1	7,225		23,843	28,969		14,747					
	Condenser	1	8,364		27,600	33,534		17,071					
Low pressure swing distillation													
Isopropanol pressure swing distillation	Feed condenser	1	7,901	3.3	26,074	31,680	0.51	16,127	2,125,662				
	Tower	1	539,856		1,781,526	2,164,554		1,101,910					
	Reboiler	1	7,179		23,691	28,785		14,654					
	Condenser	1	11,597		38,269	46,497		23,670					
	High pressure swing distillation												
	First pre-heater	1	7,917	3.3	26,126	31,743	0.51	16,159					
	Second pre-heater	1	7,400		24,420	29,671		15,104					
	Tower	1	447,603		1,477,090	1,794,665		913,610					
Reboiler	1	11,968	39,494		47,985	24,428							
Steam and water management													
Steam and water management	CO ₂ flash drum steam heater	1	33,438	3.3	110,346	134,070	0.51	68,251	1,571,228				
	Steam mechanical vapour compressors	1	706,707		2,332,134	2,833,543		1,442,472					
	Water recycle to fermentation cooler	1	11,040		36,430	44,263		22,533					
	Water recycle to SCWG gasification	1	11,227		37,051	45,016		22,916					
	IPA cooler to absorber	1	7,376		24,341	29,574		15,055					

Table S5: Capital cost estimation for the solvent plant using the Hand method.

Plant section	Major ISBL equipment item	Quantity	Purchase cost US\$	ISBL installed cost Hand factor	Installed cost (2006) US\$	CE cost index adjustment to 2019 US\$	Location factor	Total installed cost US\$	Total plant section US\$	
Feedstock pre-treatment	SCWG thermal cycle									
	High pressure pump	1	86,721	4.00	346,885	421,465	0.51	214,555	30,378,659	
	Heat pump condenser	1	618,283	3.50	2,163,991	2,629,249		1,338,472		
	Heat pump compressor	1	1,566,961	2.50	3,917,404	4,759,645		2,422,993		
	SCWG recovery HE	1	602,795	3.50	2,109,781	2,563,384		1,304,942		
	SCWG plug flow reactor	1	417,687	4.00	1,670,749	2,029,961		1,033,392		
	Vapour heater	1	235,313	3.50	823,597	1,000,670		509,411		
	Heat pump recovery HE	1	272,464	3.50	953,623	1,158,653		589,835		
	Combustion heater	1	33,243	3.50	116,351	141,367		71,966		
	Supercritical heater	1	75,606	3.50	264,622	321,516		163,674		
	Turbo-expander	1	3,717,523	2.50	9,293,807	10,746,075		5,470,505		
	Air compression after cooler	1	7,281	3.50	25,484	30,962		15,762		
	H ₂ bioreactor cooler	1	241,164	3.50	844,074	1,025,550		522,077		
	Combustion									
	H ₂ combustion feed heater	1	26,928	3.50	94,249	114,513	0.51	58,295		
	Bioreactor off-gas combustion feed heater	1	22,629	3.50	79,201	96,229		48,987		
Combustion chamber	1	2,072,893	2.00	4,145,786	4,441,914	2,261,245				
Combustion turbine	1	9,281,863	2.50	23,204,657	28,193,659	14,352,547				
Fermentation	Seed fermenters									
	Seed fermenters	1	186,818	4.00	747,274	907,937	0.51	462,204	11,210,164	
	Seed fermenter recirculation pumps	1	24,809	4.00	99,236	120,571		61,379		
	Seed fermenter HE	1	26,767	3.50	93,684	113,827		57,946		
	Production fermenters									
	Production fermenters	4	644,723	4.00	10,315,568	12,533,415	0.51	6,380,386		
	Production fermenter recirculation pumps	4	129,080	4.00	2,065,285	2,509,321		1,277,420		
	Production fermenter HE	4	197,147	3.50	2,760,053	3,353,465		1,707,148		
Centrifuge	4	204,307	2.50	2,043,071	2,482,331	1,263,680				
Product recovery from bioreactor aqueous and vapour	Absorption									
	Acetone stripper tower	1	125,909	4.00	503,634	611,916	0.51	311,508	3,076,854	
	Water stripper tower	1	106,671	4.00	426,684	518,421		263,913		
	Isopropanol pre-flash distillation tower									
	Pre-flash bottoms recovery heater	1	58,797	3.50	205,791	250,036	0.51	127,286		
	Pre-flash condensate recovery heater	1	8,196	3.50	28,686	34,854		17,743		
	Tower	1	206,398	4.00	825,592	1,003,094		510,645		
	Reboiler	1	12,468	3.50	43,637	53,019		26,991		
	Condenser	1	8,196	3.50	28,686	34,854		17,743		
	Isopropanol and acetone concentration distillation									
	Column feed heater	1	11,033	3.50	38,616	46,918	0.51	23,885		
	Tower	1	700,026	4.00	2,800,103	3,402,125		1,731,920		
Reboiler	1	9,476	3.50	33,167	40,298	20,514				
Condenser	1	11,413	3.50	39,946	48,534	24,707				
Solvent recovery	Acetone product distillation									
	Tower	1	180,458	4.00	721,832	877,026	0.51	446,468	1,138,897	
	Reboiler	1	9,772	3.50	34,201	41,555		21,154		
	Condenser	1	7,177	3.50	25,121	30,522		15,538		
	Solvent distillation									
	Pre-heater	1	7,180	3.50	25,131	30,534	0.51	15,544		
	Tower	1	245,120	4.00	980,479	1,191,282		606,446		
	Reboiler	1	7,225	3.50	25,288	30,725		15,641		
Condenser	1	8,364	3.50	29,272	35,566	18,106				
Isopropanol pressure swing distillation	Low pressure swing distillation									
	Feed condenser	1	7,901	3.50	27,655	33,600	0.51	17,105	2,559,872	
	Tower	1	539,856	4.00	2,159,425	2,623,702		1,335,648		
	Reboiler	1	7,179	3.50	25,127	30,530		15,542		
	Condenser	1	11,597	3.50	40,589	49,315		25,105		
	High pressure swing distillation									
	First pre-heater	1	7,917	3.50	27,709	33,666	0.51	17,139		
	Second pre-heater	1	7,400	3.50	25,900	31,469		16,020		
	Tower	1	447,603	4.00	1,790,412	2,175,351		1,107,406		
	Reboiler	1	11,968	3.50	41,887	50,893		25,908		
Steam and water management	Steam and water management									
	CO ₂ flash drum steam heater	1	33,438	3.50	117,033	142,195	0.51	72,387	1,229,341	
	Steam mechanical vapour compressors	1	706,707	2.50	1,766,768	2,146,623		1,092,782		
	Water recycle to fermentation cooler	1	11,040	3.50	38,638	46,946		23,899		
	Water recycle to SCWG gasification	1	11,227	3.50	39,296	47,745		24,305		
IPA cooler to absorber	1	7,376	3.50	25,816	31,367	15,968				

Table S6: Fixed operating cost for the solvent plant using the NREL method.

Labour and supervision	Salary US\$ (2020)	Number of personnel	Annual cost US\$ year ⁻¹
Plant manager	29,591	1	29,591
Plant engineer	29,977	1	29,977
Maintenance supervisor	20,406	1	20,406
Maintenance technician	14,968	3	44,903
Lab manager	21,569	1	21,569
Lab technician	14,619	1	14,619
Shift supervisor	15,267	4	61,067
Shift operators	13,373	12	160,470
Yard employees	6,184	4	24,735
Clerks and secretaries	11,488	3	34,464
TOTAL SALARIES			441,800
Labour burden	90% of total salaries		397,620
TOTAL LABOUR COST			839,421
Other overhead			Annual cost US\$ year⁻¹
Maintenance	3% of ISBL		975,639
Property insurance	0.7% of FCI		427,980
TOTAL FIXED OPERATING COST			2,243,040

Table S7: Fixed operating cost for the solvent plant using the TS method.

FIXED OPERATING COST			
Fixed operational consideration	Assessment basis	Unit (basis)	Annual cost US\$ year ⁻¹
Operating labour	Wage and salary cost for shift team members (excl. supervision)	13,373 US\$ operator ⁻¹ , 4 shift teams with 3 operators each	160,470
Supervisory labour	25	% of operating labour	40,118
Direct salary overhead	50	% of operating + supervisory	100,294
Maintenance	3	% of ISBL	1,673,462
Property taxes and insurance	1	% of ISBL	557,821
Rent of land/buildings	1	% of FCI	725,167
General plant overhead	65	% of total labour + maintenance	1,218,132
Allocated environmental charges	1	% of FCI	725,167
Interest charges (capital)	0	% of total capital investment	0
TOTAL FIXED OPERATING COST			5,200,631

Table S8: Fixed operating cost for the solvent plant using the Coulson and Richardson method.

Labour and supervision	Salary US\$ (2020)	Number of personnel	Annual cost US\$ year ⁻¹
Plant manager	29,591	1	29,591
Plant engineer	29,977	1	29,977
Maintenance supervisor	20,406	1	20,406
Maintenance technician	14,968	3	44,903
Lab manager	21,569	1	21,569
Lab technician	14,619	1	14,619
Shift supervisor	15,267	4	61,067
Shift operators	13,373	12	160,470
Yard employees	6,184	4	24,735
Clerks and secretaries	11,488	3	34,464
TOTAL OPERATING AND SUPERVISORY LABOUR COSTS			441,800
FIXED COSTS			
Fixed operational consideration	Assessment basis	Unit (basis)	Annual cost US\$ year ⁻¹
Maintenance	5	% of FCI	3,099,612
Operating labour			274,703
Laboratory costs	20	% operating labour	54,941
Supervisory labour	20	% operating labour	167,097
Plant overhead	50	% operating labour	137,352
Capital charges	10	% of FCI	0
Insurance	1	% of FCI	619,922
Local taxes	1	% of FCI	619,922
Royalties	1	% of FCI	0
FIXED COSTS			4,973,549
Sales expense	20	% of direct production costs	34,464
General overheads			
Research and development			
TOTAL FIXED OPERATING COSTS			5,008,013

Table S9: Investment analysis for the solvent plant using the Hand method for capital estimation and the TS method for fixed operating cost estimation.

Year	Project life	Detailed design	Fixed capital investment	Working capital	Fixed OPEX	Variable OPEX	Plant income	Depreciation	Corporation tax	Total cash flow	NPV	Cumulative NPV	Comments
		US\$	US\$	US\$	US\$	US\$	US\$	US\$	US\$	US\$	US\$	US\$	
2019	0	-250,000	0	0	0	0	0	0	0	-250,000	-250,000	-250,000	
2020	1	0	-44,262,454	0	0	0	0	0	0	-44,262,454	-40,238,595	-40,488,595	Plant construction and commissioning.
2021	2	0	-22,573,852	0	0	0	0	0	0	-22,573,852	-18,656,076	-59,144,670	
2022	3	0	0	6,578,665	-4,904,838	-798,965	35,292,066	-6,683,631	-5,726,158	30,440,770	22,870,601	-36,274,069	Year 0 for plant operation.
2023	4	0	0	0	-5,002,935	-814,945	35,292,066	-6,683,631	-5,697,639	23,776,548	16,239,702	-20,034,367	
2024	5	0	0	0	-5,102,993	-831,243	35,292,066	-6,683,631	-5,668,550	23,689,280	14,709,179	-5,325,188	
2025	6	0	0	0	-5,205,053	-847,868	35,292,066	-6,683,631	-5,638,879	23,600,266	13,321,735	7,996,547	
2026	7	0	0	0	-5,309,154	-864,826	35,292,066	-6,683,631	-5,608,614	23,509,472	12,064,077	20,060,624	
2027	8	0	0	0	-5,415,337	-882,122	35,292,066	-6,683,631	-5,577,744	23,416,863	10,924,139	30,984,763	
2028	9	0	0	0	-5,523,644	-899,765	35,292,066	-6,683,631	-5,546,257	23,322,401	9,890,975	40,875,738	
2029	10	0	0	0	-5,634,117	-917,760	35,292,066	-6,683,631	-5,514,140	23,226,050	8,954,648	49,830,385	
2030	11	0	0	0	-5,746,799	-936,115	35,292,066	-6,683,631	-5,481,380	23,127,771	8,106,143	57,936,528	
2031	12	0	0	0	-5,861,735	-954,837	35,292,066	-6,683,631	-5,447,966	23,027,528	7,337,280	65,273,808	
2032	13	0	0	0	-5,978,970	-973,934	35,292,066	0	-7,084,791	21,254,372	6,156,634	71,430,442	
2033	14	0	0	0	-6,098,549	-993,413	35,292,066	0	-7,050,026	21,150,078	5,569,477	76,999,919	
2034	15	0	0	0	-6,220,520	-1,013,281	35,292,066	0	-7,014,566	21,043,699	5,037,694	82,037,613	
2035	16	0	0	0	-6,344,931	-1,033,547	35,292,066	0	-6,978,397	20,935,192	4,556,108	86,593,721	
2036	17	0	0	0	-6,471,829	-1,054,218	35,292,066	0	-6,941,505	20,824,514	4,120,019	90,713,740	
2037	18	0	0	0	-6,601,266	-1,075,302	35,292,066	0	-6,903,875	20,711,624	3,725,168	94,438,907	
2038	19	0	0	0	-6,733,291	-1,096,808	35,292,066	0	-6,865,492	20,596,475	3,367,688	97,806,596	
2039	20	0	0	0	-6,867,957	-1,118,744	35,292,066	0	-6,826,341	20,479,024	3,044,076	100,850,672	
2040	21	0	0	0	-7,005,316	-1,141,119	35,292,066	0	-6,786,408	20,359,223	2,751,153	103,601,825	
2041	22	0	0	0	-7,145,422	-1,163,942	35,292,066	0	-6,745,676	20,237,027	2,486,037	106,087,863	
2042	23	0	0	0	-7,288,331	-1,187,220	35,292,066	0	-6,704,129	20,112,386	2,246,114	108,333,977	
2043	24	0	0	0	-7,434,097	-1,210,965	35,292,066	0	-6,661,751	19,985,253	2,029,015	110,362,992	
2044	25	0	0	0	-7,582,779	-1,235,184	35,292,066	0	-6,618,526	19,855,577	1,832,590	112,195,582	
2045	26	0	0	0	-7,734,435	-1,259,888	35,292,066	0	-6,574,436	19,723,307	1,654,893	113,850,475	
2046	27	0	0	-6,578,665	-7,889,124	-1,285,086	35,292,066	0	-6,529,464	13,009,727	992,352	114,842,827	

Table S10: Capital cost estimation for conventional renewable electricity generation using the Hand method.

Plant section	Major ISBL equipment item	Quantity	Purchase cost US\$	ISBL Installed cost Hand factor	Installed cost (2006) US\$	CE cost index adjustment to 2019 US\$	Location factor	Total installed cost US\$	Total plant section US\$
Electricity generation	Steam turbine	3	2,791,955	2.50	6,979,888	7,478,452	0.51	3,807,056	3,807,056

Table S11: Fixed operating cost estimation for conventional renewable electricity generation using the TS method.

FIXED OPERATING COST			
Fixed operational consideration	Assessment basis	Unit (basis)	Annual cost US\$ year ⁻¹
Operating labour	Wage and salary cost for shift team members (excl. supervision)	13,373 US\$ operator ⁻¹ , 4 shift teams with 3 operators each	13,373
Supervisory labour	25	% of operating labour	3,343
Direct salary overhead	50	% of operating + supervisory	8,358
Maintenance	3	% of ISBL	114,212
Property taxes and insurance	1	% of ISBL	38,071
Rent of land/buildings	1	% of FCI	47,588
General plant overhead	65	% of total labour + maintenance	85,103
Allocated environmental charges	1	% of FCI	47,588
Interest charges (capital)	0	% of total capital investment	0
TOTAL FIXED OPERATING COST			357,636

Table S12: Investment analysis for conventional renewable electricity generation using the Hand method for capital estimation and the TS method for fixed operating cost estimation.

Year	Project life	Detailed design	Fixed capital	Working capital	Fixed OPEX	Variable OPEX	Plant income	Depreciation	Corporation tax	Total cash flow	NPV	Cumulative NPV	Comments
		US\$	US\$	US\$	US\$	US\$	US\$	US\$	US\$	US\$	US\$	US\$	
2019	0	-25,000	0	0	0	0	0	0	0	-25,000	-25,000	-25,000	
2020	1	0	-3,397,797	0	0	0	0	0	0	-3,397,797	-3,088,907	-3,113,907	Plant construction and commissioning.
2021	2	0	-1,732,877	0	0	0	0	0	0	-1,732,877	-1,432,129	-4,546,036	
2022	3	0	0	505,010	-379,526	-864,501	14,972,100	-513,067	-3,303,751	10,929,331	8,211,368	3,665,332	
2023	4	0	0	0	-387,117	-881,791	14,972,100	-513,067	-3,297,531	10,405,661	7,107,206	10,772,538	
2024	5	0	0	0	-394,859	-899,427	14,972,100	-513,067	-3,291,187	10,386,627	6,449,278	17,221,817	
2025	6	0	0	0	-402,756	-917,415	14,972,100	-513,067	-3,284,715	10,367,213	5,852,021	23,073,838	
2026	7	0	0	0	-410,812	-935,763	14,972,100	-513,067	-3,278,114	10,347,410	5,309,858	28,383,696	
2027	8	0	0	0	-419,028	-954,479	14,972,100	-513,067	-3,271,381	10,327,212	4,817,720	33,201,416	
2028	9	0	0	0	-427,408	-973,568	14,972,100	-513,067	-3,264,514	10,306,609	4,371,008	37,572,425	
2029	10	0	0	0	-435,956	-993,040	14,972,100	-513,067	-3,257,509	10,285,594	3,965,542	41,537,967	
2030	11	0	0	0	-444,676	-1,012,900	14,972,100	-513,067	-3,250,364	10,264,160	3,597,525	45,135,492	
2031	12	0	0	0	-453,569	-1,033,158	14,972,100	-513,067	-3,243,076	10,242,296	3,263,511	48,399,003	
2032	13	0	0	0	-462,640	-1,053,822	14,972,100	0	-3,363,909	10,091,728	2,923,214	51,322,217	
2033	14	0	0	0	-471,893	-1,074,898	14,972,100	0	-3,356,327	10,068,981	2,651,477	53,973,695	
2034	15	0	0	0	-481,331	-1,096,396	14,972,100	0	-3,348,593	10,045,779	2,404,880	56,378,574	
2035	16	0	0	0	-490,958	-1,118,324	14,972,100	0	-3,340,704	10,022,113	2,181,104	58,559,678	
2036	17	0	0	0	-500,777	-1,140,690	14,972,100	0	-3,332,658	9,997,974	1,978,046	60,537,724	
2037	18	0	0	0	-510,792	-1,163,504	14,972,100	0	-3,324,451	9,973,352	1,793,795	62,331,519	
2038	19	0	0	0	-521,008	-1,186,774	14,972,100	0	-3,316,079	9,948,238	1,626,616	63,958,135	
2039	20	0	0	0	-531,428	-1,210,510	14,972,100	0	-3,307,540	9,922,621	1,474,934	65,433,070	
2040	21	0	0	0	-542,057	-1,234,720	14,972,100	0	-3,298,831	9,896,492	1,337,319	66,770,388	
2041	22	0	0	0	-552,898	-1,259,414	14,972,100	0	-3,289,947	9,869,840	1,212,470	67,982,859	
2042	23	0	0	0	-563,956	-1,284,603	14,972,100	0	-3,280,885	9,842,656	1,099,210	69,082,068	
2043	24	0	0	0	-575,235	-1,310,295	14,972,100	0	-3,271,642	9,814,927	996,466	70,078,535	
2044	25	0	0	0	-586,740	-1,336,501	14,972,100	0	-3,262,215	9,786,644	903,268	70,981,803	
2045	26	0	0	0	-598,475	-1,363,231	14,972,100	0	-3,252,599	9,757,796	818,732	71,800,535	
2046	27	0	0	-505,010	-610,444	-1,390,495	14,972,100	0	-3,242,790	9,223,360	703,537	72,504,072	

Table S13: Calculation of greenhouse gas emissions on cradle-to-gate basis for LanzaTech's anaerobic gas fermentation technology, producing acetone and ethanol.

Parameter	Value	Unit	Comment
Lower heating value for ethanol	26.70	MJ kg ⁻¹ _{ethanol}	Lower Heating Value (LHV).
Reported ethanol greenhouse gas (GHG) emissions	8.10	g _{CO2eq} MJ ⁻¹ _{ethanol}	Cradle-to-grave emissions.
Cradle-to-grave ethanol GHG emissions	0.22	kg _{CO2eq} kg ⁻¹ _{ethanol}	
Cradle-to-gate ethanol GHG emissions	-1.69	kg _{CO2eq} kg ⁻¹ _{ethanol}	Stoichiometry of ethanol combustion in excess O ₂ , forming two moles of CO ₂ .
Reported acetone GHG emissions	-2.07	kg _{CO2eq} kg ⁻¹ _{acetone}	Case A.
Cradle-to-gate GHG emissions for reported solvent mix.	-1.91	kg _{CO2eq} kg ⁻¹ _{acetone + ethanol}	Reported solvent mix, i.e. 57.3% acetone with balance ethanol on a mass basis.

References

1. L. A. H. Petersen, J. Villadsen, S. B. Jørgensen and K. V. Gernaey, *Biotechnol. Bioeng.*, 2017, **114**, (2), 344 LINK <https://doi.org/10.1002/bit.26084>