Supplementary information

A comparative life cycle analysis of electromicrobial production systems

Authors

Anthony J. Abel,[1,†] Jeremy D. Adams,[1,†] Douglas S. Clark[1,2,*]

Affiliations

1. Department of Chemical and Biomolecular Engineering, University of California, Berkeley, CA 94720, USA
2. Molecular Biophysics and Integrated Bioimaging Division, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA

[†]These authors contributed equally.
[*]Correspondence should be addressed to D.S.C (dsc@berkeley.edu)

Supplementary tables

Table S1. Base case model parameters

Parameter	Value	Units	References
Operating conditions			
P_{CO_2}	0.2	atm	--
D_{gas}	100	hr^{-1}	--
T	30 (*C. necator*)	°C	DSMZ
	35 (*S. ovata*)		DSMZ
	37 (*E. coli*)		DSMZ
Microbial growth			
C. necator (formatotrophy)			
$\mu_{max,opt}$	0.18	hr^{-1}	1
$Y'_{X/F,maz}$	0.169	mol mol^{-1}	1
$Y'_{L/F,maz}$	0.11	mol mol^{-1}	calculated
θ_F	75.11	mM	1
$K_{S,F}$	10	µM	2
K_{S,O_2}	2.5	µM	3
pH_{opt}	7	--	1
pH_{min}	4	--	4
pH_{max}	9	--	4
$c_{Na,min}$	0.2	M	5
$c_{Na,max}$	1.05	M	5
C. necator (hydrogenotrophy)			
$\mu_{max,opt}$	0.18	hr^{-1}	6
Y'_{X/H_2}	0.19	mol mol^{-1}	6
Y'_{L/H_2}	0.11	mol mol^{-1}	calculated
K_{S,H_2}	20.4	µM	7
K_{S,O_2}	2.5	µM	3

K_{S,CO_2}	9.38	μM	[7]
pH_{opt}	7	--	[1]
pH_{min}	4	--	[4]
pH_{max}	9	--	[4]
$c_{Na,min}$	0.2	M	[5]
$c_{Na,max}$	1.05	M	[5]
S. ovata (acetogenesis)			
$\mu_{max,opt}$	0.044	hr^{-1}	[8]
K_{S,H_2}	20	μM	[9]
K_{S,CO_2}	20	μM	[9]
n	0.47	--	[10]
pH_{opt}	7	--	[8]
pH_{min}	4	--	assumed
pH_{max}	9	--	assumed
$c_{Na,min}$	0.2	M	[5]
$c_{Na,max}$	1.05	M	[5]
E. coli (acetotrophy)			
$\mu_{max,opt}$	0.3	hr^{-1}	[11]
$Y'_{X/Ac}$	0.936	mol mol^{-1}	[11]
$Y'_{L/Ac}$	0.5	mol mol^{-1}	calculated
K_{S,O_2}	2.5	μM	[3]
$K_{S,Ac}$	10	μM	assumed
$K_{I,Ac}$	0.83	M	[12]
pH_{opt}	7	--	[11]
pH_{min}	4	--	[13–15]
pH_{max}	9.5	--	[13–15]
$c_{Na,min}$	0.2	M	[5]
$c_{Na,max}$	1.05	M	[5]
Acid/base reactions			
S_5	-71.0	J mol^{-1} K^{-1}	[16]
S_6	-92.4	J mol^{-1} K^{-1}	[16]
S_w	-80.66	J mol^{-1} K^{-1}	[16]
H_5	-0.12	kJ mol^{-1}	[16]
H_6	-0.4	kJ mol^{-1}	[16]
H_w	55.84	kJ mol^{-1}	[16]
K_7	1.38×10^{-4}	mol L^{-1}	[16]
k_{+1}	$\exp\left(1246.98 - \frac{6\times10^4}{T} - 183\ln(T)\right)$	s^{-1}	[17]
k_{+2}	59.44	s^{-1}	[17]
k_{+3}	2.23×10^3	L mol^{-1} s^{-1}	[17]
k_{+4}	6.0×10^9	L mol^{-1} s^{-1}	[17]
k_{+5}	10	s^{-1}	assumed
k_{+6}	10	s^{-1}	assumed
k_{+7}	10	s^{-1}	assumed
k_{+w}	2.4×10^{-5}	L mol^{-1} s^{-1}	[18]
Gas/liquid mass transfer			
$k_L a_{O_2}$	200	hr^{-1}	assumed
A_S	0.56	m^{-1}	assumed

Diffusion coefficients			
D_{CO_2}	$14.68 \times 10^{-9}\left(\frac{T}{217.206}-1\right)^{1.997}$	$m^2\ s^{-1}$	19
D_{H_2}	$\frac{2.290\times10^{-11}}{\mu^{0.819}}T$	$m^2\ s^{-1}$	2
D_{O_2}	$10\text{^}\left[-8.410+\frac{773.8}{T}-\left(\frac{506.4}{T}\right)^2\right]$	$m^2\ s^{-1}$	20
Bunsen coefficients			
A_{1,CO_2}	-60.2409	--	21
A_{2,CO_2}	93.4517	--	21
A_{3,CO_2}	23.3585	--	21
B_{1,CO_2}	2.3517×10^{-2}	--	21
B_{2,CO_2}	-2.3656×10^{-2}	--	21
B_{3,CO_2}	4.7036×10^{-3}	--	21
A_{1,O_2}	-58.3877	--	22
A_{2,O_2}	85.8079	--	22
A_{3,O_2}	23.8439	--	22
B_{1,O_2}	3.4892×10^{-2}	--	22
B_{2,O_2}	1.5568×10^{-2}	--	22
B_{3,O_2}	-1.9387×10^{-3}	--	22
A_{1,H_2}	-39.9611	--	23
A_{2,H_2}	53.9381	--	23
A_{3,H_2}	16.3135	--	23
B_{1,H_2}	2.3517×10^{-2}	--	23
B_{2,H_2}	1.7566×10^{-2}	--	23
B_{3,H_2}	-2.3010×10^{-3}	--	23
pH controller			
K_C	0.1	hr^{-1}	--
τ	60	s	--
Combustion energy			
$\Delta_r G_X^0$	-479	$kJ\ mol^{-1}$	Note 4
$\Delta_r G_E^0$	-479	$kJ\ mol^{-1}$	Note 4
$\Delta_r G_{H_2}^0$	-260	$kJ\ mol^{-1}$	Note 4
$\Delta_r G_{FFA}^0$	-240	$kJ\ mol^{-1}$	Note 4
$\Delta_r G_{LLA}^0$	-1370	$kJ\ mol^{-1}$	Note 4
$\Delta_r G_{AAA}^0$	-870	$kJ\ mol^{-1}$	Note 4
CO_2 electrolyzer			
j	140	$mA\ cm^{-2}$	24
η_F	94	%	24
V_e	3.5	V	24
$c_{FFA,eff}$	2.08	M	24
H_2 electrolyzer			
j	1000	$mA\ cm^{-2}$	25
η_F	99	%	25
V_e	2.0	V	25
Electrodialysis – lactic acid			
a_{ED}	0.5154	$kWh\ kg^{-1}$	Note 5

b_{ED}	3.7×10^{-2}	Wh L^{-1}	Note 5
$\Gamma_{\max}$	7.56	kg m^2 h^{-1}	Note 5
κ_{M}	51.5	g L^{-1}	Note 5
Electrodialysis – formic acid			
$\eta_{\mathrm{ED,F}}$	3	%	Note 5
$\Gamma_{\max}$	6.42	kg m^2 h^{-1}	Note 5
κ_{M}	26.3	g L^{-1}	Note 5

Table S2. Power breakdown for subprocesses.

Process power (kWh/kg CDW)	**Value**			
	Formatotrophic	*Knallgas*	*Acetogenic*	*Theoretical*
Substrate generation	47.26	22.61	19.55	5.32
Gas-liquid mass transfer and fluid mixing	0.48	0.43	1.38	0
Liquid heating	0.26	0.13	0.91	0
Direct air capture of CO_2	4.22	3.56	4.2	0.22
Haber-Bosch ammonia production	1.68	1.68	1.89	0.88
Chlor-alkali process (pH control)	0.38	0	4.01	0

Table S3. Parameter sensitivity

Parameter	Baseline Value	Units	Parameter -30%	Parameter +30%	Formate GWP -30%	H2 GWP -30%	Acetate GWP -30%	Hetero GWP -30%	Formate GWP +30%	H2 GWP +30%	Acetate GWP +30%	Hetero GWP +30%
Impact Model Parameters – Biomass												
BASELINE	n/a		n/a	n/a	**1.1607**	**0.6816**	**1.3509**	**1.9427**	**1.1607**	**0.6816**	**1.3509**	**1.9427**
Glucose GWP	0.95	kg co2/kg	0.665	1.235	1.1607	0.6816	1.3509	1.3727	1.1607	0.6816	1.3509	2.5127
% GWP Corn Fertilizer	0.25		0.175	0.325	1.1607	0.6816	1.3509	2.0352	1.1607	0.6816	1.3509	1.8501
Heterotroph Productivity	19.8	kg/L/yr	13.86	25.74	1.1607	0.6816	1.3509	1.9538	1.1607	0.6816	1.3509	1.9366
Glucose Yield	0.5	kg biomass/kg glucose	0.35	0.65	1.1607	0.6816	1.3509	2.649	1.1607	0.6816	1.3509	1.5623
Distance NH3 Shipped [km]	500	km	350	650	1.1593	0.6801	1.3493	1.9412	1.1622	0.683	1.3525	1.9441
Distance Nutrients Shipped [km]	500	km	350	650	1.1588	0.6777	1.3247	1.9385	1.1627	0.6855	1.377	1.9469
Distance electrolyzer materials Shipped [km]	500	km	350	650	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
Distance Bioreactors shipped [km]	500	km	350	650	1.1607	0.6815	1.3507	1.9426	1.1608	0.6816	1.3511	1.9427
Distance Glucose shipped [km]	500	km	350	650	1.1607	0.6816	1.3509	1.9257	1.1607	0.6816	1.3509	1.9596
Wind GWP	9.102	kg co2/MWh	6.3714	11.8326	1.0136	0.6034	1.266	1.9342	1.3078	0.7598	1.4358	1.9511
DAC Electricity Demand	2.02	kWh/kg CO2	1.414	2.626	1.1492	0.6719	1.3395	1.9427	1.1722	0.6913	1.3623	1.9427
Adsorbent GWP	23.7	g CO2-e/kg CO2 capture	16.59	30.81	1.1458	0.6691	1.3362	1.9427	1.1756	0.6941	1.3656	1.9427
DAC Plant GWP	15	g CO2-e/kg CO2 capture	10.5	19.5	1.1513	0.6737	1.3416	1.9427	1.1701	0.6895	1.3602	1.9427
GWP Ammonia (besides H2 electrolysis)	0.4105	kg co2/ kg nh3	0.28735	0.53365	1.1396	0.6605	1.3273	1.9065	1.1818	0.7027	1.3745	1.9788
Green Ammonia Electricity Demand	9.41	kWh/kg NH3	6.587	12.233	1.1563	0.6772	1.346	1.9351	1.1651	0.686	1.3558	1.9502
Phosphoric Acid GWP	1.012	kg CO2-e/kg	0.7084	1.3156	1.1293	0.6502	1.3158	1.9113	1.1921	0.713	1.386	1.974
NaCl GWP	0.178	kg CO2-e/kg	0.1246	0.2314	1.1575	0.6808	1.3481	1.9398	1.1639	0.6824	1.3537	1.9455
MgSO4 GWP	0.239	kg CO2-e/kg	0.1673	0.3107	1.1577	0.6786	1.3476	1.9397	1.1637	0.6846	1.3542	1.9456
CaCl2 GWP	0.611	kg CO2-e/kg	0.4277	0.7943	1.1596	0.6805	1.3496	1.9415	1.1618	0.6827	1.3521	1.9438
FeCl3 GWP	0.511	kg CO2-e/kg	0.3577	0.6643	1.1607	0.6815	1.3508	1.9426	1.1608	0.6816	1.351	1.9427
NaOH GWP minus electrolysis	0.116	kg CO2-e/kg	0.0812	0.1508	1.16	0.6714	1.2991	1.9325	1.1614	0.6917	1.4027	1.9528
HCl GWP minus electrolysis	0.127	kg CO2-e/kg	0.0889	0.1651	1.1607	0.6816	1.2987	1.9427	1.1607	0.6816	1.4031	1.9427
NaOH chlor-alkili electricity demand	1.1	kWh/kg	0.77	1.43	1.1607	0.6807	1.3464	1.9418	1.1608	0.6825	1.3554	1.9435

HCl Chlor-alkili electricity demand	1.21	kWh/kg	0.847	1.573	1.1607	0.6816	1.3464	1.9427	1.1607	0.6816	1.3554	1.9427
Iridium GWP	8860	kg Co2-e/kg	6202	11518	1.1392	0.6801	1.3496	1.9427	1.1823	0.6831	1.3522	1.9427
Carbon Fibre GWP	30.98	kg Co2-e/kg	21.686	40.274	1.1598	0.6815	1.3508	1.9427	1.1617	0.6817	1.351	1.9427
Tin GWP	5.77	kg Co2-e/kg	4.039	7.501	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
Nafion GWP	831	kg Co2-e/kg	581.7	1080.3	1.1041	0.6804	1.3499	1.9427	1.2173	0.6828	1.3519	1.9427
Polystyrene Sulfonate Cationic Resin GWP	1.76	kg Co2-e/kg	1.232	2.288	1.1603	0.6816	1.3509	1.9427	1.1611	0.6816	1.3509	1.9427
Reactor Volume	30000	L	21000	39000	1.1667	0.6869	1.368	1.944	1.1568	0.678	1.3396	1.9417
Reactor Weight:Vol	0.6235	kg/L	0.43645	0.81055	1.1466	0.6689	1.3103	1.9393	1.1749	0.6943	1.3915	1.946
Reactor Lifetime	8	yr	5.6	10.4	1.1809	0.6998	1.4089	1.9474	1.1498	0.6718	1.3197	1.9401
Steel GWP	6.89	kg CO2-e/kg	4.823	8.957	1.1466	0.6689	1.3105	1.9394	1.1748	0.6943	1.3913	1.946
Reactor Area Density	50	L/m^2	35	65	1.1883	0.7064	1.43	1.9491	1.1459	0.6682	1.3083	1.9392
Plant Lifetime	40	year	28	52	1.1883	0.7064	1.43	1.9491	1.1459	0.6682	1.3083	1.9392
Bulding GWP/m^2	595.9	kg CO2-e/kg	417.13	774.67	1.1414	0.6642	1.2955	1.9381	1.18	0.6989	1.4063	1.9472
Nitrogen Ratio	0.134	g N/ g biomass	0.0938	0.1742	1.1474	0.6375	1.3432	1.8986	1.2048	0.7256	1.3586	1.9867
Phosphorous Ratio	0.031	g P/g biomass	0.0217	0.0403	1.132	0.6529	1.3101	1.914	1.1907	0.7103	1.3916	1.9713
Sulfur Ratio	0.0105	g S/g biomass	0.00735	0.01365	1.1574	0.6783	1.3472	1.9393	1.164	0.6849	1.3546	1.946
Calcium Ratio	0.0021	g Ca/g biomass	0.00147	0.00273	1.1595	0.6804	1.3496	1.9415	1.1619	0.6828	1.3522	1.9438
Iron Ratio	0.0001	g Fe/g biomass	0.00007	0.00013	1.1607	0.6815	1.3508	1.9426	1.1608	0.6816	1.351	1.9427
Nitrient Utilization Ratio	0.95		0.665	1 *	1.2764	0.7933	1.4319	2.0577	1.1472	0.6686	1.3414	1.9292
Bioreactor Parameters – Biomass												
BASELINE	n/a		n/a	n/a	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
mu_max,opt	0.18	hr^{-1}	0.126	0.234	1.1605	0.6816	1.3509	1.9427	1.1606	0.6816	1.3509	1.9427
Y' X,F max	0.169	mol/mol	0.1183	0.2197	1.5565	0.6816	1.3509	1.9427	0.9659	0.6816	1.3509	1.9427
theta_F	75.11	mM	52.577	97.643	1.1608	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
Ks,F	10	uM	7	13	1.1607	0.6816	1.3509	1.9427	1.1608	0.6816	1.3509	1.9427
KS,O2	2.5	uM	1.75	3.25	1.1607	0.6816	1.3509	1.9427	1.1608	0.6816	1.3509	1.9427
pHmin	4		2.8	5.2	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
pHmax**	9		8	11.7	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
cNa_tox min	0.2	M	0.14	0.26	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
can_tox max	1.05	M	0.735	1.365	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427

mu_max,opt	0.18	hr^{-1}	0.126	0.234	1.1607	0.6813	1.3509	1.9427	1.1607	0.6819	1.3509	1.9427
Y' X,H max	0.19	mol/mol	0.133	0.247	1.1607	0.8412	1.3509	1.9427	1.1607	0.6075	1.3509	1.9427
Ks,H2	20.4	uM	14.28	26.52	1.1607	0.6815	1.3509	1.9427	1.1607	0.6817	1.3509	1.9427
Ks,O2	2.5	uM	1.75	3.25	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
Ks,CO2	9.38	uM	6.566	12.194	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
pHmin	4		2.8	5.2	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
pHmax**	9		8	11.7	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
cNa_tox min	0.2	M	0.14	0.26	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
cNa_tox_max	1.05	M	0.735	1.365	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
mu_max_opt	0.044	hr^{-1}	0.0308	0.0572	1.1607	0.6816	1.4586	1.9427	1.1607	0.6816	1.2938	1.9427
Ks,H2	20	uM	14	26	1.1607	0.6816	1.3496	1.9427	1.1607	0.6816	1.3547	1.9427
Ks,CO2	20	uM	14	26	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
nATP	0.47		0.329	0.611	1.1607	0.6816	1.338	1.9427	1.1607	0.6816	1.3642	1.9427
pHmin	4		2.8	5.2	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
pHmax**	9		8	11.7	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
cNa_tox min	0.2	M	0.14	0.26	1.1607	0.6816	1.3685	1.9427	1.1607	0.6816	1.3337	1.9427
cNa_tox max	1.05	M	0.735	1.365	1.1607	0.6816	1.4403	1.9427	1.1607	0.6816	1.3037	1.9427
mu_max_opt	0.3	hr^{-1}	0.21	0.39	1.1607	0.6816	1.3526	1.9427	1.1607	0.6816	1.3527	1.9427
Y' X,Ac	0.936	mol/mol	0.6552	1.2168	1.1607	0.6816	1.8509	1.9427	1.1607	0.6816	1.0851	1.9427
Ks,O2	2.5	uM	1.75	3.25	1.1607	0.6816	1.3506	1.9427	1.1607	0.6816	1.3528	1.9427
Ks,Ac	10	uM	7	13	1.1607	0.6816	1.3508	1.9427	1.1607	0.6816	1.351	1.9427
Ki,Ac	0.83	uM	0.581	1.079	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
pHmin	4		2.8	5.2	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
pHmax**	9.5		8	12.35	1.1607	0.6816	1.3509	1.9427	1.1607	0.6816	1.3509	1.9427
cNa_tox min	0.2	M	0.14	0.26	1.1607	0.6816	1.3514	1.9427	1.1607	0.6816	1.3507	1.9427
cNa_tox max	1.05	M	0.735	1.365	1.1607	0.6816	1.3544	1.9427	1.1607	0.6816	1.3506	1.9427

Parameter	Baseline Value	Units	Parameter -30%	Parameter +30%	Formate GWP -30%	H2 GWP -30%	Acetate GWP -30%	Hetero GWP -30%	Formate GWP +30%	H2 GWP +30%	Acetate GWP +30%	Hetero GWP +30%
Bioreactor Model Parameters – Lactic Acid												
BASELINE	n/a	n/a	n/a	n/a	**0.7775**	**0.4784**	**0.8952**	**1.0915**	**0.7775**	**0.4784**	**0.8952**	**1.0915**
Y' X,F max	0.169	mol/mol	0.1183	0.2197	0.8217	0.4784	0.8952	1.0915	0.7670	0.4784	0.8952	1.0915
Y' L,F max	0.11	mol/mol	0.077	0.143	0.9421	0.4784	0.8952	1.0915	0.7565	0.4784	0.8952	1.0915
mu_max_opt	0.018	hr^{-1}	0.0126	0.0234	0.7854	0.4784	0.8952	1.0915	0.7948	0.4784	0.8952	1.0915
c_Na_min	0.2	M	0.14	0.26	0.7953	0.4784	0.8952	1.0915	0.7694	0.4784	0.8952	1.0915
c_Na_max	1.05	M	0.735	1.365	1.0228	0.4784	0.8952	1.0915	0.7566	0.4784	0.8952	1.0915
Y' X,H max	0.19	mol/mol	0.133	0.247	0.7775	0.4874	0.8952	1.0915	0.7775	0.4736	0.8952	1.0915
Y' L,H max	0.11	mol/mol	0.077	0.143	0.7775	0.5243	0.8952	1.0915	0.7775	0.4541	0.8952	1.0915
mu_max_opt	0.018	hr^{-1}	0.0126	0.0234	0.7775	0.5464	0.8952	1.0915	0.7775	0.4421	0.8952	1.0915
c_Na_min	0.2	M	0.14	0.26	0.7775	0.4896	0.8952	1.0915	0.7775	0.4672	0.8952	1.0915
c_Na_max	1.05	M	0.735	1.365	0.7775	0.5395	0.8952	1.0915	0.7775	0.4431	0.8952	1.0915
mu_max_opt	0.044	hr^{-1}	0.0308	0.0572	0.7775	0.4784	0.9558	1.0915	0.7775	0.4784	0.8644	1.0915
nATP	0.47		0.329	0.611	0.7775	0.4784	0.8873	1.0915	0.7775	0.4784	0.9033	1.0915
c_Na_min	0.2	M	0.14	0.26	0.7775	0.4784	0.9059	1.0915	0.7775	0.4784	0.8846	1.0915
c_Na_max	1.05	M	0.735	1.365	0.7775	0.4784	0.9863	1.0915	0.7775	0.4784	0.8874	1.0915
Y' X,Ac	0.936	mol/mol	0.6552	1.2168	0.7775	0.4784	0.9523	1.0915	0.7775	0.4784	0.8680	1.0915
Y' L,Ac	0.5	mol/mol	0.35	0.65	0.7775	0.4784	1.2050	1.0915	0.7775	0.4784	0.7321	1.0915
mu_max_opt	0.3	hr^{-1}	0.21	0.39	0.7775	0.4784	0.9891	1.0915	0.7775	0.4784	0.8443	1.0915
c_Na_min	0.2	M	0.14	0.26	0.7775	0.4784	0.9134	1.0915	0.7775	0.4784	0.8770	1.0915
c_Na_max	1.05	M	0.735	1.365	0.7775	0.4784	1.0732	1.0915	0.7775	0.4784	0.8606	1.0915

Supplementary notes

Note 1: Optimizing full-system productivity in the acetate-mediated system

For both biomass and enzyme production, the acetotrophic portion of the acetate-mediated system is limited ultimately by O_2 gas-liquid mass transfer, as described in the main text. The feed concentration of acetate/ic acid, therefore, plays no role in determining the productivity of this reactor because the dilution rate can be adjusted in the opposite direction of a change in the feed acetate/ic acid concentration to maintain a constant productivity. Hence, the full-system productivity is maximized by maximizing the productivity of the upstream acetogenesis reactor. Acetate/ic acid productivity in the acetogenesis reactor is maximized by an intermediate normalized dilution rate of ~0.55 (Fig. S1a).

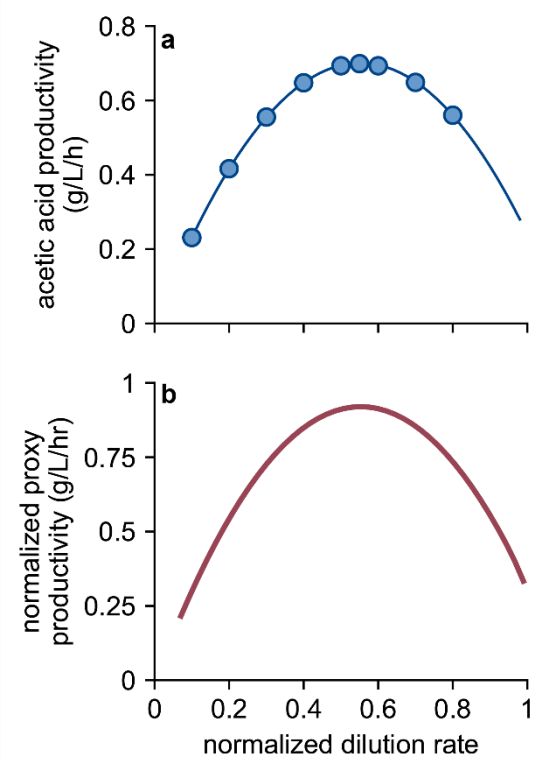

Figure S1. Optimal productivity in the acetate-mediated system. Maximum (**a**) acetate/ic acid productivity in the acetogenic reactor and (**b**) proxy full-system lactic acid productivity as a function of the normalized dilution rate in the acetogenic reactor. In both cases, the productivity is maximized at a normalized dilution rate of 0.55.

This trend is analogous to that of lactic acid production in the H_2-mediated case as described in the main text, where the product (lactic acid or acetic acid) concentration is negatively proportional to the dilution rate (in this case, $c_{\mathrm{AAA}} \propto -D_{\mathrm{liq,A}}$) such that the reactor productivity is negatively proportional to the square of the dilution rate (here, $\dot{m}_{\mathrm{AAA,A}} = D_{\mathrm{liq,A}} c_{\mathrm{AAA}}$, so $\dot{m}_{\mathrm{AAA,A}} \propto -\left(D_{\mathrm{liq,A}}\right)^2$.

The picture is more complicated for lactic acid production in this system because the acetate/ic acid feed concentration does contribute to the maximum lactic acid productivity in the acetotrophic reactor; specifically, $\dot{m}_{\mathrm{LLA,Ac}} \propto Y'_{\mathrm{L/Ac}} D_{\mathrm{liq,Ac}} c_{\mathrm{AAA,f}}$, where $c_{\mathrm{AAA,f}}$ represents the total acetate/ic acid concentration fed to the acetotrophic reactor. The maximum dilution rate is negatively proportional to the fed acetic acid concentration, that is, $D_{\mathrm{liq,Ac}} \propto -c_{\mathrm{AAA,f}}$ (see analogous description below in Note 2 for an explanation of this point), such that the productivity in the acetotrophic reactor is negatively proportional to the square of the acetate/ic acid feed concentration: $\dot{m}_{\mathrm{LLA,Ac}} \propto -\left(c_{\mathrm{AAA,f}}\right)^2$. From eq. 73 in the main text, the overall productivity of lactic acid is proportional to the productivity in the acetotrophic reactor and the ratio of the dilution rates in each reactor, equivalently $\dot{m}_{\mathrm{LLA,AA}} \propto \dot{m}_{\mathrm{LLA,Ac}} \left(\frac{D_{\mathrm{liq,A}}}{D_{\mathrm{liq,Ac}}}\right)$. The feed acetate/ic acid concentration to the acetotrophic reactor ($c_{\mathrm{AAA,f}}$) is equivalent to the exit acetate/ic acid concentration in the acetogenic reactor (c_{AAA}, above). The dilution rate in the acetotrophic reactor is negatively proportional to the feed concentration, which is in turn negatively proportional to the dilution rate in the acetogenic reactor. Hence, this dependence cancels out and $\dot{m}_{\mathrm{LLA,AA}} \propto \dot{m}_{\mathrm{LLA,Ac}}$, which indicates that $\dot{m}_{\mathrm{LLA,AA}} \propto -\left(c_{\mathrm{AAA,f}}\right)^2$, or equivalently, $\dot{m}_{\mathrm{LLA,A}} \propto -\left(D_{\mathrm{liq,A}}\right)^2$. We use the acetate feed rate ($D_{\mathrm{liq,Ac}} c_{\mathrm{AAA}}$) as a proxy for the overall productivity (since they are proportional to each other) and plot the relationship between this proxy and the dilution rate in the acetogenic reactor (Fig. S1b). Interestingly, the productivity proxy is maximized at the same normalized dilution rate (~0.55) that maximizes acetate/ic acid productivity. Hence, in all base-cases in our model, $\delta_{\mathrm{A}} = 0.55$ and $c_{\mathrm{AAA}} \approx 0.48$ M.

Note 2: Optimizing lactic acid productivity in the formate-mediated system

The productivity of lactic acid (and any generic product) is given by $D_{\mathrm{liq}} c_{\mathrm{LLA}}$. The titer, c_{LLA}, is proportional to the product of the lactic acid yield on formate ($Y'_{\mathrm{L/F}}$) and the feed concentration of formate ($c_{\mathrm{FFA,f}}$), that is, $c_{\mathrm{LLA}} \propto Y'_{\mathrm{L/F}} c_{\mathrm{FFA,f}}$. The dilution rate, D_{liq}, is typically thought of as independently controllable. However, the dilution rate is bounded by the maximum specific growth rate, μ_{max}. The maximum specific growth rate is a function of the sodium concentration, specifically, $\mu_{\mathrm{max}} \propto -c_{\mathrm{Na}}$ (eq. 47 in the main text). The sodium concentration, in turn, is a function of the lactic acid titer (specifically, $c_{\mathrm{Na}} \propto c_{\mathrm{LLA}}$) because sodium hydroxide is added to neutralize the proton liberated by lactic acid production. Hence, because c_{LLA} is proportional to $c_{\mathrm{FFA,f}}$, the maximum specific growth rate is negatively proportional to the feed concentration of formate/ic acid (that is, $\mu_{\mathrm{max}} \propto -c_{\mathrm{FFA,f}}$). This also means that the maximum dilution rate is negatively proportional to the feed concentration because the dilution rate is bounded by the specific growth rate ($D_{\mathrm{liq}} \propto -c_{\mathrm{FFA,f}}$). Together, this means the productivity of lactic acid in the formate mediated system ($\dot{m}_{\mathrm{LLA,F}}$) is negatively proportional to the squared feed concentration of formate/ic acid, that is, $\dot{m}_{\mathrm{LLA,F}} \propto -\left(c_{\mathrm{FFA,f}}\right)^2$. Hence, we should expect to see a feed formate/ic acid concentration that maximizes the lactic acid productivity. Fig. S2 shows the maximum lactic acid productivity as a function of the feed concentration of formic acid and demonstrates a maximum productivity at ~5.1 M formate/ic acid. We therefore selected a 5.1 M feed stream for formatotrophic production of lactic acid and considered the life cycle impact of an electrodialysis process to concentrate the effluent from the CO_2 electrolysis reactor.

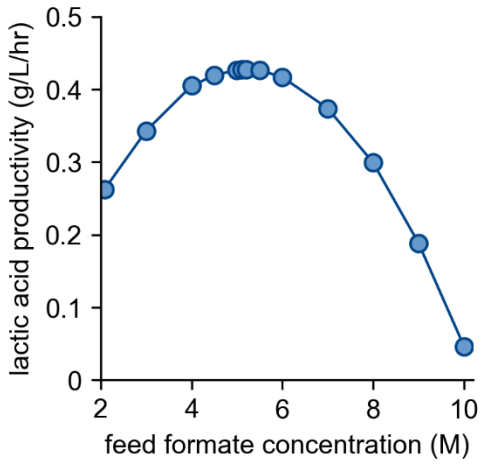

Figure S2. Optimal formate feed concentration for lactic acid productivity. Maximum lactic acid productivity as a function of the formate feed concentration. Maximum value of ~0.42 g/L/h is achieved at a feed concentration of ~5.1 M.

Note 3: Intrinsically safer operation of the H_2-mediated system

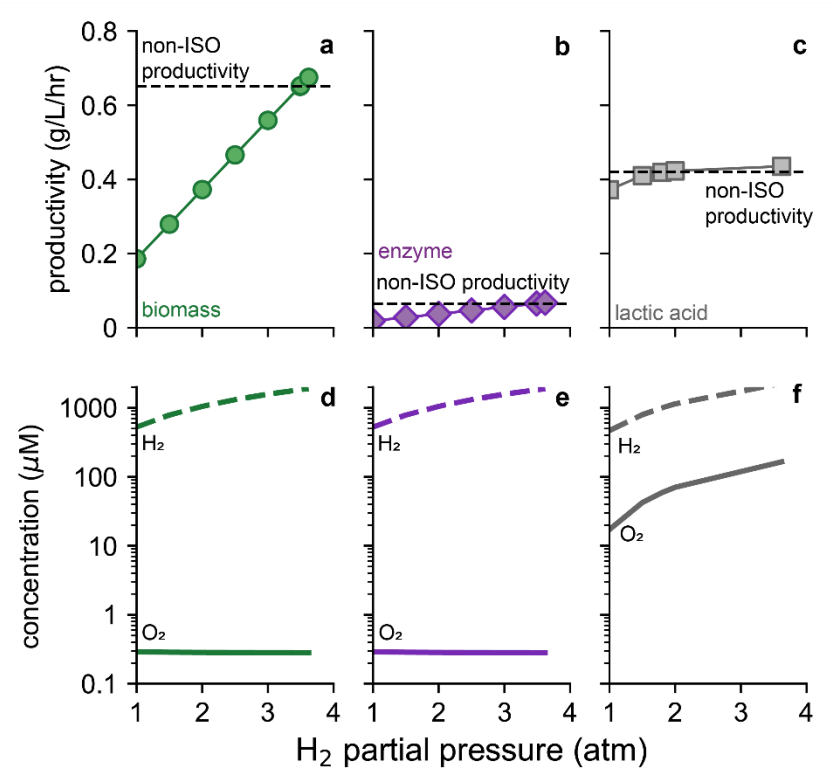

Figure S3. Intrinsically-safer operation of the H_2-mediated system. Productivity (**a**, **b**, **c**) and liquid-phase concentration of H_2 and O_2 (**d**, **e**, **f**) for the H_2-mediated EMP system under intrinsically-safer operation (ISO, p_{H2}:p_{O2} = 10:1) producing biomass (**a**, **d**), enzyme (**b**, **e**), and lactic acid (**c**, **f**). Horizontal black dashed lines in (**a**, **b**, **c**) correspond to the non-ISO (p_{H2}:p_{O2} = 1:0.21) base-case productivity for each of the three products. Low (<10 μM) O_2 concentration (solid lines in **d**, **e**, **f**) indicate O_2 gas-liquid mass transfer limitation on the productivity.

Note 4: Polylactic acid production life cycle impacts

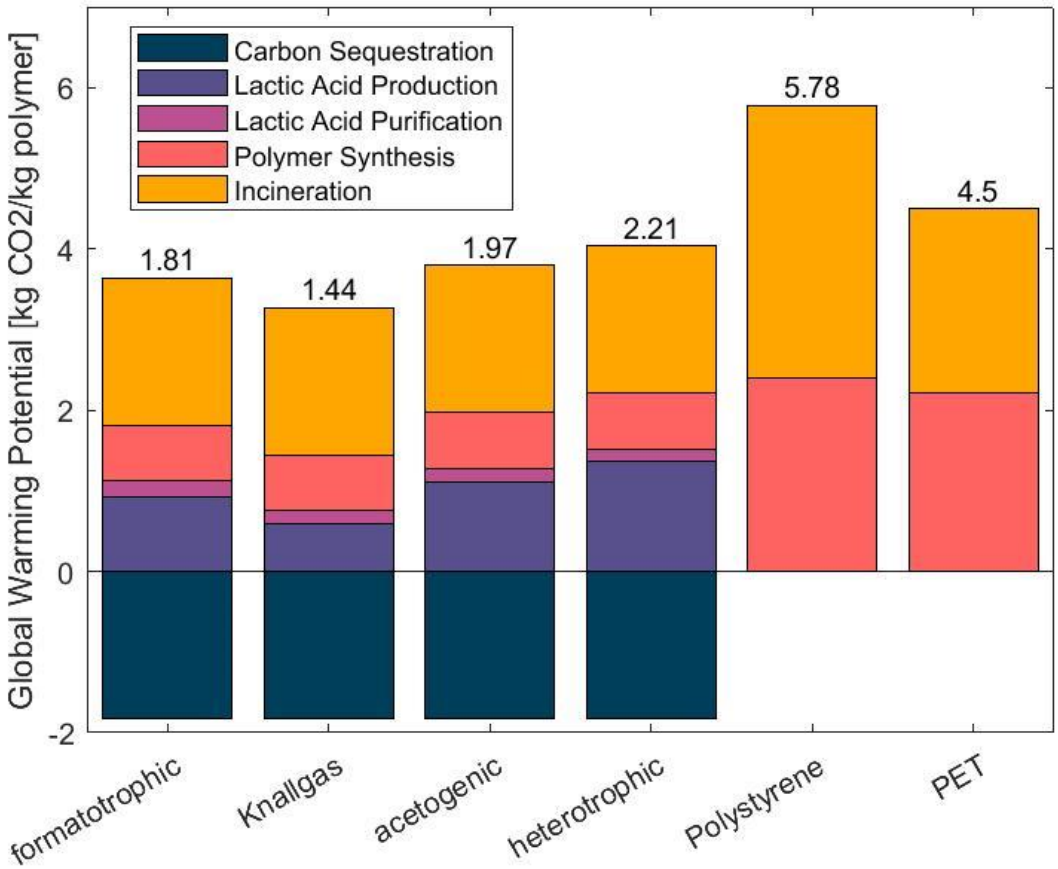

Figure S4: Life Cycle Global Warming Potential of EMP-based and traditional plastics. Life cycle (cradle-to-grave) global warming potential of polymer production of polylactic acid (PLA) in the three EMP systems and traditional bioprocesses compared to those of fossil-fuel based plastics polyethylene terephthalate (PET) and polystyrene (PS). EMP production assumes a 90% carbon efficiency (as defined in main text) and grid composed solely of wind power.

We analyzed the cradle-to-grave life cycle impact of polylactic acid (PLA) production. We split the PLA production process into five categories: carbon sequestration, lactic acid production, lactic acid purification, polymer synthesis, and end of life. The global warming potentials for the lactic acid production are identical to the results in Fig. 5c in the main text. Purification of lactic acid relies on acidifying the lactate anion produced in the bioreactor and therefore requires a stoichiometric proportion of sulfuric acid, the carbon footprint of which is obtained from the PEF dataset. We obtained data for the carbon footprint of polylactic acid polymer production from Morão and de Bie.[26] We further compared the global warming footprints to those of two major fossil-fuel based polymers: polyethylene terephthalate (PET) and polystyrene (PS). Carbon footprints for the production of these two polymers were obtained from the PEF dataset. We assume all plastics are incinerated at the end of their life and assume the carbon footprint is equal to the stoichiometric amount of carbon dioxide that would be produced by complete combustion of the polymer.

The global warming potentials of the cradle-to-grave PLA production of the three EMP systems and the traditional bioprocess reflect the same trends as for lactic acid production because the lactic acid purification and polymer synthesis steps are identical for each system. Therefore, the Knallgas bacteria-based system outcompetes the other bioprocesses in PLA production as it does in lactic acid production. All lactic acid production systems outperform the two fossil-based polymers, PET and PS, in terms of life cycle global warming potential, in the scenario shown. The acetogenic system and heterotrophic system both have comparable carbon footprints to the fossil-based plastics if the plastics are not incinerated, which is a plausible scenario given that burial is a common practice for plastic disposal. However, a true like-to-like comparison will involve incinerating these plastics to leave no waste, as PLA will ultimately biodegrade in the environment. In the scenario, all methods of PLA production have smaller carbon footprints when compared to PET and PS.

These results are for a carbon conversion efficiency of 90%, similar to current glucose-based PLA fermentation. As noted in the main text, an efficiency this high will be difficult in EMP processes. Lower carbon efficiencies in the lactic acid production step will therefore increase the total carbon footprint of PLA production. As shown in Fig. 6b in the main text, this change in GWP is also dependent on the electricity source/grid composition. As with lactic acid production, for H_2-mediated electromicrobial production of PLA to outcompete heterotroph-based processes, the process must rely on renewable electricity and must achieve a carbon efficiency of around 50%.

Note 5: calculating combustion energies

To calculate combustion energies, we adopted the strategy of Claassens *et al.*[27] Briefly, we used eQuilibrator[28] to calculate the $\Delta_r G'^0$ of the combustion reaction at a pH of 7.0 and ionic strength of 0.1 M. The biomass combustion energy was adopted from previous calculations.[29,30]

Note 6: calculating parameters for electrodialysis-based separations

Data from Hábová *et al.*[31] were used to determine parameters for membrane electrodialysis. Energy consumption as a function of lactic acid feed concentration was determined according to a linear model, eq. 87 in the main text. The linear model fit well to reported data ($R^2 = 0.73$), as shown in Fig. S4a. Lactic acid flux parameters were determined similarly and fit well to the proposed model ($R^2 = 0.85$), as shown in Fig. S4b.

Because relatively little data exist on formic acid concentration in membrane electrodialysis, we used the same dataset to estimate an average energy efficiency ($\eta_{\mathrm{ED,F}}$) of 3%. We also used the same fitting parameters but modified the values to account for the different molar masses and diffusivities of lactic acid and formic acid.

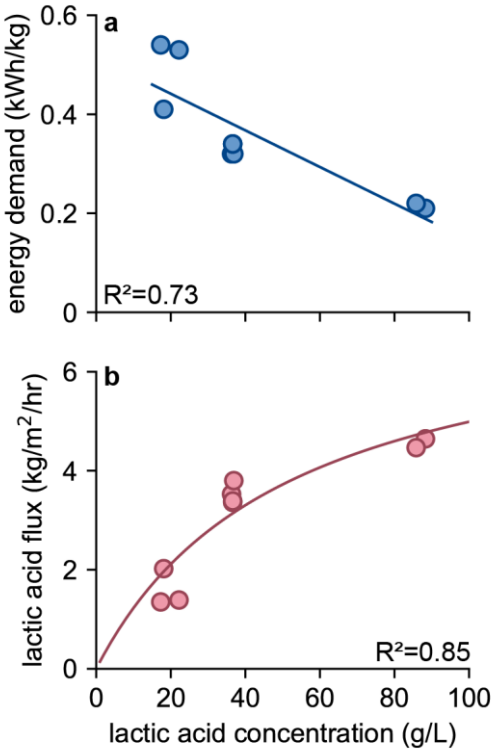

Figure S5. Fitting parameters for membrane electrodialysis. (**a**) energy demand and (**b**) through-membrane lactic acid flux for membrane electrodialysis as a function of the fed lactic acid concentration. Circles represent data from Hábová *et al.* and solid lines are fitted equations.

Note 7: reactor model parameter sensitivity calculations

When some parameters (*e.g.*, the maximum specific growth rate, $\mu_{\max,\mathrm{opt}}$) are adjusted, operating conditions such as the liquid dilution rate (D_{liq}) have different optima. In these cases, we identified the new optimal operating conditions and report system outputs based on these.

Note 8: Theoretical Energy and Material Demands of EMP Process

Table 2 in the main text displays the predicted material and energy demands for EMP processes through the three studied schemes. Also included are theoretical minimum values for each of the material and energy demands listed.

Grosz and Stephanopolous give the Gibbs Free Energy of Formation for *E. coli* as -46.0 kJ/mol C [29]:

$$\mathrm{C}_{(s)} + 0.885\mathrm{H}_{2(\mathrm{g})} + 0.12\mathrm{N}_{2(\mathrm{g})} + 0.245\mathrm{O}_{2(\mathrm{g})} \rightarrow \mathrm{CH}_{1.77}\mathrm{O}_{0.49}\mathrm{N}_{0.24(s)} \qquad \Delta G_{\mathrm{X}}^{0} = -46.0\ \mathrm{kJ/mol}$$

To determine Gibbs free energies for reactions relevant to the EMP systems, however, manipulations can be made. As CO_2, rather than solid carbon, and ammonia, rather than nitrogen

gas, are fed into the EMP system, the chemical equation above may be linearly combined with the equation for formation of CO_2:

$$CO_{2(g)} \rightarrow C_{(s)} + O_{2(g)} \qquad \Delta G^0 = +394.4\ \text{kJ/mol}$$

as well as the equation for the formation of ammonia

$$NH_{3(l)} \rightarrow \frac{1}{2}N_{2(g)} + \frac{3}{2}H_{2(g)}\ \ \Delta G^0 = +26.5\ \text{kJ/mol}$$

The free energy of biomass from CO_2, H_2, and NH_3, as it occurs in an electromicrobial system, is therefore

$$CO_2 + 0.525H_2 + 0.24NH_3 \rightarrow CH_{1.77}O_{0.49}N_{0.24} + 0.755O_2\ \Delta G^0 = 354.8\ \text{kJ/mol}$$

When considering water, rather than hydrogen gas, as a reactant for the EMP system,

$$H_2O_{(l)} \rightarrow \frac{1}{2}O_{2(g)} + H_{2(g)}\ \ \Delta G^0 = +274.1\ \text{kJ/mol}$$

the equation becomes

$$CO_2 + 0.525H_2O + 0.24NH_3 \rightarrow CH_{1.77}O_{0.49}N_{0.24} + 1.02O_2\ \Delta G^0 = +479\ \text{kJ/mol}$$

Therefore, the theoretical energy input required to produce biomass is 479 kJ/mol C of biomass. Using a biomass molar mass of 25 g/mol C, and converting the energy to kWh, this energy requirement on a mass basis is 5.32 kWh/kg biomass.

Carbon Demand

The carbon demand to produce biomass is simply determined by stoichiometry. As one mole of CO_2 is fixed per carbon mole of biomass (MW=25.0 g/mol), 1.76 kg CO_2 are required per mole of biomass.

Assuming CO_2 is fed to the EMP reactor at 1 atm, and is fixed from atmospheric CO_2, the minimum energy required to produce this CO_2 is equal to the Gibbs Free Energy required to concentrate from 400 pm to pure CO_2. Assuming CO_2 behaves as an ideal gas, this free energy at standard temperature is:

$$\Delta G^0 = -RT\ln\left(\frac{1\ \text{atm}}{0.0004\ \text{atm}}\right) = 19.4\frac{\text{kJ}}{\text{mol}} = 0.12\frac{\text{kWh}}{\text{kg}\ CO_2} = 0.22\ \frac{\text{kWh}}{\text{kg Biomass}}$$

Nitrogen Demand

The theoretical ammonia demand is obtained by stoichiometry, assuming one mole of ammonia is required per mole of nitrogen fixed in biomass, using the biomass equation $CH_{1.77}O_{0.49}N_{0.24}$. Therefore, 0.24 mol of ammonia per carbon mole of biomass, or 0.163 kg NH_3 per kg biomass, is required.

The minimum energy required to produce this ammonia using nitrogen gas (from air) and water (as is the case in green ammonia production) can be determined from the Gibbs Free Energy of the following reaction:

$$\frac{1}{2}\mathrm{N}_{2(g)} + \frac{3}{2}\mathrm{H_2O}_{(l)} \rightarrow \mathrm{NH}_{3(\mathrm{l})} + \frac{3}{4}\mathrm{O}_{2(g)} \qquad \Delta G^0 = 329.1\ \mathrm{kJ/mol}$$

Using the ammonia to biomass ratio determined above, the energy required in nitrogen fixation for 1 kg of biomass is 0.88 kWh.

Total NaOH and HCl

As the net equation for the formation of biomass (see above) involves no net consumption/generation of protons, the theoretical required mass of NaOH and HCl is 0. The theoretical energy required to produce these pH control agents is therefore also 0.

Total Process Electricity

The theoretical total process electricity is equal to the sum of the theoretical energy requirements of the constitutive subprocesses (electrolysis/bioreactor electricity, NH_3 generation electricity, CO_2 generation electricity, and NaOH/HCl generation electricity).

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