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Supplementary Material: Baseline Cost Analysis of Energy Wastewater Treatment with Preliminary Feasibility Analysis of Critical Mineral Recovery

Chad Able [1,2], Thomas Schmitt, [1,2] Nicholas Siefert, [1] and Alison Fritz [3,*]

Supplementary S1. Compositions for Leachate and Produced Water Simulations

The compositions for the inlet and outlet streams in the leachate and produced water simulations are detailed in the subsections below.

Supplementary S1.1. Landfill Leachate Compositions

The median landfill leachate composition is outlined in Table S1.

Table S1. Median values for landfill leachate from CPInfo; critical mineral values are bolded.

Parameter	Value	Parameter	Value	Parameter	Value
Aluminum, mg/L	0.09	**Manganese, mg/L**	0.73	Bicarbonate, mg/L	69
Arsenic, mg/L	0.014	**Zinc, mg/L**	0.0093	**Antimony, mg/L**	0.000167
Boron, mg/L	8.15	**Nickel, mg/L**	0.0048	Selenium (VI), mg/L	0.103641
Barium, mg/L	0.0553	Copper, mg/L	0.00047	Thallium, mg/L	7.00×10^{-5}
Calcium, mg/L	450	Carbon, organic, mg/L	2.8	Uranium, mg/L	0.00233
Chloride, mg/L	113	EC (field), umho/cm	3955	Ammonia, mg/L	0.15
Fluoride, mg/L	0.445	Iron, mg/L	0.0498	Hardness–total, mg/L	1000
Potassium, mg/L	93	Selenium, mg/L	0.023	Total suspended solids, mg/L	4.2
Lithium, mg/L	1.045	Bromide, mg/L	11.3	Nitrogen, Kjeldahl, mg/L	0.62
Magnesium, mg/L	29.05	Eh, mV	211	Nitrite + nitrate, mg/L	1.2
Molybdenum, mg/L	0.283	Alkalinity, mg/L	140	Alpha, pCi/L	31
Sodium, mg/L	308	Chemical oxygen demand, mg/L	20.2	Beta, pCi/L	490.5
Nitrate nitrogen, mg/L	2.8	Hardness-Ca, mg/L	450	pH (lab), SU	7.715
Oxygen reduction potential, mV	199	TDS, mg/L	4335	Turbidity (field), NTU	4.335
pH (field), SU	8.8	Arsenic (III), mg/L	0.0051	Dissolved oxygen (ppm), mg/L	7.475
Silica, mg/L	6.1	Arsenic (other species), mg/L	0.000196	Electrical conductivity (lab), umho/cm	6300
Sulfate, mg/L	1600	Arsenic (V), mg/L	0.006163	**Chromium, mg/L**	0.0002
Strontium, mg/L	4.539	**Cobalt, mg/L**	0.000935	Chromium (VI), mg/L	0.000679
Carbon, inorganic, mg/L	6.234501	Carbonate, mg/L	47.45	**Vanadium, mg/L**	0.0048

Not all of these values are used as inputs to the OLI Studio software—those inputs are summarized in Table S2.

Table S2. Inputs for landfill leachate to OLI Studio.

Parameter	Value	Parameter	Value
Total dissolved solids, mg/L	4335	NH_3, mg/L	0.15
SeO_4^{-2}, mg/L	0.5503	Na^{+1}, mg/L	308
CO_3^{-2}, mg/L	47.45	K^{+1}, mg/L	93
SiO_2, mg/L	6.1	Ca^{+2}, mg/L	450
$B(OH)_3$, mg/L	46.6188	Mg^{+2}, mg/L	29.05
$Sb(OH)_5$, mg/L	2.83×10^{-4}	Sr^{+2}, mg/L	4.539
U, mg/L	2.33×10^{-3}	Ba^{+2}, mg/L	0.0553
Fe^{+2}, mg/L	0.0498	Al^{+3}, mg/L	0.09

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Co^{+2}, mg/L	9.35 × 10^{-4}	Cu^{+2}, mg/L	4.7 × 10^{-4}
Mn^{+2}, mg/L	0.73	Mo^{+3}, mg/L	0.283
Ni^{+2}, mg/L	4.8 × 10^{-3}	Ti^{+1}, mg/L	7 × 10^{-5}
VO_2^{+1}, mg/L	7.815 × 10^{-3}	Zn^{+2}, mg/L	9.3 × 10^{-3}
Li^{+1}, mg/L	1.045	Cl^{-1}, mg/L	113
SO_4^{-2}, mg/L	1600	HCO_3^{-1}, mg/L	69
AsO_4^{-3}, mg/L	0.011427	AsO_3^{-3}, mg/L	8.367 × 10^{-3}
CrO_4^{-2}, mg/L	4.46 × 10^{-4}	Br^{-1}, mg/L	11.3
F^{-1}, mg/L	0.445	NO_3^{-1}, mg/L	12.4

Some changes of note:

- Silica and sulfate values are used (silicon and sulfur are ignored).
- Arsenic is computed as proportional As(V) and As(III) using the median values of arsenic, As(V) and As(III).
- Selenium is computed as selenate.
- Boron is computed as boric acid.
- Chromium is computed as chromate.
- Vanadium is computed as pervanadyl.
- Antimony is computed as antimony pentoxide.

The total dissolved solids (TDS) value is not used directly and is simply a placeholder. During reconciliation, TDS is recalculated—the reconciled TDS is 2723.17 mg/L (which is the value used in WaterTAP). The full reconciled stream is input into OLI Flowsheet simulations.

For sensitivity analyses, only single components are changed to either their 25th percentile value, 75th percentile value, or median from the CoDaRT tool [21] (except for bulk runs, which change the dominant cation and anion). The change, as well as the reconciled TDS, is outlined in Table S3.

Table S3. Sensitivity values and reconciled TDS values for landfill leachate.

Simulation	New Value	Reconciled TDS
Median	-	2723.17 mg/L
25th percentile Li	Li, 0.41 mg/L	2718.03 mg/L
75th percentile Li	Li, 4.7225 mg/L	2804.12 mg/L
CoDaRT Li	Li, 3.43005 mg/L	2793.85 mg/L
25th percentile Mg	Mg, 9.8475 mg/L	2695.61 mg/L
75th percentile Mg	Mg, 93 mg/L	3092.71 mg/L
CoDaRT Mg	Mg, 29.7 mg/L	2726.42 mg/L
Bulk 25th percentile	Ca, 234.13 mg/L; SO_4, 1249 mg/L	2147.82 mg/L
Bulk 75th percentile	Ca, 720.5 mg/L; SO_4, 2100 mg/L	3225.68 mg/L
CoDaRT bulk	Ca, 440 mg/L; SO_4, 1600 mg/L	2689.28 mg/L

These CoDaRT data, in turn, are shown in Table S4 for landfill leachate. The best r^2 value is chosen using the data from CPInfo for landfill leachate. This r^2 value is defined below:

$$r^2 = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2}$$

where:

- y_i = true value;
- $\hat{y}_i$ = predicted value;
- $\bar{y}$ = average value.

For lithium and magnesium, this is the run using four features and five classifiers (that is, four independent numeric variables and up to five independent binary (derived from string) variables), and for bulk concentration (calcium and sulfate), this is the run using two features and five classifiers. This is further discussed in the user's guide for the CoDaRT tool [21].

Table S4. CoDaRT results for different constituents.

Constituent	R^2 (2 Features, 0 Classes)	R^2 (4 Features, 0 Classes)	R^2 (2 Features, 5 Classes)	R^2 (4 Features, 5 Classes)
Li	0.782	0.668	−0.041	0.867
Mg	0.894	0.943	0.889	0.967
Ca	0.916	0.82	0.925	0.791
SO4	0.974	0.98	0.975	0.96

Using the reconciled median feed, the outlet streams are shown in Table S5. These are results from OLI Flowsheet. The brine contains some suspended solids—the value is slightly higher than the brine's total TDS in the manuscript.

Table S5. Permeate and brine compositions from the median OLI Flowsheet run for landfill leachate.

Parameter (mg/L)	Permeate 1	Permeate 2	Brine
Al(+3)	8.01×10^{-6}	1.30×10^{-5}	0.017655
As(+3)	4.32×10^{-4}	7.62×10^{-3}	1.36×10^{-3}
As(+5)	4.73×10^{-5}	7.04×10^{-4}	3.19×10^{-3}
B(+3)	0.827967	14.183	3.89×10^{-3}
Ba(+2)	9.39×10^{-6}	7.97×10^{-6}	0.130855
Br(−1)	0.096629	1.36988	8.65×10^{-3}
C(+4)	0.205133	18.1604	0.018282
Ca(+2)	0.694211	1.48583	0.084731
Cl(−1)	0.807972	11.5982	0.091828
Co(+2)	8.63×10^{-7}	1.16×10^{-5}	0.093851
Cr(+6)	7.21×10^{-7}	1.36×10^{-5}	0.119147
Cu(+2)	1.30×10^{-5}	3.31×10^{-4}	0.18149
F(−1)	5.05×10^{-3}	0.0709953	0.973099
Fe(+2)	5.35×10^{-5}	1.11×10^{-3}	2.37976
H(+1)	1.12×10^{5}	1.12×10^{5}	8.55468
K(+1)	0.587457	7.07715	5.49433
Li(+1)	3.97×10^{-3}	0.0613926	5.92183
Mg(+2)	0.027223	0.367928	88.7409
Mn(+2)	6.76×10^{-4}	9.14×10^{-3}	14.2732
Mo(+3)	1.61×10^{-3}	0.0190736	20.3317
N(−3)	1.34×10^{-3}	0.012527	50.2782
N(+5)	0.14929	1.96973	53.4938
Na(+1)	1.58752	18.2888	131.029
Ni(+2)	4.45×10^{-6}	6.01×10^{-5}	241.484
O(−2)	8.85×10^{5}	8.85×10^{5}	218.213
S(+6)	1.15664	6.97569	8167.36
Sb(+5)	2.27×10^{-6}	3.27×10^{-5}	567.984
Se(+6)	8.97×10^{-4}	0.0141623	1803.71
Si(+4)	0.058131	1.33356	2186.99
Sr(+2)	6.74×10^{-3}	0.0185426	10851.4
Tl(+1)	4.62×10^{-7}	5.74×10^{-6}	5984.96

V(+5)	6.05×10^{-5}	1.11×10^{-3}	1.11×10^{5}
Zn(+2)	2.73×10^{-5}	1.34×10^{-4}	9.01×10^{5}

For brevity, the TDS of each stream in the sensitivity analysis is compared to the median in Table S6. The breakdown of critical minerals is shown in the manuscript in Section 3.4.

Table S6. TDS of landfill leachate sensitivities.

Run	Permeate 1 TDS (mg/L)	Permeate 2 TDS (mg/L)	Brine TDS (mg/L)
Median	13.6894	164.557	28,026.4
25th percentile Li	13.6642	163.984	27,927.9
75th percentile Li	13.5998	169.183	28,594.0
CoDaRT Li	13.7744	167.558	28,395.7
25th percentile Mg	12.5246	162.329	26,140.7
75th percentile Mg	14.2312	175.427	34,287.6
CoDaRT Mg	13.6928	164.657	28,090.0
25th percentile bulk	13.5623	164.55	30,935.7
75th percentile bulk	14.7728	177.566	28,044.9
CoDaRT bulk	13.5692	163.687	28,025.0

Supplementary S1.2. Impoundment Leachate Compositions

The median impoundment leachate is detailed in Table S7.

Table S7. Impoundment leachate median composition from CPInfo; critical minerals are bolded.

Parameter	Value	Parameter	Value	Parameter	Value
Aluminum, mg/L	0.0292	Strontium, mg/L	2.315	Mercury, mg/L	1.00E−06
Arsenic, mg/L	0.3665	Temperature, °C	19.55	TSS, mg/L	2.2
Boron, mg/L	1.49	Thallium, mg/L	2.41E−05	Rhenium, mg/L	3.94E−05
Barium, mg/L	0.169438	**Vanadium, mg/L**	0.000144	Silicon, mg/L	4.138
Calcium, mg/L	81.72	**Zinc, mg/L**	0.00109	Arsenic (III), mg/L	0.002631
Cadmium, mg/L	0.000377	**Lithium, mg/L**	0.0346	Arsenic (V), mg/L	0.052824
Chloride, mg/L	13.255	Carbon, organic, mg/L	5.65	Carbonate, mg/L	0.16257
Cobalt, mg/L	0.000368	Phosphate, mg/L	1.568	Bicarbonate, mg/L	41.90136
Chromium, mg/L	0.000955	TDS, mg/L	1010	**Antimony, mg/L**	0.000138
Copper, mg/L	0.000255	Carbon, inorganic, mg/L	44.1	Uranium, mg/L	0.0109
EC (field), umho/cm	742.5	Eh, mV	138	Alpha, pci/l	31
Iron, mg/L	0.0284	**Fluoride, mg/L**	1.555	Beta, pci/l	490.5
Potassium, mg/L	9.245559	Nitrate nitrogen, mg/L	0.716	pH (lab), SU	7.715
Magnesium, mg/L	14.21	Sulfur, mg/L	24.65	Turbidity (field), NTU	4.335
Manganese, mg/L	0.273	Phosphorus, mg/L	0.5301	Dissolved oxygen (ppm), mg/L	7.475
Molybdenum, mg/L	0.2595	Silica, mg/L	6.87	EC (lab), umho/cm	6300
Sodium, mg/L	45.9	pH (field), SU	7.87		
Nickel, mg/L	0.0015	Sulfate, mg/L	109.7105		

Not all of these values are used as inputs to the OLI Studio software—those inputs are summarized in Table S8.

Table S8. Inputs for impoundment leachate to OLI Studio.

Parameter	Value	Parameter	Value
Total dissolved solids, mg/L	1010	Ni^{+2}, mg/L	1.5×10^{-3}
SiO_2, mg/L	6.87	Ti^{+1}, mg/L	2.41×10^{-5}
$B(OH)_3$, mg/L	8.52	VO^{+2}, mg/L	2.34×10^{-4}
$Sb(OH)_5$, mg/L	2.34×10^{-4}	Zn^{+2}, mg/L	1.09×10^{-3}
Na^{+1}, mg/L	45.9	Li^{+1}, mg/L	0.0346

K^{+1}, mg/L	9.24556	U^{+3}, mg/L	0.0109
Ca^{+2}, mg/L	81.72	Hg^{+2}, mg/L	1×10^{-6}
Mg^{+2}, mg/L	14.21	Rh^{+3}, mg/L	3.94×10^{-5}
Sr^{+2}, mg/L	2.315	Cl^{-1}, mg/L	13.255
Ba^{+2}, mg/L	0.169438	SO_4^{-2}, mg/L	109.711
Fe^{+2}, mg/L	0.0284	HCO_3^{-1}, mg/L	41.9014
Al^{+3}, mg/L	0.0292	AsO_4^{-3}, mg/L	0.68
Cd^{+2}, mg/L	3.77×10^{-4}	CrO_4^{-2}, mg/L	2.55×10^{-4}
Co^{+2}, mg/L	3.68×10^{-4}	PO_4^{-3}, mg/L	1.568
Cu^{+2}, mg/L	2.55×10^{-4}	F^{-1}, mg/L	1.555
Mn^{+2}, mg/L	0.273	NO_3^{-1}, mg/L	3.17
Mo^{+3}, mg/L	0.2595	CO_3^{-2}, mg/L	0.16257

Similar changes are made as with landfill leachate; however, only As(V) is used. The median value for As(V) is 20 times larger than the median for As(III), so it is assumed that only As(V) is present in solution.

For sensitivity analyses, only single components are changed from their initial values—the new values and the impact on TDS are shown in Table S9.

Table S9. Sensitivity values and reconciled TDS values for impoundment leachate.

Simulation	New Value	Reconciled TDS
Median	-	485.7 mg/L
25th percentile Mg	Mg, 9.399 mg/L	466.3 mg/L
75th percentile Mg	Mg, 18.6 mg/L	506.4 mg/L
Bulk 25th percentile	Ca, 64.02 mg/L; SO_4, 68.486 mg/L	470.5 mg/L
Bulk 75th percentile	Ca, 180.25 mg/L; SO_4, 480 mg/L	865.1 mg/L

The outlet streams are shown in Table S10 using the reconciled median feed.

Table S10. Permeate and brine compositions for the median OLI Flowsheet simulation for impoundment leachate.

Parameter (mg/L)	Permeate 1	Permeate 2	Brine
Al(+3)	4.03×10^{-6}	1.74×10^{-5}	0.034093
As(+5)	1.73×10^{-3}	0.020796	7.18984
B(+3)	0.151641	2.2477	24.4778
Ba(+2)	8.80×10^{-6}	7.54×10^{-6}	0.295209
C(+4)	0.265151	12.9065	145.925
Ca(+2)	0.101477	1.12282	1588.89
Cd(+2)	3.50×10^{-7}	3.46×10^{-6}	7.43×10^{-3}
Cl(−1)	0.061905	0.61971	260.007
Co(+2)	3.39×10^{-7}	3.32×10^{-6}	7.26×10^{-3}
Cr(+6)	2.56×10^{-7}	4.13×10^{-6}	2.25×10^{-3}
Cu(+2)	8.15×10^{-6}	1.27×10^{-4}	4.76×10^{-3}
F(−1)	9.39×10^{-3}	0.02141	28.4515
Fe(+2)	3.01×10^{-5}	3.42×10^{-4}	0.559892
H(+1)	1.12×10^{5}	1.12×10^{5}	1.12×10^{5}
Hg(+2)	4.19×10^{-8}	0.503883	1.90×10^{-5}
K(+1)	0.057485	1.15×10^{-3}	181.033
Li(+1)	1.29×10^{-4}	0.128867	0.679761
Mg(+2)	0.012942	2.45×10^{-3}	280.222
Mn(+2)	2.49×10^{-4}	0.012557	5.3836

Mo(+3)	1.45×10^{-3}	0.24493	5.08558
N(+5)	0.024953	1.97007	13.4522
Na(+1)	0.233035	1.35×10^{-5}	900.574
Ni(+2)	1.37×10^{-6}	8.85×10^{5}	0.02958
O(−2)	8.85×10^{5}	2.48×10^{-8}	8.90×10^{5}
P(+5)	-	-	1.01×10^{-5}
Rh(+3)	2.52×10^{-7}	2.25×10^{-6}	7.71×10^{-4}
S(+6)	0.133701	1.4192	1989.94
Sb(+5)	1.23×10^{-6}	1.26×10^{-5}	2.69×10^{-3}
Si(+4)	0.064622	1.09273	61.1707
Sr(+2)	2.69×10^{-3}	0.014927	45.6477
Tl(+1)	1.57×10^{-7}	1.42×10^{-6}	4.72×10^{-4}
U(+3)	9.82×10^{-5}	3.64×10^{-4}	0.213118
V(+4)	1.45×10^{-6}	2.73×10^{-5}	3.46×10^{-3}
Zn(+2)	5.58×10^{-6}	1.16×10^{-5}	0.021412

The TDS of each stream in the sensitivity analysis is compared to the median in Table S11.

Table S11. TDS of impoundment leachate sensitivities.

Run	Permeate 1 TDS (mg/L)	Permeate 2 TDS (mg/L)	Brine TDS (mg/L)
Median	2.42066	28.2404	6706.09
25th percentile Mg	2.40954	28.1146	6247.17
75th percentile Mg	2.42059	28.3636	7126.15
25th percentile bulk	2.23442	28.3037	6707.59
75th percentile bulk	3.21932	28.0549	6697.87

Supplementary S1.3. Combustion Residual Leachate Treatment Standards

The treatment standards for combustion residual leachate are shown in Table S12. These are shown for the federal standard as well as the most stringent regional standard, outlined in earlier work on this topic [2].

Table S12. Combustion residual leachate treatment standards.

Parameter	Federal Standard	Zone 8 (Washington) Standard [2]
Total Suspended Solids, ppm	30	30
Oil/grease, ppm	15	15
Arsenic, ppb	8	-
Mercury, ppt	356	10
Copper, ppb	-	89
Selenium, ppb	-	5.6
Chlorine, ppb	-	12.4
Chromium, ppm	-	0.2
Zinc, ppm	-	1

Supplementary S1.4. Produced Water Compositions

The median values for produced water from the Permian Basin from the United States Geological Survey (USGS) data set are shown in Table S13.

Table S13. Median values for the Permian Basin produced water from the USGS data set; critical minerals are bolded.

Parameter	Value	Parameter	Value
Depth (upper), ft	6749	Bromine, mg/L	224
Depth (lower), ft	7408	Calcium, mg/L	3127.5
Depth (well), ft	7020	Carbonate, mg/L	48.885
Elevation, ft	2895.5	Chlorides, mg/L	59,200
Temperature, F	143.45	Iodine, mg/L	10
pH, SU	6.95	Iron, mg/L	21
Specific gravity	1.077	**Lithium, mg/L**	10.75
Resistivity, Ohm m	0.086	**Magnesium, mg/L**	889.115
Conductivity, μS/cm	138,000	**Manganese, mg/L**	0.885
TDS, mg/L	101,336	Potassium, mg/L	402.87
Ammonia, mg/L	96	Silicon, mg/L	12
Barium, mg/L	2.355	Sodium, mg/L	31,275
Boron, mg/L	19.51	Strontium, mg/L	123.755
Bicarbonate, mg/L	231.005	Sulfate, mg/L	1438.375

The input to OLI Studio is shown in Table S14.

Table S14. Input for produced water to OLI Studio.

Parameter	Value	Parameter	Value
Total dissolved solids, mg/L	1.01336×10^5	Br^{-1}, mg/L	224
SiO_2, mg/L	25.7	CO_3^{-2}, mg/L	48.885
$B(OH)_3$, mg/L	111.6	I^{-1}, mg/L	10
Na^{+1}, mg/L	31,275	Fe^{+2}, mg/L	21
K^{+1}, mg/L	402.87	NH_4^{+1}, mg/L	96
Ca^{+2}, mg/L	3127.5	Li^{+1}, mg/L	10.75
Mg^{+2}, mg/L	889.115	Mn^{+2}, mg/L	0.885
Sr^{+2}, mg/L	123.755	Cl^{-1}, mg/L	59,200
Ba^{+2}, mg/L	2.355	SO_4^{-2}, mg/L	1438.38
HCO_3^{-1}, mg/L	231.005		

The SiO_2 value and $B(OH)_3$ value are calculated from molar weight conversions from Si and B, respectively.

For sensitivity analyses only, single components are changed from their initial values—the changes to those values and the reconciled TDS are shown in Table S15.

Table S15. Reconciled TDS values for input streams for produced water sensitivity analyses.

Simulation	New Value	Reconciled TDS
Median	-	99,304 mg/L
25th percentile Li	Li, 5.76 mg/L	99,315.5 mg/L
75th percentile Li	Li, 17.48 mg/L	99,288.4 mg/L
CoDaRT Li	Li, 9.22 mg/L	99,307.5 mg/L
25th percentile Mg	Mg, 357.533 mg/L	100,665 mg/L
75th percentile Mg	Mg, 2003.77 mg/L	98,778.9 mg/L
CoDaRT Mg	Mg, 895.13 mg/L	99,298.6 mg/L
Bulk 25th percentile	Na, 14,891.8 mg/L; Cl, 24,977.3 mg/L	51,916.6 mg/L
Bulk 60th percentile	Na, 39,360 mg/L; Cl, 76,260.2 mg/L	127,426 mg/L
CoDaRT bulk	Na, 31,055.4 mg/L; Cl, 59,200 mg/L	99,304 mg/L

These CoDaRT data are derived from the machine learning results from the CoDaRT tool; the r^2 values are shown in Table S16. The lithium data are from the run with two features, five classes, and the magnesium data are from the run with four features, five classes. The bulk data use the run with two features and zero classes.

Table S16. CoDaRT results for produced water runs.

Constituent	R^2 (2 Features, 0 Classes)	R^2 (4 Features, 0 Classes)	R^2 (2 Features, 5 Classes)	R^2 (4 Features, 5 Classes)
Li	0.184	0.209	0.442	0.425
Mg	0.57	0.705	0.7	0.762
Na	0.947	0.975	0.963	0.98
Cl	0.995	0.57	0.994	0.159

The outlet streams are shown in Table S17 using the reconciled median feed.

Table S17. Distillate and brine streams from the median-feed produced water simulation.

Parameter (mg/L)	Distillate	Brine
B(+3)	0.0281998	41.4271
Ba(+2)	-	5.00423
Br(−1)	-	475.986
C(+4)	102.396	0.590061
Ca(+2)	-	6645.74
Cl(−1)	5.08804×10^{-5}	1.26×10^{5}
Fe(+2)	-	44.6237
H(+1)	1.11×10^{5}	1.03×10^{5}
I(−1)	-	21.2494
K(+1)	-	856.074
Li(+1)	-	22.8431
Mg(+2)	-	1889.31
Mn(+2)	-	1.88057
N(−3)	103.105	40.7615
Na(+1)	-	71227.1
O(−2)	8.82×10^{5}	8.21×10^{5}
S(+6)	-	1020.24
Si(+4)	1.74×10^{-7}	25.5271
Sr(+2)	-	262.972

For brevity, the TDS of the distillate and brine streams are shown in Table S18 for all sensitivities.

Table S18. TDS of produced water sensitivities.

Run	Distillate TDS (mg/L)	Brine TDS (mg/L)
Median	574.099	208,433
25th percentile Li	576.511	208,684
75th percentile Li	576.504	208,622
CoDaRT Li	578.274	208,124
25th percentile Mg	595.141	209,069
75th percentile Mg	568.694	205,931
CoDaRT Mg	591.252	208,662
25th percentile bulk	600.409	105,282
60th percentile bulk	554.685	272,237

CoDaRT bulk	576.509	208,657

Supplementary S2. Detailed Design Parameters and Costing Data

The following appendices contain more detailed design parameters and costing data used in each treatment system, as well as the costing data used for critical mineral pricing.

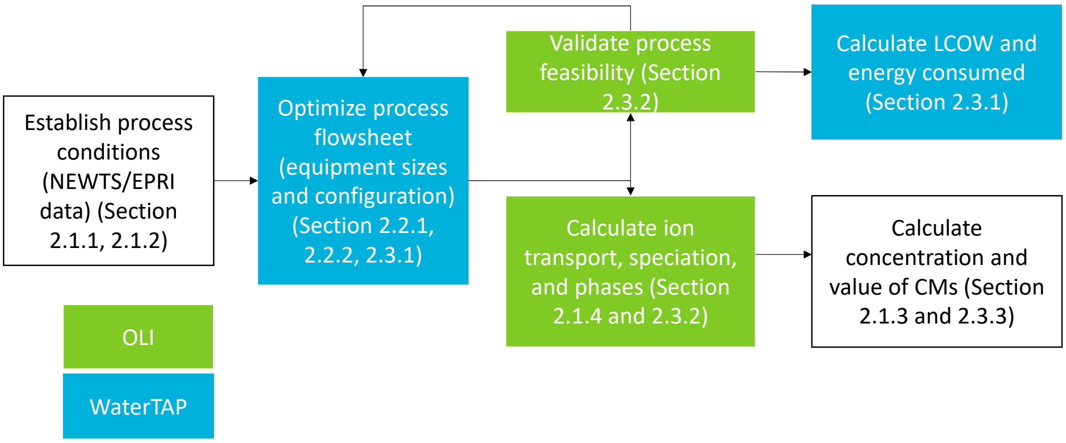

Figure S1. Methods to establish case studies, perform process optimization, and calculate the levelized cost of water (LCOW) of treatment and value of critical minerals in the concentrate using OLI (green) and WaterTAP (blue). The data are first used to calculate the median values for leachate and produced water, along with relevant concentration profile sensitivities. The WaterTAP simulation is then created with this concentration data using the parameters for the performance and cost simulations. OLI Studio data are integrated into this WaterTAP model through reconciliation and a parallel OLI Flowsheet model is used to calculate the resultant brine for critical mineral calculations and validate the WaterTAP simulation. The WaterTAP simulation ultimately calculates the LCOW and other cost values.

Supplementary S2.1. Leachate Treatment System Data

The parameters for the leachate treatment system are shown in Table S19.

Table S19. Leachate treatment system design and costing parameters.

Parameter	Value	Source
Landfill leachate flow rate, gpm	61.8	[8]
Impoundment leachate flow rate, gpm	242	[8]
Reconciled landfill leachate feed TDS, mg/L	2723	-
Reconciled impoundment leachate feed TDS, mg/L	485.7	-
Feed pressure, Pa	101,325	-
Feed temperature, K	298.15	-
Pump efficiency	0.8	-
Pump outlet pressure, MPa	3	-
Membrane 1 volumetric recovery	90%	-
Membrane 2 volumetric recovery	50%	-
Permeate pressure, Pa	101,325	-
BW30-400 water permeability coefficient (A), m/Pa/s	9.63×10^{-12}	[38]
BW30-400 salt permeability coefficient (B), m/s	5.58×10^{-8}	[38]
SW30-HRLE 400 water permeability coefficient (A), m/Pa/s	3.75×10^{-12}	[39]
SW30-HRLE 400 salt permeability coefficient (B), m/s	2.1×10^{-7}	[39]
BWRO equipment cost, USD 2023/m^2	23	[40-43]
SWRO equipment cost, USD 2023/m^2	25	[44, 45]

Pump equipment cost, USD 2023/W	2.2	[43,46]
Settling tank equipment cost, USD 2023/L/s	1800	[46,47]
Membrane replacement cost factor	0.143	[46,29]
Antiscalant cost, USD 2023/L feed	4.5×10^{-6}	[46]

The flow rates are brought from earlier work on national landfill and impoundment leachate volumes [3]. The TDS values are reconciled in OLI studio using the initial values from the Combustion Product Information Database (Supplementary 1, Tables S1 and S7). Ambient conditions are used both for the feed and permeate conditions. The pump outlet pressure was set to 3 MPa (30 bar) to facilitate the selected membrane recoveries at the given TDS in WaterTAP.

The BW30-400 (400 square feet active area) is used for the first membrane and the SW30-HRLE 400 (high rejection, low energy, 400 square feet active area) is used for the second membrane.

The membrane replacement cost factor is dimensionless and multiplied by the cost of the membrane each year to estimate replacement costs.

The water and salt permeability coefficients are used in the WaterTAP simulation. The OLI Flowsheet simulation calculates its own A and B coefficients based on the predetermined salt rejections in the software. For the BWRO (DOW/BW30-400) the salt rejection is set to 99.5% NaCl at 2000 mg/L, and for the SWRO (DOW/SW30HR LE-400) the salt rejection is set to 99.75% NaCl at 32,000 mg/L and 91% $B(OH)_3$ at 5 mg/L. The OLI and WaterTAP simulations therefore differ on their A and B coefficients—this comparison is shown in Table S20. The A coefficients from OLI are converted from units of g/s/m²/Pa using the density of water (997 kg/m³).

Table S20. WaterTAP and OLI permeability coefficients.

Parameter	WaterTAP Value	OLI Value
BW30-400 water permeability coefficient (A), m/Pa/s	9.63×10^{-12}	9.96×10^{-12}
BW30-400 salt permeability coefficient (B), m/s	5.58×10^{-8}	6.32×10^{-8}
SW30-HRLE 400 water permeability coefficient (A), m/Pa/s	3.75×10^{-12}	3.10×10^{-12}
SW30-HRLE 400 salt permeability coefficient (B), m/s	2.1×10^{-7}	2.21×10^{-8} (NaCl), 8.72×10^{-7} ($B(OH)_3$)

Supplementary S2.2. Produced Water Treatment System Data

The parameters for the produced water treatment system are shown below.

Table S21. Produced water treatment system design and costing parameters.

Parameter	Value	Source
Produced water flow rate, gpm	235.8	[13]
Reconciled feed TDS, mg/L	99,304	-
Feed pressure, Pa	101,325	-
Feed temperature, K	298.15	-
Pump efficiency	0.8	-
Feed pump outlet pressure drop, Pa	7000	-
HX outlet pressure drop, Pa	7000	-
Brine/Distillate pump pressure drop, Pa	4000	-
Brine outlet temperature, K	345.15	-
Mass recovery	50%	-
Evaporator U (kW/m²/°C)	3	[48]
Brine heat exchanger (HX) U (kW/m²/°C)	2	[17]
Distillate HX U (kW/m²/°C)	2	[17]
Compression ratio	1.4	[49]

Compressor efficiency	70%	[22]
Evaporator material factor	2.9	[50]
HX material factor	2.9	[50]
HX equipment cost, USD 2023/m^2	399.2	[17]
Evaporator equipment cost, USD 2023/m^2	1331	[17]
Compressor equipment cost, USD 2023/kg/s	14,820	[17,51]
Pump cost, USD 2023/W	2.2	[43,46]

The flow rate for produced water is calculated using 100 wells at the average well volume for the Permian Basin [13]. Some values are brought in as their defaults from WaterTAP [17]. The material factor is used from Analysis, Synthesis, and Design of Chemical Processes [50] for a stainless steel heat exchanger; this is varied in the sensitivity analysis from a 1 (for carbon steel) to a 5 (for nickel alloy).

The output parameters prior to cost optimization are shown in Table S22. During optimization, the compression ratio and vapor outlet temperature are allowed to vary—these results are shown in the manuscript.

Table S22. Outlet parameters calculated from OLI Flowsheet and WaterTAP simulations prior to cost optimization.

Outlet Property	OLI Flowsheet Value	WaterTAP Value
Brine flow rate	25.19 m^3/h	25.14 m^3/h
Brine TDS	208,581 mg/L	186,002 ppm
Distillate flow rate	28.64 m^3/h	28.78 m^3/h
Distillate TDS	578.704 mg/L	-
Brine HX area x U	6.433×10^8 J/K/h	4.778×10^8 J/K/h
Distillate HX area x U	2.974×10^9 J/K/h	6.030×10^8 J/K/h
Compressed vapor pressure	40.77 kPa	40.72 kPa
Compressed vapor temperature	387.34 K	385.77 K
Compressor work	630.72 kW	519.128 kW
Brine HX area	-	66.36 m^2
Distillate HX area	-	83.75 m^2
Evaporator area	-	489.38 m^2

Supplementary S3. PrOMMiS Costing Method and Changes

The Process Optimization and Modeling for Minerals Sustainability (PrOMMiS) costing team has built a Python package for developing dynamic flowsheet simulations using WaterTAP [17] as a base method. The costing method used in this package [24] was developed for a solvent extraction system for rare earth elements; adapting this costing method for the treatment systems discussed in this work thus involves some significant changes to the method, which are outlined below.

Supplementary S3.1. Capital Cost

The equipment costs are used to calculate the bare erected cost, which is used in subsequent capital cost calculations:

$$C_{BEC} = \sum f_{BEC} C_{equip}$$

where:

- C_{equip} = equipment cost (calculated from WaterTAP base methods) [52];
- f_{BEC} = bare erected equipment factor, set to 1.58 for this work [29];
- C_{BEC} = bare erected cost.

This value is used to calculate the total plant cost in the following calculation:

$$C_{TPC} = C_{BEC} + C_{TIC} + C_{other}$$

where:

- C_{TIC} = total installation cost;
- C_{other} = any other plant costs (this is set to 0 in this work);
- C_{TPC} = total plant cost.

The total installation cost is made up of multiple cost categories:

$$C_{TIC} = C_{anc} + C_{build} + C_{EPCM} + C_{cont}$$

where:

- C_{anc} = ancillary cost;
- C_{build} = building cost;
- C_{EPCM} = engineering, procurement and construction management (EPCM) cost;
- C_{cont} = contingency cost (set to 0.15 × C_{BEC}).

Each of these costs are made up of other cost categories (save for the contingency cost), which are all themselves functions of the bare erected cost.

For ancillary costs:

$$C_{anc} = C_{pipeM\&L} + C_{elecM\&L} + C_{inst} + C_{serv}$$

where:

- $C_{pipeM\&L}$ = piping materials and labor cost (set to 0.2 × C_{BEC});
- $C_{elecM\&L}$ = electrical materials and labor cost (set to 0.2 × C_{BEC});
- C_{inst} = instrumentation cost (set to 0.08 × C_{BEC});
- C_{serv} = plant services cost (set to 0.15 × C_{BEC}).

For building costs:

$$C_{build} = C_{procb} + C_{auxb} + C_{sic}$$

where:

- C_{procb} = process building cost (set to 0.4 × C_{BEC});
- C_{auxb} = auxiliary building cost (set to 0.15 × C_{BEC});
- C_{sic} = site improvements cost (set to 0.1 × C_{BEC}).

For EPCM costs:

$$C_{EPCM} = C_{eic} + C_{fec} + C_{pmcc}$$

where:

- C_{eic} = equipment installation cost (set to 0.17 × C_{BEC});
- C_{fec} = field expenses cost (set to 0.12 × C_{BEC});
- C_{pmcc} = project management and construction cost (set to 0.3 × C_{BEC}).

The total plant cost is used to calculate the total overnight cost; in the PrOMMiS method, these are equivalent:

$$C_{TOC} = C_{TPC}$$

where C_{TOC} is the total overnight cost.

The total as-spent cost is calculated as a function of the total overnight cost:

$$C_{TASC} = f_{TASC/TOC} C_{TOC}$$

where:

- $f_{TASC/TOC}$ = TASC/TOC factor, set to 1.207 for a 1-year capital expenditure, 3% capital escalation, and a weighted average cost of capital (WACC) of 7.25% [28];
- C_{TASC} = total as-spent cost.

This total as-spent cost is ultimately used to calculate the annualized capital cost:

$$C_{annual,c} = f_{crf} C_{TASC}$$

where:

- f_{crf} = capital recovery factor, set to 0.0769 for an after tax WACC (ATWACC) of 6.54% and a plant life of 30 years [28];
- $C_{annual,c}$ = annualized capital cost.

Supplementary S3.2. Fixed Operating Costs

The fixed operating costs for the PrOMMiS costing method are ultimately calculated using the following equation:

$$C_{fop} = C_{labor} + C_{MM} + C_{QA/QC} + C_{admin} + C_{patent} + C_{prop} + C_{other} + C_{WaterTAP}$$

where:

- C_{labor} = annual labor cost;
- C_{MM} = maintenance and material cost;
- $C_{QA/QC}$ = quality assurance and control cost;
- C_{admin} = admin and support labor cost;
- C_{patent} = sales patenting and research cost (set to 0 in this work);
- C_{prop} = property taxes and insurance cost;
- C_{other} = other fixed costs (set to 0 in this work);
- $C_{WaterTAP}$ = fixed costs arising from the unit costing models in the WaterTAP base costing method [52];
- C_{fop} = fixed operating cost.

The labor costs are calculated using the following equation:

$$C_{labor} = \left(\sum N_{op,i} C_{oprate,i}\right) \times (1 + \%_{burden}) \times t_{shift} \times N_{shifts} \times N_{days} \times R_{eci}$$

where:

- $N_{op,i}$ = number of operators of type i per shift (only two laborers are used in this work);
- $C_{oprate,i}$ = hourly labor rate for the ith operator type (set to USD 24.81/h) [25];
- $\%_{burden}$ = labor burden (set to 0.25);
- t_{shift} = shift length in hours (set to 8);
- N_{shifts} = number of shifts (set to 3);
- N_{days} = number of operating days in a year (set to 365 but modulated using the utilization factor, discussed in the manuscript);
- R_{eci} = ratio of the employment cost index (ECI) from Q2 2022 (154.0) and the average of the ECI for the four quarters of 2023 (159.4, 161.1, 162.7, 164.4) [26].

The PrOMMiS costing method distinguishes between operating and technical labor by default; however, for the smaller treatment systems shown here, no distinction is made in the flowsheet (as there is only one type of labor).

Other costs are functions of the operating labor or total plant costs, save for patent costs:

- C_{MM} = set to 0.02 × C_{TPC};
- $C_{QA/QC}$ = set to 0.1 × C_{labor};
- C_{admin} = set to 0.2 × C_{labor};

- C_{patent} = set to 0.005 × C_{sales}, the total sales revenue (set to 0 in this work);
- C_{prop} = set to 0.01 × C_{TPC}.

For this work, the WaterTAP costs only include one fixed operating cost that falls outside of the above costs; for membrane replacement, the replacement cost is set to 0.143 × the membrane cost (calculated using the WaterTAP base costing method) [46, 52, 29].

Supplementary S3.3. Variable Operating Costs

The variable operating cost is calculated using the following equation:

$$C_{vop} = \sum C_{vop,r,i} + C_{other} + C_{po} + C_{land} + C_{chem} + C_{waste}$$

where:

- $C_{vop,r,i}$ = variable operating cost of the ith resource;
- C_{other} = other variable costs (set to 0 in this work);
- C_{po} = plant overhead cost;
- C_{land} = annualized land cost (set to 0 in this work);
- C_{chem} = any additional chemical costs (set to 0 in this work—chemicals are included under resources);
- C_{waste} = any additional waste costs (set to 0 in this work—waste production is included under resources);
- C_{vop} = variable overhead cost.

For each resource, the variable operating cost is calculated as follows:

$$C_{vop,r} = C_r \dot{n}_r t_{shift} N_{shifts} N_{days}$$

where:

- C_r = price of the resource;
- $\dot{n}_r$ = consumption rate of the resource (or production for waste disposal).

These resources include electricity, antiscalant, and liquid and solid waste disposal in this work. The plant overhead cost is calculated using the following equation:

$$C_{po} = 0.2\ (C_{fop} + C_{vop,power} + C_{land} + \sum C_{vop,chem,i} + \sum C_{vop,waste,i} + C_{chem} + C_{waste})$$

where:

- $C_{vop,power}$ = variable operating cost of electricity;
- $C_{vop,chem,i}$ = variable operating cost of the ith chemical;
- $C_{vop,waste,i}$= variable operating cost of the ith waste disposal type.

Supplementary S3.4. Annualized Cost and Levelized Cost of Water (LCOW)

The annualized plant cost is calculated as the sum of the three cost categories:

$$C_{annual} = C_{annual,c} + C_{fop} + C_{vop}$$

where C_{annual} is the annualized plant cost. This is used to calculate the LCOW in the following relation:

$$LCOW = \frac{C_{annual}}{f_{util} Q}$$

where:

- f_{util} = utilization factor (set to 1 but varied in sensitivity analyses);
- Q = flow rate of treated water (permeate or distillate).

Supplementary S4. OLI Flowsheets and Parameters

This section describes the flowsheets created in OLI for the purpose of analyzing the feasibility of treatment and the composition of the brine in both systems.

Supplementary S4.1. Leachate Treatment

An image of the flowsheet is shown in Figure S2.

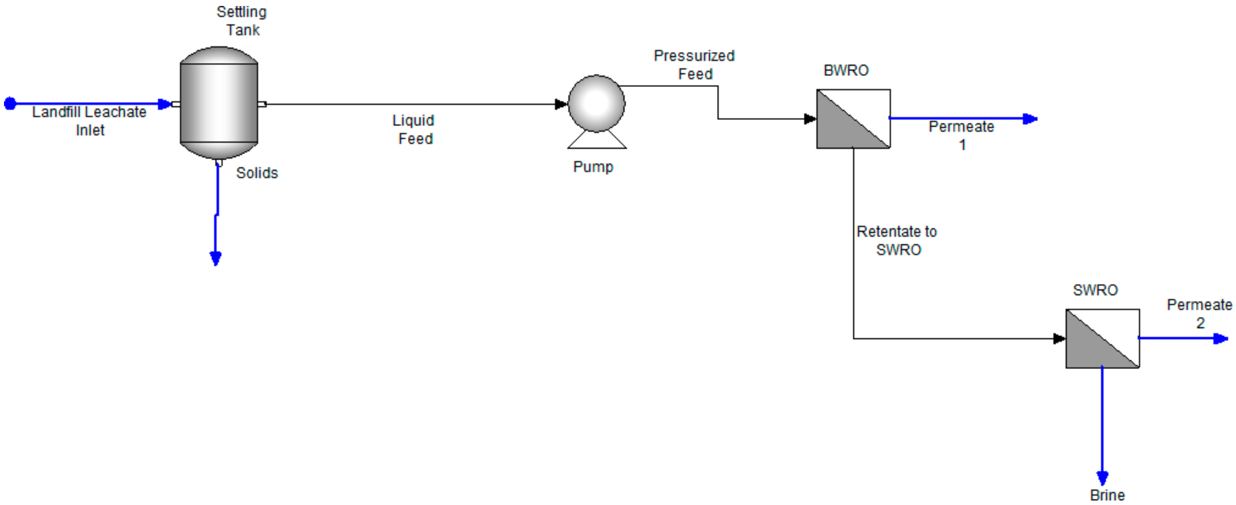

Figure S2. OLI Flowsheet simulation for leachate treatment.

For this flowsheet, the inlet is first brought to the settling tank for solids removal. It is assumed that the solids stream is 100 percent solid (0 percent liquid); however, it is also assumed that the liquid feed stream still contains 1 × 10^{-5} solids by mass to simulate a small degree of entrainment.

The pump pressure is set to 30 bar (same as the WaterTAP simulation) with 80 percent pump efficiency.

The brackish water reverse osmosis (BWRO) membrane is set to use as many vessels as needed to achieve a permeate recovery of 90 percent by volume; this is achieved using the DOW/BW30-400 membrane in the OLI Flowsheet simulation.

The retentate is fed to the seawater reverse osmosis (SWRO) block, which achieves a 50 percent recovery by volume using the DOW/SW30HR LE-400 membrane.

For analyses with the WaterTAP simulation, it was desired to assess the degree of solids created in the retentate; for this, an additional simulation was created, as shown in Figure S3.

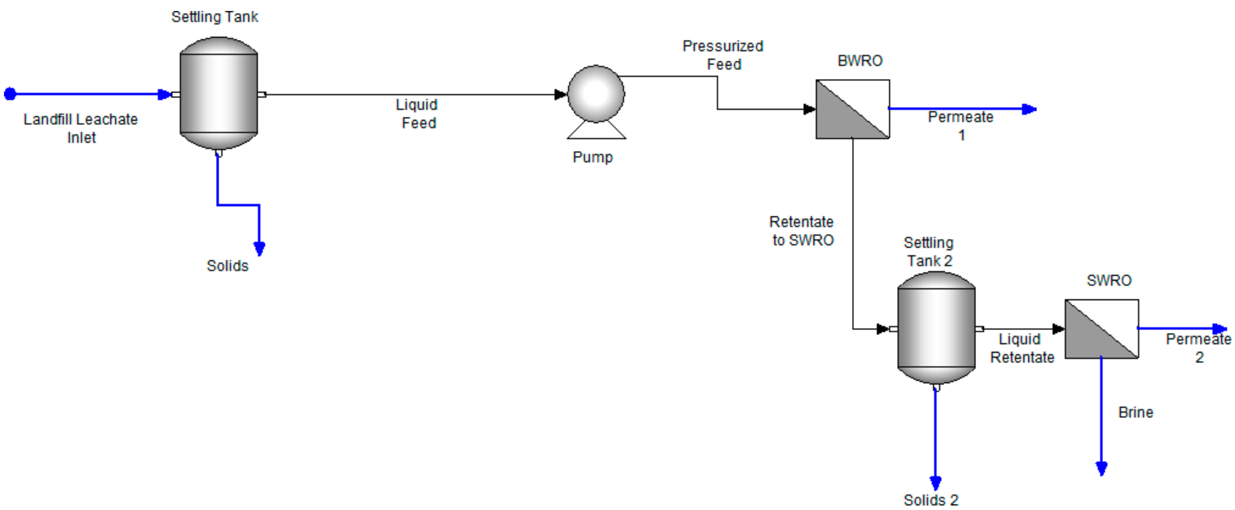

Figure S3. OLI Flowsheet simulation to estimate solids removal.

This is also performed in the WaterTAP simulation to shift the TDS to match the retentate in the OLI Flowsheet simulation. It should be noted that the settling tank shown here is not costed (as it is not real), but it is simply used to bring the WaterTAP and OLI Flowsheet results in line with one another.

Supplementary S4.2. Produced Water Treatment

An image of the flowsheet is shown in Figure S4.

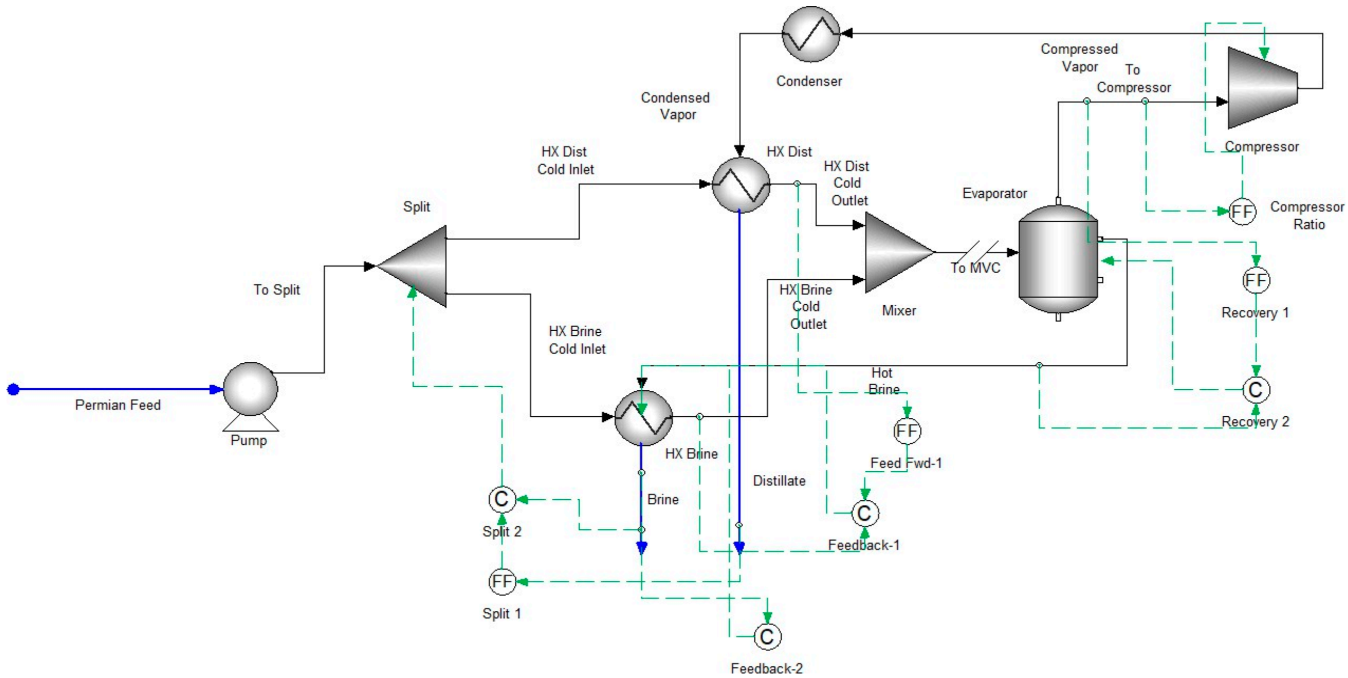

Figure S4. OLI Flowsheet for produced water treatment.

The feed is fed through a low-pressure pump (discharge pressure of 115.33 kPa) before being split between the brine and distillate heat exchangers (HX Brine and HX Dist). This split is controlled using the "Split 2" controller shown in Figure S4. This controller uses the "Split 1" controller to keep the brine and distillate outlet temperatures within 10 degrees of one another—"Split 1" thus feeds a temperature goal value to "Split 2".

The brine and distillate heat exchangers are set to a discharge temperature of 340.95 K (from the WaterTAP simulation)—this is further modulated by the "Feedback-1" controller to keep their discharge temperatures in line with one another (to within 4 degrees). An additional controller "Feedback-2" can also act on the brine HX discharge temperature to keep the brine temperature between 27 and 47 °C (to ensure a minimum temperature approach of 2 °C in the exchangers). Both of these controllers are turned on or off as needed during the different feed sensitivities. In addition, the condenser is modulated between 0% and 1×10^{-5}% vapor to ensure convergence.

The outlets to these exchangers are then mixed (adiabatically, with no mixing tank in OLI Flowsheet) before being fed to the evaporator. The stream "To MVC" is the tear stream for the simulation, initially set to 340.95 K and 115.33 kPa as well as the flow rate used in the manuscript.

The evaporator block is simply a "separator" in OLI Flowsheet—this sets the vapor temperature to 348.15 K. The vapor/liquid split is set using the "Recovery 1" and "Recovery 2" controllers, which ultimately set the mass flow rates equal to one another. The vapor is then compressed, using the "Compressor Ratio" controller (set to 1.67 from the

WaterTAP optimization) to set the discharge pressure. The compressed vapor is then sent to the condenser block (setting the vapor fraction to 0) before being fed to the distillate heat exchanger.

Supplementary S5. Critical Mineral Recovery Values

The full value of the critical minerals present in landfill leachate is shown in Table S23. Much of the value of this brine is from Li and Mg. The value (in USD/m³ feed) is significantly lower than the LCOW from Section 3.3.1 (USD 8.57/m³); thus, the cost of treatment is not likely to be offset by the value of critical minerals at the median concentration values for landfill leachate.

Table S23. Landfill leachate recovery values.

Element	Mass (kg/Year)	Value (USD 2023/Year)	Value (USD 2023/m³ Brine)	Value (USD 2023/m³ Feed)	Value (USD 2023/m³ Permeate)
Aluminum	0.111	USD 0.32	USD 0.00	USD 0.00	USD 0.00
Arsenic	1.28	USD 5.64	USD 0.00	USD 0.00	USD 0.00
Antimony	0.0200	USD 0.25	USD 0.00	USD 0.00	USD 0.00
Barium (as barite)	1.40	USD 0.21	USD 0.00	USD 0.00	USD 0.00
Cobalt	0.115	USD 4.30	USD 0.00	USD 0.00	USD 0.00
Chromium	0.0244	USD 0.16	USD 0.00	USD 0.00	USD 0.00
Fluoride (as fluorspar)	221	USD 79.47	USD 0.01	USD 0.00	USD 0.00
Lithium	128	USD 5872.74	USD 0.94	USD 0.05	USD 0.05
Magnesium	3570	USD 39,314.28	USD 6.26	USD 0.32	USD 0.34
Manganese	89.6	USD 0.45	USD 0.00	USD 0.00	USD 0.00
Nickel	0.589	USD 12.73	USD 0.00	USD 0.00	USD 0.00
Vanadium	0.577	USD 11.76	USD 0.00	USD 0.00	USD 0.00
Zinc	1.14	USD 3.82	USD 0.00	USD 0.00	USD 0.00
Total	4010	USD 45,306.13	USD 7.22	USD 0.37	USD 0.39

The sensitivities for landfill leachate are shown in Table S24. Machine learning data are additionally brought in from the CoDaRT tool—the median Li value shifts the brine value considerably but has a negligible impact on the value of the feed. Even at the highest level (USD 1.07/m³ feed), this would not be justified based on the cost of treatment; however, the brine value is significant enough to potentially warrant recovery if this type of volume reduction is already being employed at a landfill leachate treatment site.

Table S24. Feed sensitivities for CM recovery values for landfill leachate.

Parameter	Mass (kg/Year)	Value (USD 2023/Year)	Total Value (USD 2023/m³ Brine)	Total Value (USD 2023/m³ Feed)
Median Li	128	USD 5872.74	USD 7.22	USD 0.37
25th percentile Li	50.1	USD 2304.15	USD 6.65	USD 0.34
75th percentile Li	577	USD 26,538.42	USD 10.51	USD 0.54
CoDaRT median Li	420	USD 19,275.71	USD 9.35	USD 0.48
Median Mg	3570	USD 39,314.28	USD 7.22	USD 0.37
25th percentile Mg	1210	USD 13,327.27	USD 3.08	USD 0.16
75th percentile Mg	11,417	USD 125,851.90	USD 21.00	USD 1.07
CoDaRT median Mg	3650	USD 40,193.97	USD 7.36	USD 0.37

The impoundment leachate values are shown in Table S25. The total value of this brine is higher due to the difference in mass; however, this is weighted even more heavily towards Mg and is lower in USD/m³ feed. At USD 0.17/m³ (compared to the LCOW of USD 2.87/m³), there is limited potential for critical mineral recovery to offset treatment costs.

Table S25. Impoundment leachate recovery values.

Element	Mass (kg/Year)	Value (USD 2023/Year)	Value (USD 2023/m³ Brine)	Value (USD 2023/m³ Feed)	Value (USD 2023/m³ Permeate)
Aluminum	0.832	USD 2.38	USD 0.00	USD 0.00	USD 0.00
Arsenic	175	USD 773.36	USD 0.03	USD 0.00	USD 0.00
Antimony	0.0655	USD 0.81	USD 0.00	USD 0.00	USD 0.00
Barium (as barite)	12.2	USD 1.84	USD 0.00	USD 0.00	USD 0.00
Cobalt	0.177	USD 6.63	USD 0.00	USD 0.00	USD 0.00
Chromium	0.0548	USD 0.37	USD 0.00	USD 0.00	USD 0.00
Fluoride (as fluorspar)	2850	USD 1026.79	USD 0.04	USD 0.00	USD 0.00
Lithium	16.6	USD 762.80	USD 0.03	USD 0.00	USD 0.00
Magnesium	6840	USD 75,353.94	USD 3.09	USD 0.16	USD 0.16
Manganese	131	USD 0.66	USD 0.00	USD 0.00	USD 0.00
Nickel	0.722	USD 15.59	USD 0.00	USD 0.00	USD 0.00
Vanadium	0.0845	USD 1.72	USD 0.00	USD 0.00	USD 0.00
Zinc	0.522	USD 1.75	USD 0.00	USD 0.00	USD 0.00
Total	10,000	USD 77,948.64	USD 3.20	USD 0.16	USD 0.17

As the dominant factor, a sensitivity was performed on the value of Mg in Table S26. In USD/m³ brine, the value does change considerably, even at the peak; however, the value in USD/m³ feed is substantially lower than the cost of treatment.

Table S26. Impoundment leachate magnesium sensitivity.

Parameter	Mass (kg/Year)	Value (USD 2023/Year)	Total Value (USD 2023/m³ Brine)	Total Value (USD 2023/m³ Feed)
Median Mg	6840	USD 75,353.94	USD 3.20	USD 0.16
25th percentile Mg	4520	USD 49,841.92	USD 2.15	USD 0.11
75th percentile Mg	8950	USD 98,633.82	USD 4.15	USD 0.21

The produced water recovery value is shown in Table S27. Unlike leachate, the value may be substantial enough to warrant treatment for recovery's sake.

Table S27. Produced water recovery values.

Element	Mass (kg/Year)	Value (USD 2023/Year)	Value (USD 2023/m³ Brine)	Value (USD 2023/m³ Feed)	Value (USD 2023/m³ Distillate)
Barium (as barite)	1880	USD 281.64	USD 0.00	USD 0.00	USD 0.00
Lithium	5040	USD 231,985.28	USD 1.05	USD 0.49	USD 0.92
Magnesium	417,000	USD 4,597,874.08	USD 20.83	USD 9.80	USD 18.25
Manganese	415	USD 2.08	USD 0.00	USD 0.00	USD 0.00
Total	**424,000**	**USD 4,830,143.08**	**USD 21.88**	**USD 10.30**	**USD 19.18**

The sensitivities are shown in Table S28. The magnesium value is far more impactful, creating a brine worth USD 47.90/m³.

Table S28. Produced water CM sensitivities.

Parameter	Mass (kg/Year)	Value (USD 2023/Year)	Total Value (USD 2023/m³ Brine)	Total Value (USD 2023/m³ Feed)
Median Li	5040	USD 231,985.28	USD 21.88	USD 10.30
25th percentile Li	2700	USD 124,301.07	USD 21.41	USD 10.07
75th percentile Li	8200	USD 377,218.92	USD 22.57	USD 10.60
CoDaRT median Li	4330	USD 198,967.95	USD 21.70	USD 10.23
Median Mg	417,000	USD 4,597,874.08	USD 21.88	USD 10.30
25th percentile Mg	168,000	USD 1,848,902.45	USD 9.42	USD 4.44
75th percentile Mg	940,000	USD 10,362,030.64	USD 47.90	USD 22.58
CoDaRT median Mg	419,000	USD 4,628,976.88	USD 22.04	USD 10.36

Supplementary S6. Exergy Analysis

An exergy analysis was conducted on the MVC system for produced water (Figure S5) to understand potential improvements in system performance to reduce overall costs. Additional streams were added to the OLI flowsheet to conduct the analysis. A summary of the outputs and calculations is contained in the Supplementary Data excel file. The analysis found that the total electrical energy into system via pumps and compressor is 1011 kW, minimum theoretical work of separation is 102 kW, the exergy efficiency is 10% and exergy efficiency if all thermal heat is used is 13%. A breakdown of exergy destruction across the system is shown in Table S29.

Table S29. Breakdown of exergy destruction.

	Brine HX	Distillate HX	MVC	Compressor and Pump	ChemExergy Remaining	Thermal Exergy Remaining or Lost to Env
Exergy (kW)	55	68	538	219	102	29
Percent Contribution	5.4%	6.7%	53.3%	21.6%	10.1%	2.9%

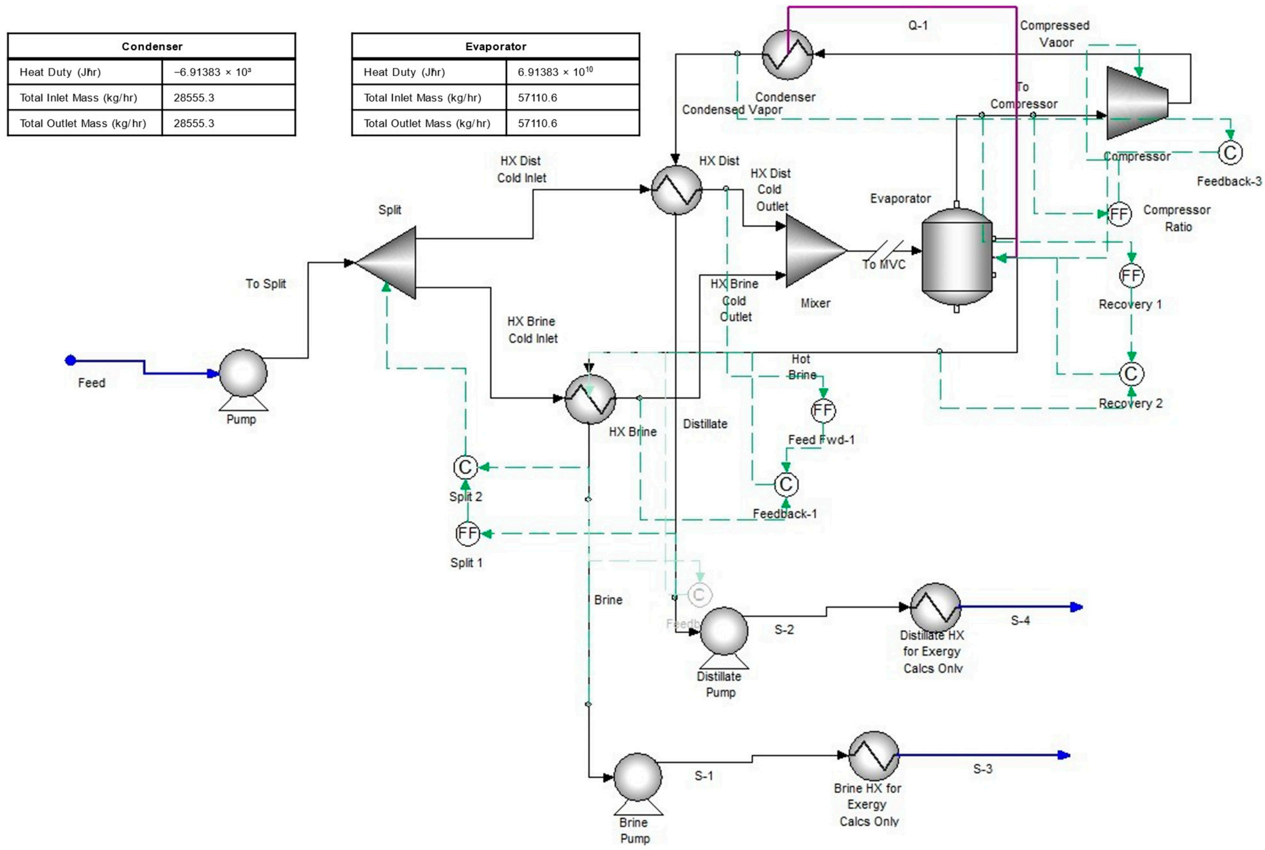

Figure S5. OLI Flowsheet for exergy analysis.