Supplementary material

Environmental and life cycle assessment of lithium carbonate production from Chilean Atacama brines

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1. Life Cycle Inventory

We present below further information of the life cycle inventory of lithium carbonate production, including effects of brine extraction, evaporation, and chemical production processes. The inputs and outputs of each individual unit process were modelled in Sphera software[1] and were calculated from the whole process net input and output data based on the process flow diagram (Fig.1). A summary of the lithium carbonate production input and output inventory is presented in Tables A1 and A2.

Table A1. Brine extraction and evaporation

Description	Input	Output	Unit	Ecoinvent 3.9.1 process and comments
Pumped brine	327		kg	
Diesel	9.44×10^{-5}		kW h	Diesel, burned in diesel-electric generating set
Electrical energy	1.442		kW h	SING electricity grid mix
Heavy fuel oil	1.02×10^{-6}		kW h	Electricity from heavy fuel oil
Precipitation	1.03		kg	Water, harvested from rainwater
Fresh water	18.7		kg	Pumped from four water wells
Reinjected brine		79.1	kg	
Evaporated water		177	kg	
Lithium brine		3.3	kg	
Waste salts		68.9	kg	Wastes are accumulated at the edge of the salar
Waste water		18.7	kg	

Table A2. Lithium carbonate chemical production

Description	Input	Output	Unit	Ecoinvent 3.9.1 process and comments
Lithium brine	3.3		kg	Concentrated lithium brine, at plant
Transportation	230		km	Transport, freight, lorry 16-32 tonne
Hydrochloric acid	0.04		kg	Hydrochloric acid (32 %)
Fresh water	12.5		kg	Water, ultrapure
Boron		0.0305	kg	Boric acid, anhydrous, powder
Extraction solvent	0.014		kg	2-Ethyl-1,3-hexanediol
Organic diluent	0.055		kg	Solvent 100, > 99 % Trimethylbenzenes
Sodium hydroxide	3.36		kg	Sodium hydroxide, 50 % in H_2O
Sodium carbonate	1.81		kg	Sodium carbonate, 30 % in H_2O
Lime milk	2.85×10^{-3}		kg	Lime water, 20 % in H_2O
$CaCO_3$		8.59×10^{-3}	kg	
$Mg(OH)_2$		1.43×10^{-5}	kg	
$MgCO_3$		0.17	kg	
Liquefied petroleum gas	4.64×10^{-10}		kg	Liquefied petroleum gases and other gaseous hydrocarbons, except natural gas
Natural gas	4.89×10^{-8}		m^3	Natural gas, liquefied
Heavy fuel oil	7.86×10^{-7}		kW h	Electricity from heavy fuel oil
Electricity	0.349		kW h	Northern Chilean electricity grid mix
Mother liquor		7.95	kg	
Evaporated water		0.119	kg	Evaporated by drying process
Liquid waste		11.8	kg	
Lithium carbonate		1	kg	

2. Waste management

The parameters used in waste management modelling are presented in this section.

Table A3. Parameters of waste management

Description	Value	Unit	Description
$H_{p\ (\mathrm{unlined})}$	18.2	m	Wastewater depth and depth of loose sediment.[2]
D_{fc}	0.10	m	Thickness of consolidated sediment layer.[3]
D_{clog}	0.50	m	Thickness of clogged soil layer.[3]
K_{fc}	1.26×10^{-9} to 1.77×10^{-9}	$m\ s^{-1}$	Saturated hydraulic conductivity of the consolidated sediment.[3]
K_{clog}	10 % K_{soil}	$m\ s^{-1}$	Saturated hydraulic conductivity of the clogged soil.[3]
K_{soil}	1×10^{-6}	$m\ s^{-1}$	Saturated hydraulic conductivity of native soil.[4]
$H_{p\ (\mathrm{single\ lined})}$	18.3	m	Wastewater depth and depth of loose sediment.[2]
D_{liner}	0.916	m	Thickness of liner.[2]
K_{liner}	1×10^{-9}	$m\ s^{-1}$	Saturated hydraulic conductivity of liner.[2]
A	10^{-5} to 10^{-4}	m^2	A defect area for liner.[5]
K_s	1×10^{-9}	$m\ s^{-1}$	Hydraulic conductivity of the low-permeability soil underlying the geomembrane.[2]
H	≤ 0.3	m	The leachate head above the geomembrane component of the composite liner.[5]
P	1	Number per acre	Density of installation defects.[5]
S	537.9	m^2	Footprint of surface impoundment.[6]

3. Evaporation modelling

The parameters used in evaporation modelling are presented in Table A4. The temperature and relative humidity (RH) were sourced from SQM Meteorología Estación Meteorológica KCL[7]; the bright sunshine hours per day (n), the latitude of the site (Ø) and the maximum possible duration of daylight (N) were sourced from Meteo Chile, Estación Cerro Moreno Antofagasta Ap. (230001), which is the nearest available meteorology station to the study area.[8]

Table A4. Parameters used in evaporation modelling.

Parameter / Unit	January	February	March	April	May	June	July	August	September	October	November	December
Number	1	2	3	4	5	6	7	8	9	10	11	12
T / °C	17.31	17.84	18.02	15.77	12.81	8.32	8.81	12.61	14.76	16.53	17.32	18.90
n / hours	11.43	10.83	10.17	9.24	7.33	6.94	6.48	7.25	6.69	6.94	8.19	9.85
Ø / rad	-0.411	-0.411	-0.411	-0.411	-0.411	-0.411	-0.411	-0.411	-0.411	-0.411	-0.411	-0.411
N / hours	13.48	12.91	12.10	11.26	10.62	10.36	10.55	11.14	11.96	12.80	13.42	13.64
R_s / MJ m^{-2} d^{-1}	23.99	23.97	23.69	22.79	20.95	20.42	20.27	21.29	21.27	21.46	22.01	22.88
R_s / kW h $m^{-2}d^{-1}$	6.66	6.66	6.58	6.33	5.82	5.67	5.63	5.91	5.91	5.96	6.11	6.36
R_A / MJ $m^{-2}d^{-1}$	33.70	33.79	33.37	32.32	31.15	30.59	31.01	32.13	33.24	33.76	33.73	33.62
R_A / kW h $m^{-2}d^{-1}$	9.36	9.38	9.27	8.98	8.65	8.50	8.61	8.92	9.23	9.38	9.37	9.34
RH / %	25.86	32.80	36.31	24.05	17.46	14.94	15.55	13.48	12.96	17.46	13.75	12.83
E_{PEN} / mm d^{-1}	8.47	7.72	7.47	6.78	5.69	4.60	4.70	5.87	6.71	7.55	7.95	8.58

4. Evaporation correction

Detailed parameters used to implement the evaporation correction are presented in Table A5. The salinity reduction coefficient is related to the liquid density, calculated from equation 1.[9]

$$y = -3.7628x^2 + 6.3353x - 1.5725 \; (R^2 = 0.9775) \tag{1}$$

Table A5. Parameters used to implement the evaporation correction.

Description	Value	Unit	Description
K_e	0.7	1	Pond coefficient (dimensionless), which equals to 0.7[9]
K_s	0.55	1	Salinity reduction coefficient (dimensionless)
E_t	-	mm day^{-1}	Evaporation rate of each scenario
X	1.223	g cm^{-3}	Average density of brine[10]

5. Water balance

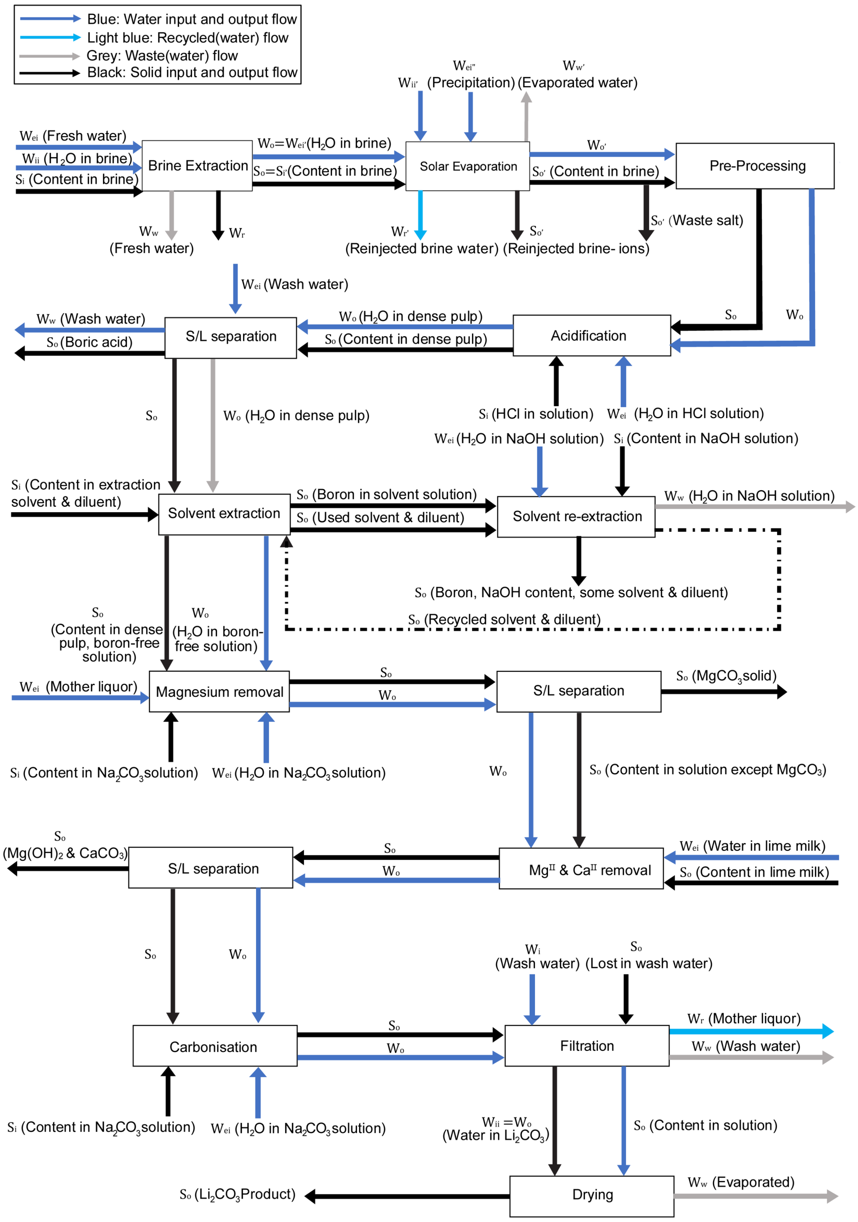

Fig. A1. Water balance flow chart of lithium carbonate production from brine.

6. Water Footprint

The detailed contributions to water footprint are shown in Fig. 9 in the article and the specific numbers for each contribution are summarised in Table A6 in the order of production.

Table A6. Contributions to water footprint.

Description	Scenario 1	Scenario 2	Scenario 3	Unit
Precipitation	1.03	1.03	1.03	kg per kg Li_2CO_3
Electricity supply at salar	0.623	0.623	0.623	
Heavy fuel oil usage at salar	1.65×10^{-6}	1.65×10^{-6}	1.65×10^{-6}	
Diesel usage at salar	2.47×10^{-5}	2.47×10^{-5}	2.47×10^{-5}	
Evaporated water	176.81	163.08	202.74	
Water pump operation	0.736	0.736	0.736	
Fresh water usage at salar	18.7	18.7	18.7	
Electricity supply at plant	0.163	0.163	0.163	
Heavy fuel oil usage at plant	1.27×10^{-6}	1.27×10^{-6}	1.27×10^{-6}	
Liquefied petroleum gas usage	3.91×10^{-9}	3.91×10^{-9}	3.91×10^{-9}	
Liquefied natural gas usage	4.22×10^{-8}	4.22×10^{-8}	4.22×10^{-8}	
Hydrochloric acid usage	0.087	0.311	0.025	
Market for soda ash	29.19	152.60	12.37	
Market for quicklime	1.98×10^{-3}	1.04×10^{-2}	8.42×10^{-4}	
Market for ultrapure water	5.91	24.48	3.32	
Sodium hydroxide solution production	105.12	551.69	44.74	

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