nature energy

Supplementary information https://doi.org/10.1038/s41560-024-01676-7

Techno-economic assessment of thin lithium metal anodes for solid-state batteries

In the format provided by the authors and unedited

Table of Contents

Supplementary Methods

Production Costs

The production costs of the thermally evaporated Li metal anodes can be broken down into nine categories:

- **Li_2CO_3:** the raw Li source material used in this techno-economic assessment (see Methods - Lithium Cost)
- **Processing Li_2CO_3:** the cost to convert the raw Li source into pure Li for thermal evaporation (see Methods - Lithium Cost)
- **Labour:** required to operate and maintain the thermal evaporator
- **Electricity:** to power the thermal evaporator
- **Depreciation:** the initial capital expenditure spread over 7 years
- **Variable overhead:** see Methods - Variable Overhead Cost
- **General Sales and Administration Cost:** see Methods - General Sales and Administration Cost
- **Financing:** The cost to borrow the money required for capital expenditure (see Methods - Financing)
- **Other Manufacturing Costs:** see Methods - Other Manufacturing Costs

Lithium Utilisation

Thermal evaporation can achieve high utilisation rates and small thickness variations when line sources are used. The lithium utilisation and film thickness variation that can be achieved using thermal evaporation have been estimated in this work with a deposition model. To achieve no more than 4% thickness variation across the entire film, a line source with a width 0.24 m larger than the substrate is required. With this setup, deposition efficiencies greater than 82% can be achieved for 1.2 m substrates, which increases with increasing substrate width.

In order to determine the percentage of the thermally evaporated lithium that can be successfully utilised, it is necessary to develop a simple model of the thermal evaporation system to describe how lithium deposition rate varies with position.

First we consider a small surface source, shown schematically in Supplementary Fig. 3a. The lithium deposition rate, t, is highest immediately above the source, at position $x = 0$. The normalised deposition rate varies with position, x, and source-substrate separation, H, according to Supplementary Eq. 1:[1]

$$\frac{t(x)}{t(0)} = \frac{1}{\left(1 + \left(\frac{x}{H}\right)^2\right)^2} \tag{1}$$

The normalised deposition rate from a surface source is plotted in Supplementary Fig. 3b for $H = 8$ cm, which is a typical source-substrate separation for other thermal evaporation technologies produced by Emerson and Renwick. It is evident that the deposition rate varies significantly with position, so larger, line sources are required for more homogeneous deposition over larger areas, as shown schematically in Supplementary Fig. 3a. Each infinitesimal element of the line source behaves like a surface source, and the contribution to the deposition rate, $t_{x'}$, due to the infinitesimal element of the source at x' varies with position x according to Supplementary Eq. 2:

$$t_{x'}(x) \propto \frac{1}{\left(1+\left(\frac{x-x'}{H}\right)^2\right)^2} \tag{2}$$

The total deposition rate distribution from the line source can then be calculated by integrating over all infinitesimal elements along the width of the source, W_{source}, according to Supplementary Eq. 3:[1,2]

$$t(x) \propto \int_{-a}^{a} \frac{1}{\left(1+\left(\frac{x-x'}{H}\right)^2\right)^2}\, dx', \qquad a = \frac{1}{2}W_{\text{source}} \tag{3}$$

Completing this integration results in the deposition rate distribution given in Supplementary Eq. 4, which has again been normalised to the maximum deposition rate at $x = 0$.

$$\frac{t(x)}{t(0)} = \frac{\frac{1}{2}\arctan\left(\frac{x+a}{H}\right) - \frac{1}{2}\arctan\left(\frac{x-a}{H}\right) + \frac{aH(a^2+H^2-x^2)}{((x+a)^2+H^2)((x-a)^2+H^2)}}{\arctan\left(\frac{a}{H}\right) + \frac{aH}{a^2+H^2}} \tag{4}$$

The deposition efficiency can then be estimated according to Supplementary Eq. 5, which considers the total amount of lithium that is deposited onto the substrate, with width $W_{\text{substrate}}$, compared to the total amount emitted from the source.

$$\text{Efficiency}\,(\%) = \frac{\int_{-\frac{1}{2}W_{\text{substrate}}}^{\frac{1}{2}W_{\text{substrate}}} t(x)\, dx}{\int_{-\infty}^{\infty} t(x)\, dx} \times 100 \tag{5}$$

The thickness variation across the deposited film can also be estimated according to Supplementary Eq. 6. This determines the percentage reduction in thickness at the extreme edges of the substrate, where the film is thinnest, compared to the maximum thickness in the centre.

$$\text{Variation}\,(\%) = \left(1 - \frac{t\left(\frac{1}{2}W_{\text{substrate}}\right)}{t(0)}\right) \times 100 \tag{6}$$

Emerson and Renwick already produce thermal evaporators with $W_{\text{substrate}} = 1.2$ m and $W_{\text{source}} = 1.44$ m, so this configuration is modelled in Supplementary Fig. 3c, giving a deposition efficiency of 82.92% and a thickness variation of 3.98%. It is therefore assumed that all of the substrate can be used, and the lithium utilisation is also 82.92%.

An additional configuration with $W_{\text{substrate}} = 3$ m and $W_{\text{source}} = 3.24$ m was also modelled to estimate the lithium utilisation in a system more suitable for gigafactory-scale production. As shown in Supplementary Fig. 3d, this gives a similar thickness variation of 4.02% and a higher lithium utilisation of 92.41%.

This line source model has been implemented in Python and is available as a supplementary file. It can be used to estimate deposition efficiency and thickness variation for any combination of H, W_{source} and $W_{\text{substrate}}$.

Machine Costing

First 1.2 m machine = $5 million
First 3 m machine = $6.5 million (30% more)
Second 1.2 m machine = $3.5 million (30% less, as does not need to be designed anymore)
Second 3 m machine = $4.55 million (30% less, as does not need to be designed anymore)
Bulk Order of 1.2 m machine = $1.75 million (50% less than second machine due to economies of scale)
Bulk Order of 3.0 m machine = $2.275 million (50% less than second machine due to economies of scale)
Average gigafactory has an output of 35 GWh yr^{-1}, and would need 744 1.2 m machines to meet that output, or 298 3 m machines.

744×1.2 m machine = $744 \times \$1.75$ million per machine (50% of the cost of the second machine) = \$1302 million order
298×3 m machine = $298 \times \$2.275$ million per machine (50% of the cost of the second machine) = \$677.95 million order

Supplementary Tables

Supplementary Table 1 Maximum excess lithium allowed with at different loading capacities to achieve an energy density of 1000 Wh L^{-1}. Target efficiency required to achieve 75% capacity retention after 1250 cycles

Areal Capacity mAh cm^{-2}	**Maximum Excess Lithium Thickness** µm	**N Capacity from Li Foil** mAh cm^{-2}	**N Capacity from NMC** mAh cm^{-2}	**N:P Ratio** —	**Target Efficiency** %
2	Cannot achieve 1000 Wh L^{-1}	—	2.352	1.176	99.964
3	Cannot achieve 1000 Wh L^{-1}	—	3.529	1.176	99.964
4	1	0.206	4.705	1.228	99.961
5	12	2.474	5.881	1.671	99.936
5.4	17	3.505	6.351	1.825	99.929
6	23	4.742	7.057	1.967	99.923
7	34	7.011	8.233	2.178	99.915
8	45	9.279	9.410	2.336	99.909

Supplementary Table 2 Labour, variable overheads and general sales and administration costs scaling factors.[3–14]

Country	Scaling Factor
Argentina	0.31871
Australia	1.28153
Austria	1.03251
Belgium	1.09202
Bulgaria	0.22252
Canada	1.21524
Chile	0.3714
China	0.33745
Colombia	0.17205
Croatia	0.25435
Czechia	0.42349
Denmark	1.34949
Estonia	0.48519
Finland	0.97946
France	0.87525
Germany	0.95398
Hungary	0.28436
Ireland	1.11166
Italy	0.66169
Japan	0.68569
Latvia	0.41891
Lithuania	0.50601
Luxembourg	1.58847
Mexico	0.19723
Netherlands	1.09709
Nicaragua	0.07442
Norway	1.35481
Poland	0.33873
Portugal	0.42651
Romania	0.32916
Russian Federation	0.22358
Serbia	0.16069
Singapore	1.08033
Slovakia	0.36215
Slovenia	0.62517
Spain	0.61098
Sweden	0.94841
Switzerland	1.94005
Ukraine	0.12455
United Kingdom	1.00000
United States	1.54439

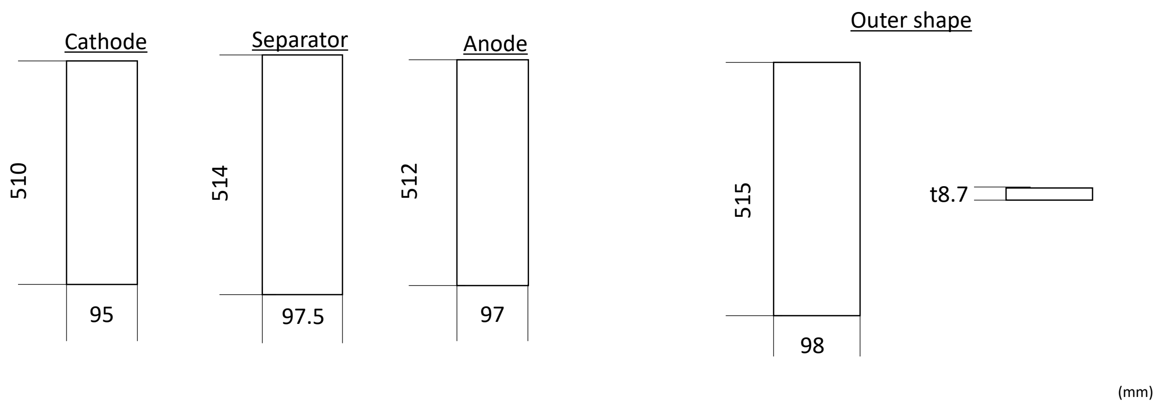
Supplementary Table 3 Total carbon emissions from electricity and total electricity consumption of the USA states, with the resulting carbon emissions per electricity unit.[15,16]

State	Million Tonnes of CO_2	Billion kWh	gCO_2 kWh^{-1}
Alabama	47.2	85.6	551
Alaska	2.8	6	466
Arizona	34.3	81.2	423
Arkansas	28.5	48.7	586
California	35.3	247.2	143
Colorado	30.6	56.4	542
Connecticut	9.2	27.7	333
Delaware	1.8	11.5	154
District of Columbia	0.0	10.1	0
Florida	91.2	241.6	378
Georgia	40.9	137.4	297
Hawaii	5.8	8.9	649
Idaho	2.0	25.3	79
Illinois	52.4	135.7	386
Indiana	68.8	99.7	690
Iowa	24.1	52.9	456
Kansas	22.2	40.5	549
Kentucky	56.9	74.5	764
Louisiana	30.4	90.8	335
Maine	1.3	11.6	109
Maryland	11.2	59.3	189
Massachusetts	6.1	50.8	121
Michigan	52.9	99.8	530
Minnesota	21.2	66.6	318
Mississippi	25.2	48	525
Missouri	60.2	77.8	774
Montana	12.5	15	831
Nebraska	19.8	32.3	613
Nevada	13.7	39	351
New Hampshire	2.1	10.9	193
New Jersey	13.3	73.1	182
New Mexico	17.1	25.4	674
New York	25.0	141.4	177
North Carolina	40.1	135.7	296
North Dakota	27.4	22.9	1198
Ohio	68.5	147.7	463
Oklahoma	26.7	64.5	415
Oregon	8.2	54.1	152
Pennsylvania	77.5	143.3	541
Rhode Island	3.4	7.4	456
South Carolina	25.0	79.8	314
South Dakota	2.4	13	184
Tennessee	24.0	99.6	241
Texas	180.3	435.6	414
Utah	29.9	32.7	916
Vermont	0.0	5.4	1
Virginia	24.4	125.2	195
Washington	9.8	88.2	112
West Virginia	59.0	32.8	1798
Wisconsin	35.0	69.4	504
Wyoming	34.1	15.8	2157
State total	1542.0	3805.9	405

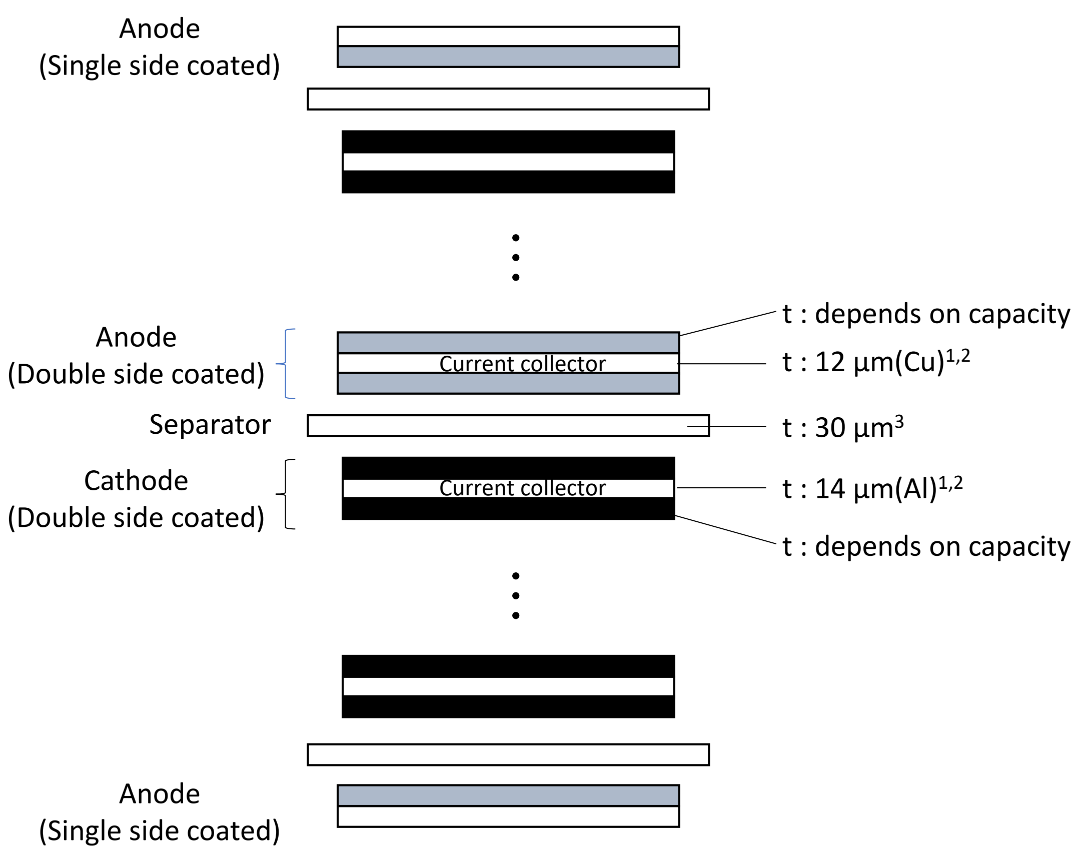
Supplementary Table 4 Results of lithium thermal evaporation trials.

Pressure (mbar)	**Duration (s)**	**Film Thickness (μm)**	**Deposition Rate (nm s^{-1})**
7.00×10^{-5}	1200	248	206.7
5.40×10^{-5}	120	53	441.7
5.00×10^{-5}	70	12	171.4
8.00×10^{-5}	210	31	147.6
8.00×10^{-5}	210	27	128.6
5.00×10^{-4}	210	25	119.0
4.90×10^{-4}	210	13	61.9
6.90×10^{-5}	210	27	128.6
6.60×10^{-4}	250	35	140.0
4.97×10^{-4}	480	26	54.2
6.19×10^{-5}	210	27	128.6
6.58×10^{-5}	240	63	262.5
5.21×10^{-4}	210	38	181.0
4.76×10^{-4}	540	25	46.3
5.56×10^{-5}	240	26	108.3
5.27×10^{-5}	120	17	141.7
5.69×10^{-4}	210	23	109.5
5.20×10^{-4}	540	20	37.0
3.90×10^{-5}	120	14	116.7
1.66×10^{-4}	240	11	45.8

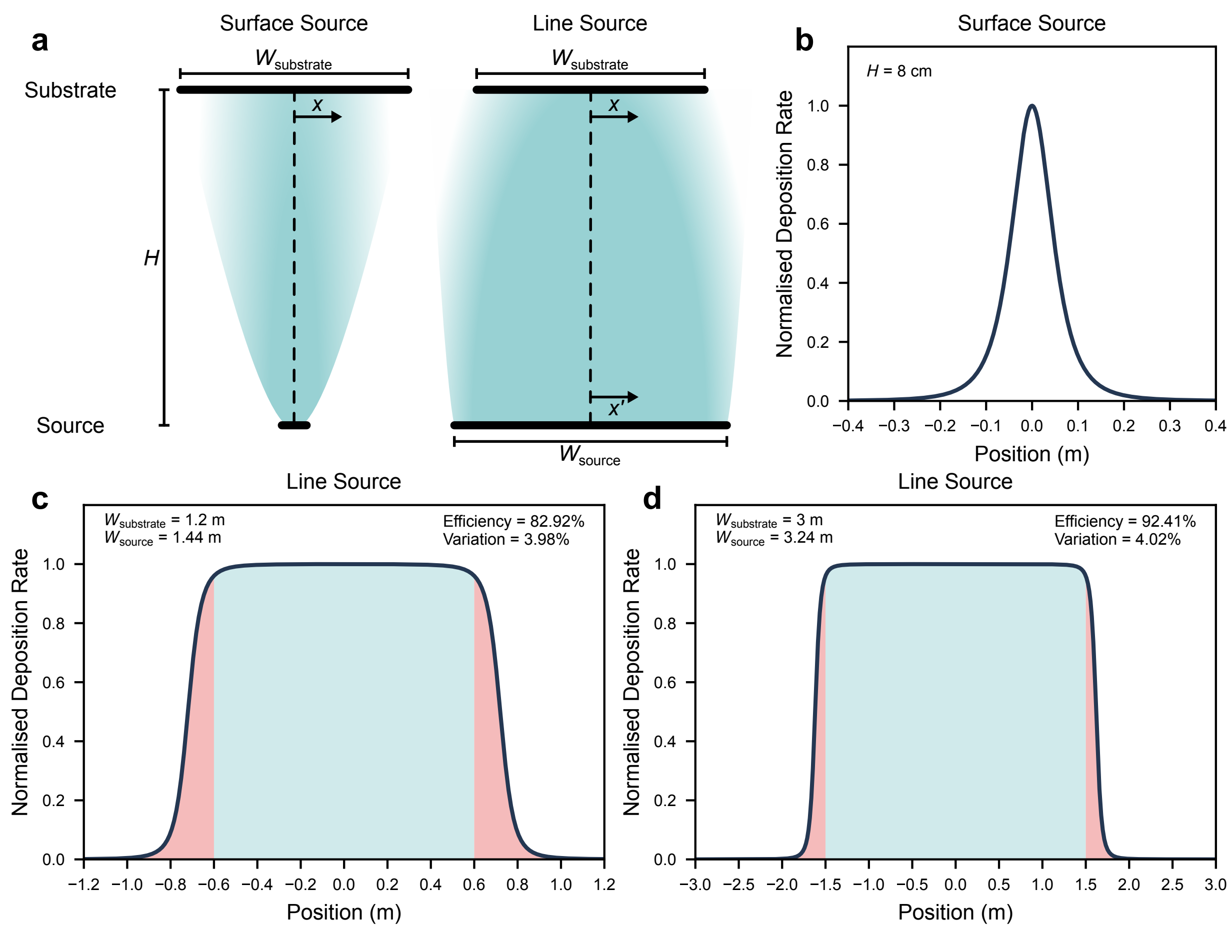
Supplementary Figures



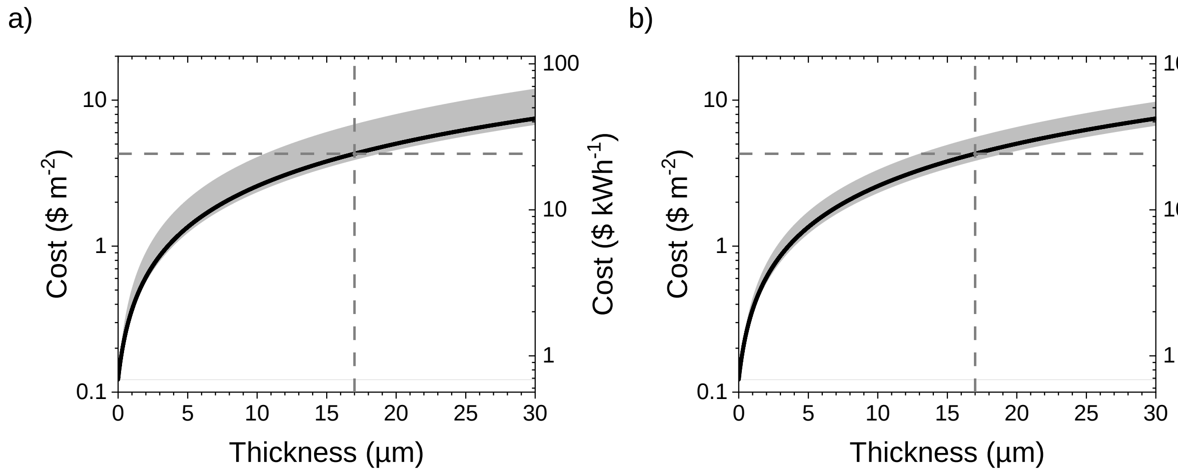
Supplementary Fig. 1 Cell geometry used for energy density calculation,[17,18] all dimensions are in mm and are based on reported cell dimensions for the Volkswagen ID.3.



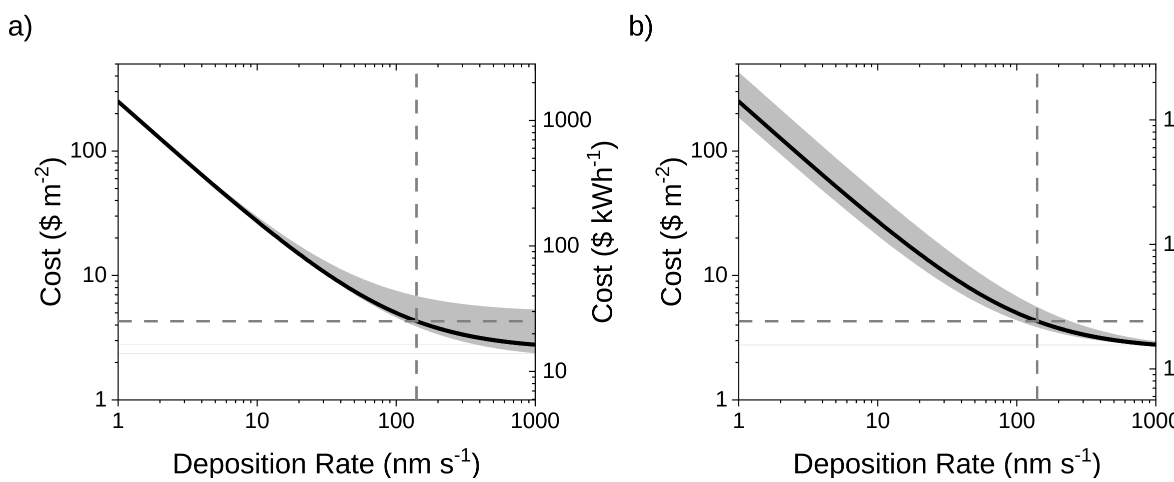
Supplementary Fig. 2 Cell geometry used for energy density calculation,[17,18] dimensions are based on reported cell dimensions for the Volkswagen ID.3, with solid electrolyte separator size taken from reported literature value.[19]



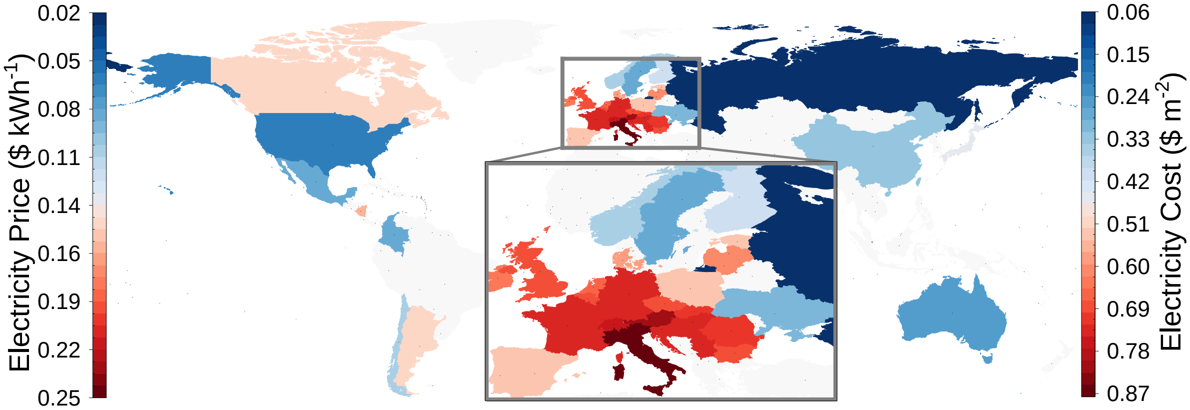
Supplementary Fig. 3 a) Schematic diagrams of modelled thermal evaporation sources, showing the geometry of a surface and a line source. b) The modelled normalised deposition rate from a surface source as a function of position along x with a source-substrate separation, $H = 8$ cm. c, d) The modelled normalised deposition rate from a line source as a function of position along x with $H = 8$ cm. c) Substrate width, $W_{\text{substrate}} = 1.2$ m, source width, $W_{\text{source}} = 1.44$ m. d) $W_{\text{substrate}} = 3$ m, $W_{\text{source}} = 3.24$ m. The lithium deposited on the substrate is highlighted in green, while the waste is highlighted in red. Full model details are provided in the Supplementary Methods



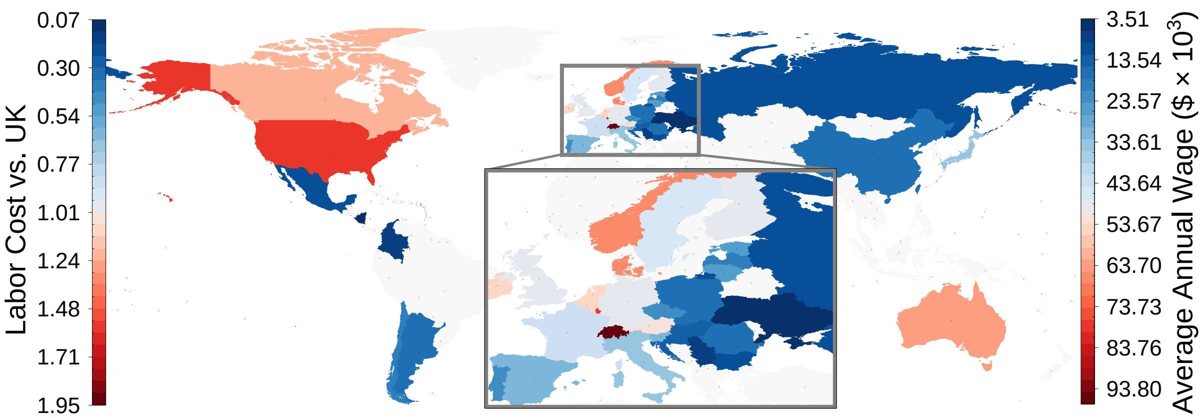
Supplementary Fig. 4 The effect on production costs at different thicknesses of varying a) Li_2CO_3 (grey area depicts Li_2CO_3 price variation between February 2023 and February 2024, with the solid black line representing the price used in this techno-economic assessment)[20,21] and b) electricity prices (grey area depicts UK electricity price between November 2021–2023, with the solid black line representing the 2 year average of the UK, France and Germany).[22] The dotted line in each depicts 17 µm Li metal anodes used in this techno-economic assessment.



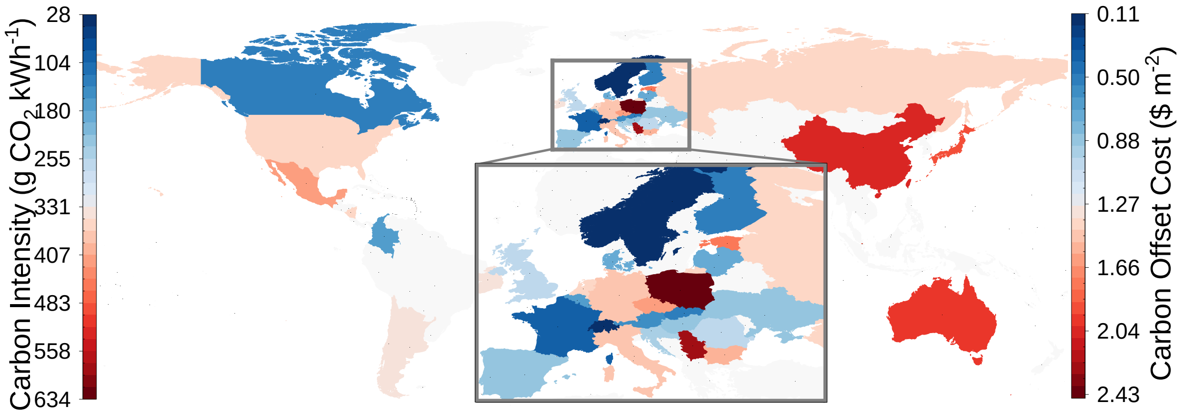
Supplementary Fig. 5 The effect on production costs at different deposition rates of varying a) Li_2CO_3 (grey area depicts Li_2CO_3 price variation between February 2023 and February 2024, with the solid black line representing the price used in this techno-economic assessment)[20,21] and b) electricity prices (grey area depicts UK electricity price between November 2021–2023, with the solid black line representing the 2 year average of the UK, France and Germany).[22] The dotted line in each depicts a deposition rate of 140 nm s^{-1} used in this techno-economic assessment.



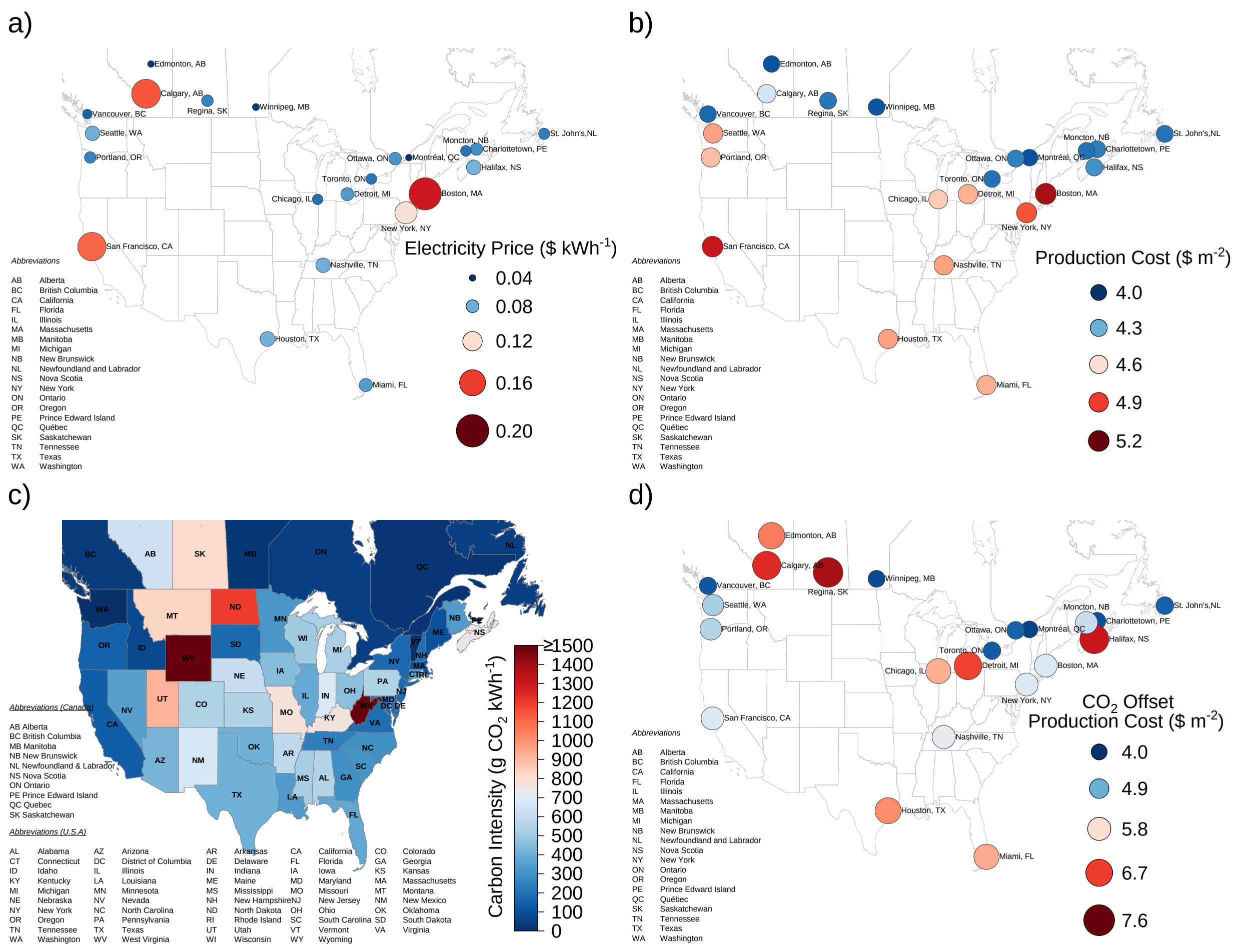
Supplementary Fig. 6 Average international electricity prices, November 2021 – November 2023. All data comes from the IEA, with the exception of China and Canada which comes from Global Petrol Prices and Hydro-Québec, respectively.[22–24]



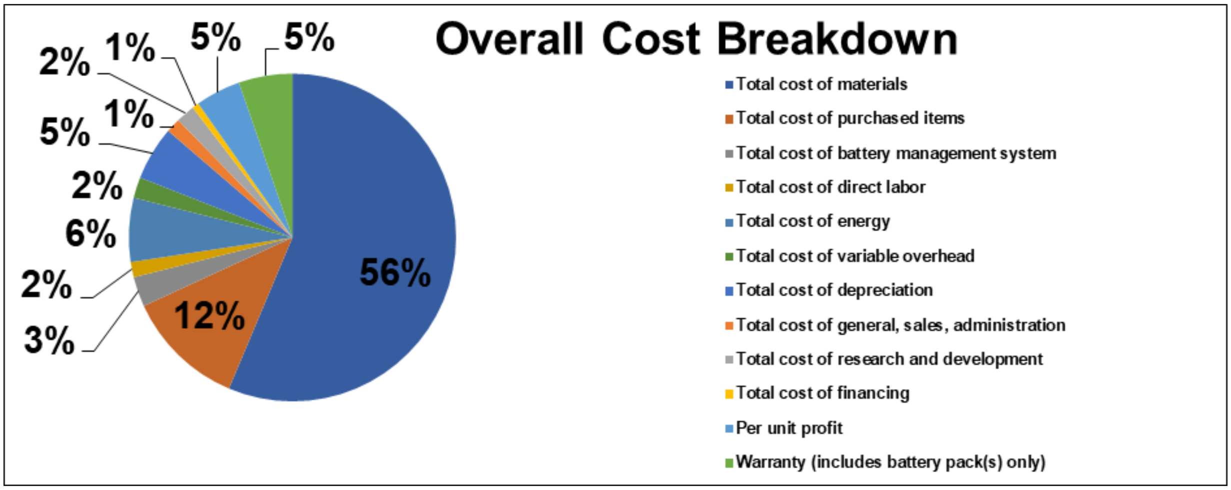
Supplementary Fig. 7 Proportional international labour costs vs. the UK 2022 average salaries (with the exception of Chile, Colombia and Ukraine) for OECD countries are taken form OECD data,[3] data for other nations is taken from a governmental source.[3–14] For Chile and Colombia, 2021 OECD data is used and compared to 2021 OECD UK data, as 2022 data for these countries is not available. Ukraine pay data is taken January 2022 and extrapolated to an annual salary.



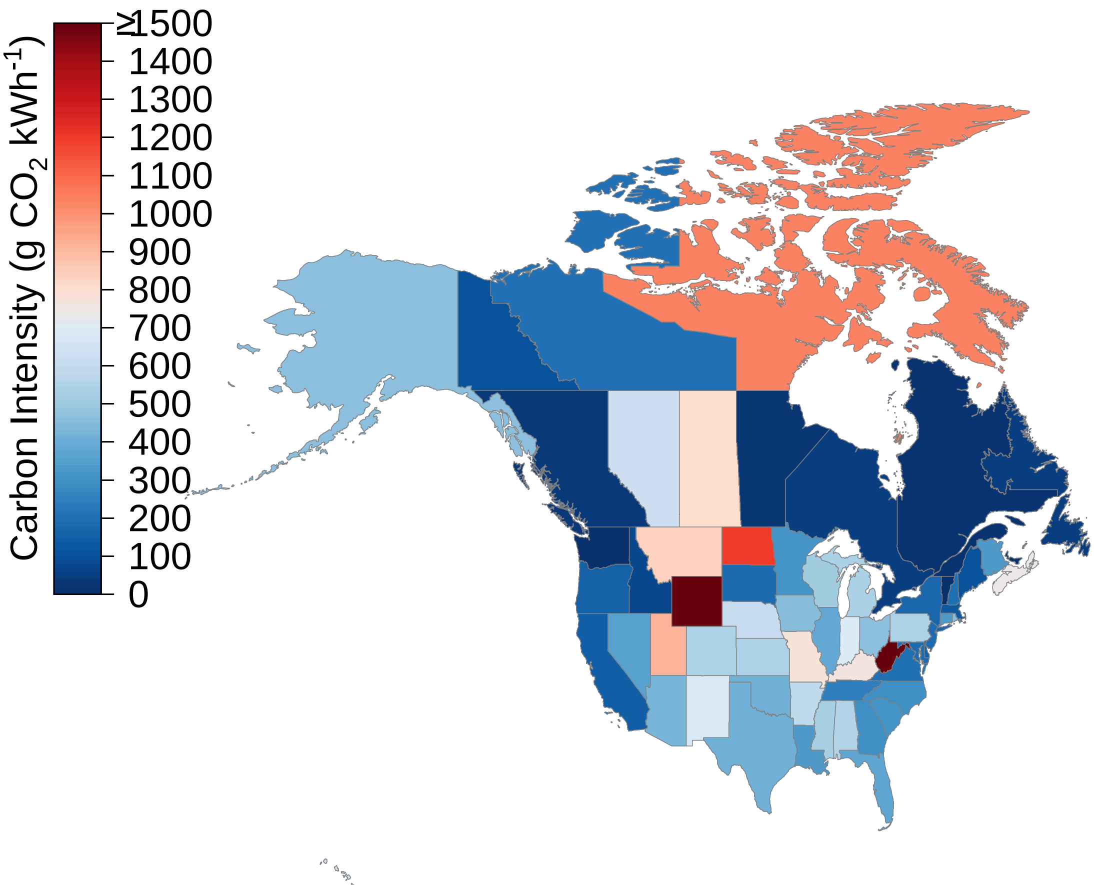
Supplementary Fig. 8 Global variation in carbon emissions for electricity production,[25] and the cost to offset the carbon emissions of 3.83 kWh m^{-2} of electricity required to produce of 17 µm thermally evaporated Li metal anodes when costed at €1000 to remove a tonne of CO_2.[26]



Supplementary Fig. 9 Variation in costs across the USA and Canada: a) variation in electricity price,[13,27] b) resulting variation in 17 µm Li anode production costs, c) variation in carbon intensity of electricity supplies[15,16,28] and d) the resulting variation in carbon offset 17 µm Li anode production costs.



Supplementary Fig. 10 BatPac cost breakdown to demonstrate the proportion of costs attributed to general sales and administration, variable overhead and financing.[29]



Supplementary Fig. 11 Variation in carbon intensity of electricity supplies across all states of the USA and territories and provinces of Canada.[15,16,28]

Supplementary References

References

[1] Wang, B. *et al.* Simulation and Optimization of Film Thickness Uniformity in Physical Vapor Deposition. *Coatings* **8**, 325 (2018).

[2] Villa, F. & Pompa, O. Emission Pattern of Real Vapor Sources in High Vacuum: An Overview. *Appl. Opt.* **38**, 695–703 (1999).

[3] Organisation for Economic Co-operation and Development. OECD.stat - Average Annual Wages. URL `https://stats.oecd.org/index.aspx?r=402626`.

[4] National Statistical Institute Bulgaria. National Statistical Institute. URL `https://www.nsi.bg/bg`.

[5] National Bureau of Statistics of China. China Statistical Yearbook. URL `https://www.stats.gov.cn/sj/ndsj/2022/indexeh.htm`.

[6] Croatian Bureau of Statistics. Croatian Bureau of Statistics. URL `https://dzs.gov.hr/`.

[7] Banco Central De Nicaragua. Banco Central De Nicaragua. URL `https://www.bcn.gob.ni/`.

[8] Institutul National de Statistica. Institutul National de Statistica. URL `https://insse.ro/cms/`.

[9] Russian Federal State Statistics Service. Russian Federal State Statistics Service. URL `https://rosstat.gov.ru/`.

[10] Statistical Office of the Republic of Serbia. Average salaries and wages per employee. URL `https://www.stat.gov.rs/en-US/`.

[11] Department of Statistics Singapore. Department of Statistics Singapore. URL `https://www.singstat.gov.sg/`.

[12] State Statistics Service of Ukraine. State Statistics Service of Ukraine. URL `https://www.ukrstat.gov.ua/`.

[13] Organisation for Economic Co-operation and Development. OECD Data - Exchange Rates. URL `https://data.oecd.org/conversion/exchange-rates.htm#indicator-chart`.

[14] XE. Trusted Global Currency Converter Money Transfers. URL `https://www.xe.com/`.

[15] U.S. Energy Information Administration. Electricity sales to ultimate customers, total and residential, total and per capita, ranked by state, 202. Tech. Rep. (2022).

[16] U.S. Energy Information Administration. Electric power energy-related carbon dioxide emissions. Tech. Rep. (2023). URL `https://www.eia.gov/environment/emissions/state/`.

[17] Wassiliadis, N. *et al.* Quantifying the state of the art of electric powertrains in battery electric vehicles: Range, efficiency, and lifetime from component to system level of the Volkswagen ID.3. *eTransportation* **12** (2022).

[18] Günter, F. J. & Wassiliadis, N. State of the Art of Lithium-Ion Pouch Cells in Automotive Applications: Cell Teardown and Characterization. *Journal of The Electrochemical Society* **169**, 030515 (2022).

[19] Lee, Y. G. *et al.* High-energy long-cycling all-solid-state lithium metal batteries enabled by silver–carbon composite anodes. *Nat. Energy* **5**, 299–308 (2020).

[20] Exchange, L. M. About Lithium. URL https://www.lme.com/en/Metals/EV/About-Lithium.

[21] Fastmarkets. Lithium Prices. URL https://www.fastmarkets.com/newgen/battery-materials/lithium/lithium-prices/.

[22] IEA. Real-time electricity tracker – data tools. URL https://www.iea.org/data-and-statistics/data-tools/real-time-electricity-tracker.

[23] Global Petrol Prices.com. China electricity prices.

[24] Hydro-Québec. 2023 Comparison of Electricity Prices in Major North American Cities (2023). https://www.hydroquebec.com/data/documents-donnees/pdf/comparison-electricity-prices.pdf.

[25] Our World in Data. Carbon intensity of electricity per kilowatt-hour. URL https://ourworldindata.org/grapher/carbon-intensity-electricity?tab=table&time=earliest..2020&country=$\sim$DEU.

[26] Dow, J. World's largest direct air carbon capture facility will reduce CO2 by .0001 percent. URL https://electrek.co/2022/06/28/worlds-largest-direct-air-carbon-capture-facility-will-reduce-co2-by-0001/.

[27] Hydro Québec. Comparison of Electricity Prices in Major North American Cities. Tech. Rep. (2023). URL https://www.hydroquebec.com/business/customer-space/rates/comparison-electricity-prices.html.

[28] Government of Canada. Pre-publication: Updated carbon intensities for Canadian grid electricity and excess electricity to grid processes. URL https://www.canada.ca/en/environment-climate-change/services/managing-pollution/fuel-life-cycle-assessment-model/updated-carbon-intensity-electricity.html.

[29] Knehr, K. W., Kubal, J. J., Nelson, P. A. & Ahmed, S. Battery performance and cost modeling for electric-drive vehicles: A manual for batpac v5. 0. Tech. Rep., Argonne National Lab.(ANL), Argonne, IL (United States) (2022).