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The importance of chemical reagents for the electric vehicle battery supply chain

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Batteries are essential for climate change mitigation, yet their supply chains face persistent challenges related to raw material supply risks and sustainability concerns. Here, we address an often-overlooked aspect of the battery supply chain: the extensive use of chemical reagents in raw materials processing, cathode synthesis, and cell recycling. Using a life cycle approach, we quantified the reagent intensity of eight lithium-ion and next-generation battery cell chemistries, defined as the total amount of reagents required across the supply chain to produce 1 kWh of battery cell capacity, and estimated the associated life cycle greenhouse gas (GHG) emissions and incurred costs. We found pronounced but heterogeneous reagent intensities, ranging from 7 to 39 kg per kWh of cell capacity. With growing battery demand, reagent requirements are projected to rise sharply, potentially reaching 14–26% of current production volumes for sulfuric acid, 4–8% for quicklime, 8–14% for sodium hydroxide, 5–43% for hydrochloric acid, and 3–14% for soda ash by 2040. Sulfuric acid, the most consumed reagent, creates a critical dependency on the fossil fuel industry and faces future availability risks as fossil fuel use declines, compounded by the current lack of viable substitutes in minerals leaching. We further show that reagents are non-negligible contributors to the carbon footprint and production costs of battery cells, accounting for 9–13% and 5–8%, respectively. Greener production methods for chemical reagents represent a key opportunity to further reduce the carbon footprint of batteries.

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1. Batteries are essential technologies for climate change mitigation. Across the battery supply chain, spanning raw material processing, cathode synthesis, and cell recycling, large quantities of chemical reagents are required, including inorganic chemicals (*e.g.*, sulfuric acid, sodium hydroxide, soda ash, *etc.*) and solvents.
2. These reagents play a crucial role in enabling battery production while also contributing non-negligibly to the carbon footprint and costs of batteries. Supply constraints and price volatility in chemical reagent markets could therefore increase battery costs and slow deployment, whereas adopting greener production routes for these reagents offers opportunities to reduce the carbon footprint of batteries.
3. Understanding future demand and supply dynamics of chemical reagents is therefore crucial for the battery industry. Equally important is the exploration of alternative production routes to ensure sustainable and reliable reagent provision.

Introduction

Batteries are essential technologies for climate change mitigation, playing a fundamental role in decarbonizing the power and transportation sectors through their use in renewable electricity storage and electric vehicles (EVs). The demand for global battery cells for EVs is projected to grow from about 1 TWh in 2024 to 5–8 TWh by 2040.^{1,2} While the climate benefits of EVs are well established,^{3–5} the battery supply chain con-

tinues to face challenges due to risk of supply disruptions and environmental concerns associated with the mining and processing of battery raw materials.^{6,7} Rising battery demand is often highlighted as the major driver of increased demand for key minerals, including lithium, cobalt, nickel, manganese, and graphite.^{8,9} As a result, a growing body of research is focusing on the global availability and cost of these minerals, alongside supply potentials and risks,^{10,11} associated environmental and social impacts,¹² and the potential of recycling to address these challenges.^{9,13} Moreover, growing attention is devoted to energy consumption for manufacturing cells in gigafactories and their environmental implications.^{1,14,15}

Large quantities of chemical reagents are also required across the battery supply chain. We define a reagent as a compound that facilitates chemical reactions, either by directly

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reacting with other substances or by serving as a medium that enables or supports the reaction process. Following Pearse,¹⁶ we consider inorganic chemicals and solvents within this scope. Key inorganic chemicals such as sulfuric acid, quicklime, sodium hydroxide, and soda ash are extensively used in the processing of raw materials used for battery cathodes, anodes, and electrolytes.^{16,17} For example, producing 1 kg of battery-grade lithium carbonate from brines may require 0.5–1 kg of sodium hydroxide and 2–39 kg of soda ash, among other reagents.¹⁸ The synthesis of precursors (pCAM) and cathode active materials (CAM) requires sodium hydroxide as a precipitating agent (1–2 kg per kWh cell capacity) and solvents for cathode slurry preparation.^{19,20} Moreover, battery cell recycling can involve reagent-intensive hydrometallurgical processes, requiring substantial amounts of sulfuric acid (*e.g.*, 4–6 kg per kg cell treated) and sodium hydroxide, among others (see Methods for further details on reagent use throughout the battery supply chain).^{21,22}

Therefore, alongside the rapid expansion of raw materials supply, cell manufacturing, and recycling, growing battery demand will also drive a parallel increase in reagent consumption. This raises important questions about future demand–supply dynamics. For example, some lithium projects in Argentina have already expressed concerns about securing reliable supply of soda ash.²³ Several studies have also warned of potential sulfuric acid shortages, given its close ties to the fossil fuel industry and vulnerability to disruptions from the energy transition.^{24,25} Preliminary estimates suggest that meeting the US 2030 battery-grade materials production targets could require up to 0.5% of current US production for sodium hydroxide and sulfuric acid and 2% for hydrochloric acid.²⁶ While these figures may appear modest, these chemicals are widely used by a myriad of industrial sectors, creating significant competition for supply.

Reagent use also carries environmental and economic implications for the battery industry. They contribute to the environmental footprint of battery raw materials, including greenhouse gas (GHG) emissions and water scarcity,^{18,27,28} and are recognized as environmental hotspots in battery recycling processes.²⁹ However, because reagent-related emissions are typically embedded within the life cycle emissions of upstream processes (*e.g.*, cathode materials' production), the contribution of various reagents to the carbon footprint of battery cells has so far remained largely overlooked. Economically, historical market data reveal both high reagent price volatility and substantial regional disparities (see SI Excel S5). For example, sulfuric acid median market prices over the past decade have ranged from 55 to 112 USD per tonne in China and the European Union, respectively.³⁰ Whether such fluctuations in reagent prices could directly affect the production cost of battery cells remains underexplored.

Achieving a sustainable battery supply chain requires a holistic perspective that goes well beyond battery materials and cell manufacturing and recycling. Chemical reagents are an essential component, yet they have received relatively limited attention in the literature. We contribute to closing this gap by

analysing the use of chemical reagents across the supply chain of eight battery cell chemistries: four nickel–manganese–cobalt chemistries (NMC532, NMC622, NMC811, and NMC900), nickel–cobalt–aluminium (NCA), lithium–iron–phosphate (LFP), sodium-ion battery (SIB) based on nickel–iron–manganese layered oxide (NaNFM442), and solid state battery (SSB) based on NMC900 cathode chemistry with oxide solid electrolyte. We first quantify the reagent intensity of each battery cell, defined as the total amount of reagents required to produce 1 kWh of battery cell capacity (capacity-based reagent intensity) or 1 kg of battery cell (mass-based reagent intensity). Adopting a life cycle approach, the scope encompasses reagents used for (1) processing primary raw materials into battery-grade materials, as well as (2), reagents necessary to synthesize pCAM and CAM (Fig. S1). We also quantify the reagent intensity associated with battery cell production from recycled materials. We then combine these reagent intensities with future battery cell demand estimates to quantify reagent requirements through 2040 under various scenarios and compare these projections with current reagent production volumes to uncover future supply implications. We also provide an overview of the contribution of these reagents to the carbon footprint and production costs of battery cells and conclude by discussing implications as well as avenues for research and development.

Battery cells are reagent-intensive

The reagent intensity accounts for the most prominent reagents used across the battery cell supply chain, including sodium hydroxide, soda ash (light), sulfuric acid, hydrochloric acid, hydrofluoric acid, nitric acid, limestone, quicklime, ammonia, organic solvents, and *N*-methyl-2-pyrrolidone (NMP) (see Methods for details on reagent selection).

Producing 1 kWh of battery cell capacity requires between 7 and 39 kg of these reagents, depending on the cell chemistry (Fig. 1). NMC and NCA cells have comparable reagent intensities, ranging from 21 to 28 kg per kWh. The production of cathode materials, particularly nickel sulfate and cobalt sulfate, has the largest reagent requirement, driven by substantial use of sulfuric acid and limestone in their hydrometallurgical processing. SSB cells are the most reagent-intensive due to the combined use of nickel sulfate in the cathode and lithium metal in the anode. Lithium metal is produced through electrolysis of lithium chloride, which in turn is produced from reagent-intensive lithium carbonate. In contrast, LFP cells have the lowest reagent intensity as their olivine intercalation method does not require reagent-intensive nickel or cobalt sulfate. SIB cells also fall on the lower end, requiring 16 kg of reagents per kWh, most of which are used in producing nickel sulfate for the cathode.

We also quantified the mass-based reagent intensity by considering the cell-specific energy density, which ranges from 0.175 to 0.315 kWh per kg for LFP and SSB, respectively (SI Excel S1). Producing 1 kg of battery cell requires between 1



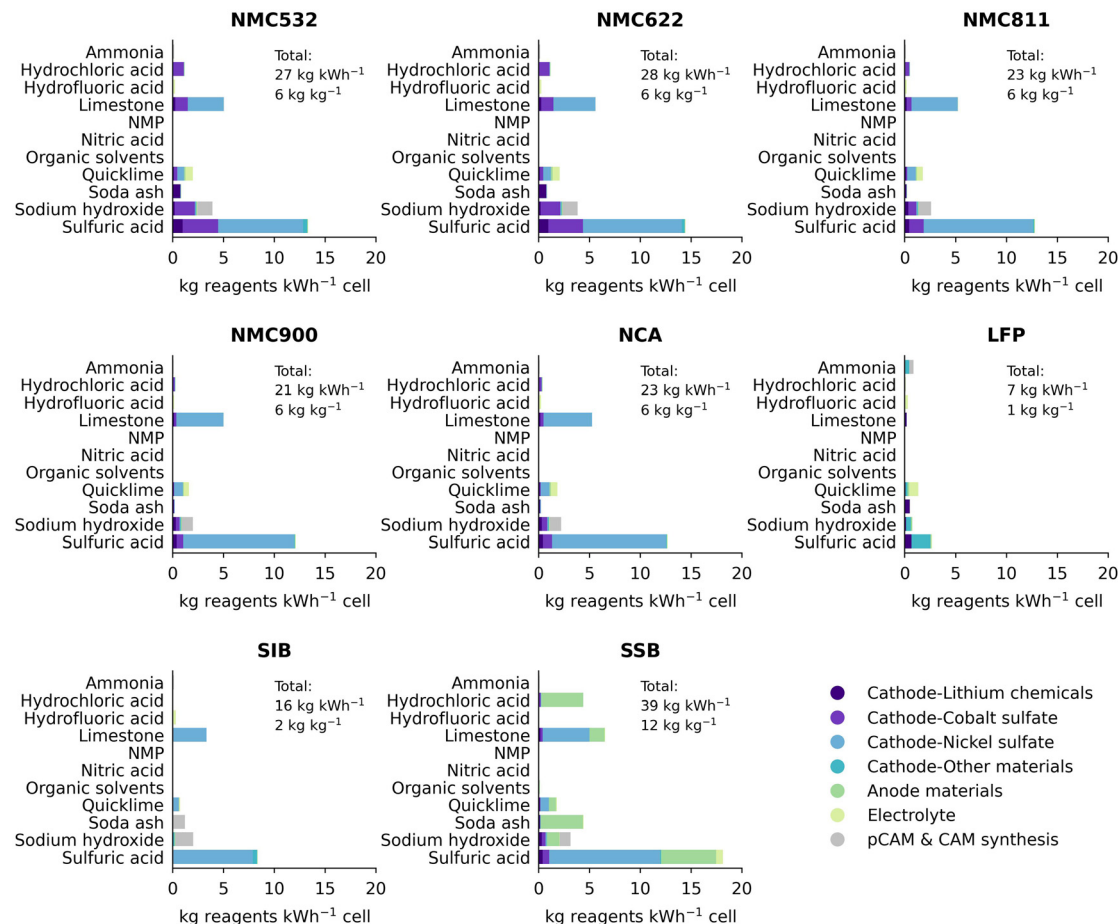


Fig. 1 Reagent intensity of battery cells. Reagent intensity is defined as the total amount of reagents required over the supply chain to produce 1 kWh of battery cell capacity or 1 kg of battery cell. The stacked bars indicate the stage of the supply chain where the reagent is consumed. NMC: nickel–manganese–cobalt. NCA: nickel–cobalt–aluminium. LFP: lithium–iron–phosphate. SIB: sodium-ion battery based on nickel–iron–manganese layered oxide (NaNFM442). SSB: solid state battery based on NMC900 cathode chemistry and oxide solid electrolyte.

and 12 kg of reagents, with LFP showing the lowest intensity and SSB the highest. This trend aligns with the capacity-based intensity observed across all cell chemistries.

Sulfuric acid is the most prominent reagent across all chemistries, ranging from 3 to 18 kg per kWh. The high consumption of sulfuric acid is largely due to its role in leaching processes to produce cobalt sulfate (requiring 6.0 kg of sulfuric acid per kg of battery-grade material), nickel sulfate (5.8 kg), lithium carbonate (1.4 kg), and lithium hydroxide (1.2 kg). Limestone (calcium carbonate) is the second most used reagent across all chemistries but LFP, primarily due to the substantial quantities used in the production of nickel sulfate and cobalt sulfate. Quicklime (calcium oxide), which is derived from limestone calcination, is also used in raw materials' processing and reported separately (we converted hydrated lime into the equivalent amount of quicklime). Sodium hydroxide is the third most used reagent in the manufacturing of NMC and NCA cells, driven by its use in raw materials' processing as well as important quantities used in pCAM synthesis (between 0.83 and 1.46 kg kWh⁻¹ cell capacity).³¹ Hydrochloric acid is used in important quantities for SSB cells, largely for produ-

cing lithium chloride used in lithium metal anodes, and for low-nickel NMC cells, owing to their higher use of cobalt sulfate. Soda ash is used in relatively small quantities, with higher consumption in low-nickel NMC and LFP cells due to their greater use of lithium chemicals, where soda ash is used in precipitation processes, and in SIB cells, where it is used in the cathode. The other reagents are consumed only in minor quantities. Organic solvents and toxic NMP, used as a solvent in cathode synthesis, have negligible net requirements due to their high recovery and reuse rates.

Recycling has mixed effects on reagent requirements

Recycling of battery cells enables the recovery of battery-grade materials, thereby reducing dependence on primary raw materials and avoiding the reagents required in their processing.²¹ However, recycling processes themselves also rely on reagents, whose type and quantity vary widely depending on the treatment pathway (pyrometallurgy, hydrometallurgy, or direct



recycling), cell chemistry, and specific process configuration. We quantified the reagent intensity associated with the production of battery cells from recycled materials obtained *via* hydrometallurgical recycling. This pathway accounted for 90% of global battery recycling capacity in 2023, and is expected to maintain a dominant role by 2030.³² We further evaluated both optimistic and conservative recycling efficiencies (*i.e.*, 90% vs. 50% for lithium, 98% vs. 85% for nickel, 98% vs. 90% for cobalt, and 98% vs. 84% for manganese).^{22,33,34}

Although hydrometallurgical recycling still requires substantial inputs of sulfuric acid and sodium hydroxide, using recycled materials to produce new battery cells reduces reagent intensity by 55–59% for NMC and NCA cells under optimistic recycling efficiency assumptions (Fig. 2). The use of most reagents decreases substantially, by between 37% and 97%, depending on the reagent and cell chemistry. In contrast, sodium hydroxide consumption increases by 12–63%, indicating a greater reliance on this reagent in hydrometallurgical recycling compared with primary materials processing. Under conservative recycling efficiencies, reagent intensities are only 1–15% higher than those observed in the optimistic case. This relatively modest sensitivity to recycling efficiency can be attributed to the consistently high recovery rates of nickel and cobalt (even under conservative assumptions), which dominate reagent use in the upstream processing of primary raw materials.

Surprisingly, for LFP cells, we find that incorporating recycled materials nearly doubles reagent intensity. Sulfuric acid and sodium hydroxide requirements increase by factors of 2.1 and 4.1, respectively. This increase is because LFP cells do not contain reagent-intensive nickel sulfate or cobalt sulfate. As a result, while hydrometallurgical recycling requires substantial amounts of reagents, for LFP, it recovers only lithium carbon-

ate and therefore offers limited reductions in reagent demand. This finding is consistent with prior studies reporting substantially lower environmental and economic benefits from recycling LFP cells compared with NMC and NCA, as LFP does not recover high-impact materials such as nickel and cobalt.^{22,35,36} However, it should be noted that we applied the same recycling process across all cell chemistries, assuming identical reagent consumption per kg of treated cell. While this assumption aligns with common practice in the literature, it has been highlighted that mainstream hydrometallurgical processes are not yet optimized for the specific composition of LFP cells.^{29,35} In this context, direct recycling is often proposed as an alternative pathway for LFP cells. Although direct recycling is expected to require fewer reagents than hydrometallurgical recycling, it remains at an early stage of technological development.

Moreover, we considered only the recovery of cathode materials. More advanced recycling processes, including direct recycling, promise higher recycling rates and the recovery of graphite and the electrolyte.^{35,37} However, we note that these components contribute minimally to the overall reagent intensity of battery cells. Finally, recycling has not been considered for SIB and SSB cells, as they remain in the early stages of development and dedicated recycling processes have yet to be established.³⁸

Reagent requirements to meet global battery cell demand

We estimated global reagent requirements from 2018 to 2040 by combining the cell-specific reagent intensities with four global battery cell deployment scenarios reported by Degen *et al.*¹ The

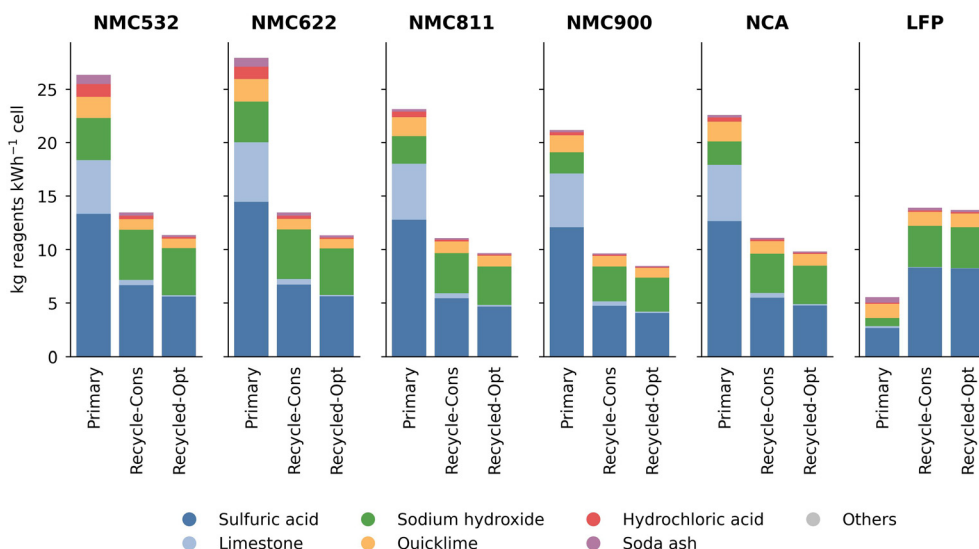


Fig. 2 Reagent intensity of NMC, NCA, and LFP cells produced from primary vs. recycled materials. Reagent intensity is defined as the total amount of reagents required over the supply chain to produce 1 kWh of battery cell capacity or 1 kg of battery cell. For recycled materials, two cases are considered: a conservative (Recycle-Cons) and an optimistic (Recycle-Opt) recycling situation, reflecting different element-level recycling efficiencies (*i.e.*, 90% vs. 50% for lithium, 98% vs. 85% for nickel, 98% vs. 90% for cobalt, and 98% vs. 84% for manganese). NMC: nickel–manganese–cobalt. NCA: nickel–cobalt–aluminium. LFP: lithium–iron–phosphate.



four scenarios, displayed in Fig. 3, assume that battery cell demand grows from 113 GWh in 2018 to 5470 GWh by 2040, with varying assumptions about the market shares of different battery cell chemistries (see the colour key in Fig. 3) while also accounting for future battery recycling (dashed lines in Fig. 3).

Assuming constant cell reagent intensities, annual demand could rise between 2025 and 2040 from 9 to 26–68 Mt for sulfuric acid, from 5 to 11–36 Mt for lime (limestone plus quicklime), from 2 to 7–15 Mt for sodium hydroxide, from 0.5 to 0.6–10 Mt for hydrochloric acid, and from 0.6 to 1–10 Mt for soda ash (Fig. 3). The projected 2040 demands represent 14–26% of today's global production for sulfuric acid, 4–8% for lime, 8–14% for sodium hydroxide, 5–43% for hydrochloric acid, and 3–14% for soda ash. The wide demand ranges reflect differences in reagent intensities of the battery cell chemistries assumed in each scenario. As expected, demand growth is consistently highest under a large deployment of SSB cells (NEXT scenario) and lowest when LFP cells dominate the market (LFP scenario). Recycling has only a modest influence on the demand for sulfuric acid, hydrochloric acid, and soda ash, but has a more pronounced effect in reducing lime demand, while increasing sodium hydroxide demand. However, it should be noted that availability of end-of-life EV batteries for recycling is expected to only become relevant post-2035,³² whereas our analysis extends only to 2040 due to the lack of battery cells deployment scenarios beyond that year.

The amount of reagents used to produce battery-grade materials and to recycle battery cells may change over time

due to changes in resource characteristics and processing technologies. For example, declining ore grades for lithium or the increasing use of laterite ores for nickel sulfate production could drive up the amount of reagents required,^{18,39} whereas optimization of chemical reactions could reduce them. We tested the sensitivity of our projections by assuming $\pm 1\%$ and $\pm 4\%$ annual variations in cell-specific reagent intensities (Fig. S2). A $\pm 1\%$ annual variation results in a cumulative change of +25% and -20% in reagent intensities by 2040 relative to 2018. Focusing on reagents whose 2040 demand exceeds 10% of current market volumes, we find that a cumulative 20% reduction would not reduce their global demand below this threshold. In contrast, a cumulative 25% increase (e.g., potentially driven by factors such as declining ore grades) could push several additional reagents above the threshold, including sulfuric acid in the LFP scenario or lime in the NCX and NEXT scenarios. Assuming a $\pm 4\%$ annual variation leads to much larger cumulative changes by 2040, corresponding to a 59% decrease and a 137% increase in reagent intensity. In the case of a decrease, global demand for sulfuric acid and sodium hydroxide would remain well below 10% of current market volumes. Conversely, the increase scenario would push the demand for nearly all reagents above the threshold across all scenarios, except for soda ash in the LFP and NCX scenarios. Therefore, in addition to battery cell demand and chemistry shares, the evolution of raw material processing and cell recycling technologies will play a major role in shaping future reagent demand.

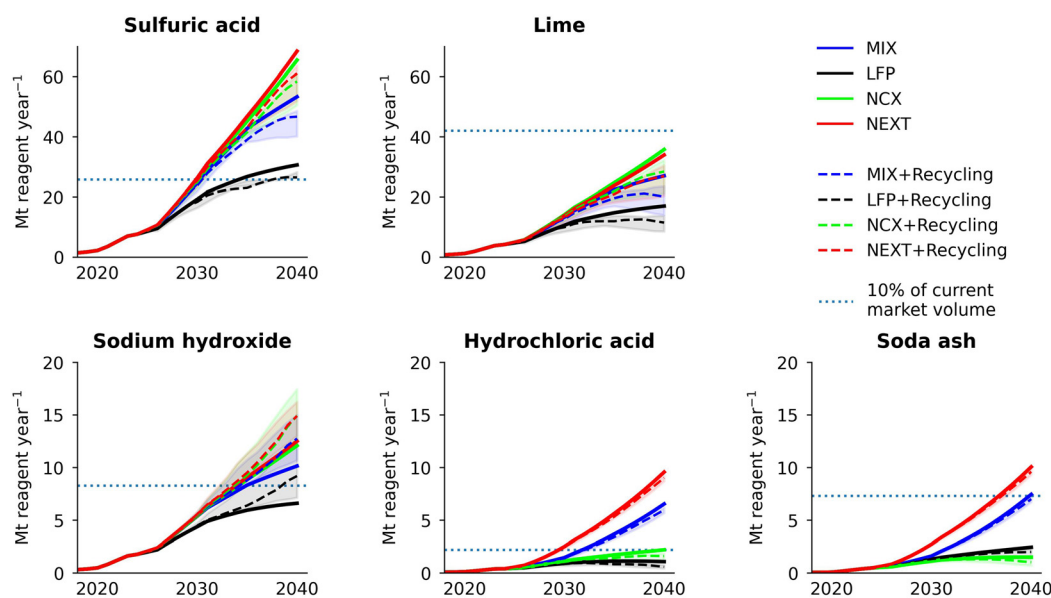


Fig. 3 Global requirements for selected reagents from 2018 to 2040 under different battery chemistry deployment scenarios. The scenarios represent different market share trajectories of battery chemistries: MIX: a balanced situation where all chemistries have similar market shares by 2040. LFP: LFP cells dominate the market, reaching 70% market share by 2040. NCX: NMC and NCA cells dominate the market with a combined market share of 95% by 2040. NEXT: SIB and SSB cells achieve 60% market share by 2040. In all scenarios, battery cell demand is assumed to increase from 113 GWh in 2018 to 5470 GWh by 2040.²¹ Solid lines indicate demand met solely from primary raw materials, while dashed lines include contributions from recycled materials (optimistic recycling efficiency assumptions); shaded bands show the range resulting from minimum and maximum battery lifetime assumptions. Lime includes the sum of limestone and quicklime.



Contribution of reagents to the battery cell carbon footprint and production costs

Reagent production can be highly carbon-intensive due to energy-intensive processes and direct process emissions. To assess the contribution of reagents to the carbon footprint of battery cells, we first quantified the cradle-to-gate life cycle GHG emissions associated with the production of reagents needed per kWh of battery cell capacity. Consistent with a life cycle perspective, this assessment accounts for GHG emissions arising from all relevant inputs (*i.e.*, energy and raw materials) and outputs (*i.e.*, direct emissions, waste, *etc.*). The resulting reagent-specific GHG emissions were then compared with the cradle-to-gate carbon footprint of the corresponding battery cells.²⁰

Producing the reagents needed for 1 kWh of battery cell capacity can cumulatively generate between 6 and 12 kg CO₂-eq, with the lower bound corresponding to LFP cells and the upper to NMC622 (Fig. 4). Meanwhile, the average carbon footprint of the studied cells ranges from 60 to 88 kg CO₂-eq per kWh corresponding to the NMC900 and NMC532 cells, respectively.²⁰ Thus, reagents alone can account for 9–13% of these emissions.

Sodium hydroxide is the main contributor to reagent-related GHG emissions for NMC, NCA, and SIB cells. Although its use intensity is relatively low (Fig. 1), sodium hydroxide has a comparatively high average carbon footprint of 1.1 kg CO₂-eq

per kg, with more than 95% of these emissions originating from electricity consumption in the electrolysis process.⁴⁰ Quicklime and sulfuric acid are the next most important contributors, with impacts of similar magnitude. Sulfuric acid has a relatively low carbon footprint (0.18 kg CO₂-eq per kg) but is used in large quantities. In contrast, the calcination of limestone to produce quicklime is highly carbon-intensive, emitting about 1.1 kg CO₂-eq per kg. Soda ash is another carbon-intensive reagent, averaging 1.3 kg CO₂-eq per kg, and contributes notably to low-nickel NMC and SIB cells. For LFP cells, ammonia (included within “Others” in Fig. 4) makes a substantial contribution, reflecting the higher use of ammonium hydroxide in pCAM synthesis.

The carbon footprint of reagent production can vary widely depending on factors such as the production location, owing to differences in electricity grid mixes, type of fuels used, and production routes. The error bars in Fig. 4 illustrate how this variability in life cycle GHG emissions of reagent production (represented by minimum and maximum values reported in the literature) affects the carbon footprint of battery cells. Shifting reagent sourcing from high- to low-carbon routes could reduce GHG emissions by 4.2–8.3 kg CO₂-eq per kWh, equivalent to 5–9% of the cells’ total carbon footprint. Although these reductions may appear modest, future mitigation measures in the chemical industry can lower reagent carbon footprints even beyond today’s low-carbon benchmarks.

Based on 2016–2025 median commodity market spot prices for China, USA, and Europe, the cost of procuring the required

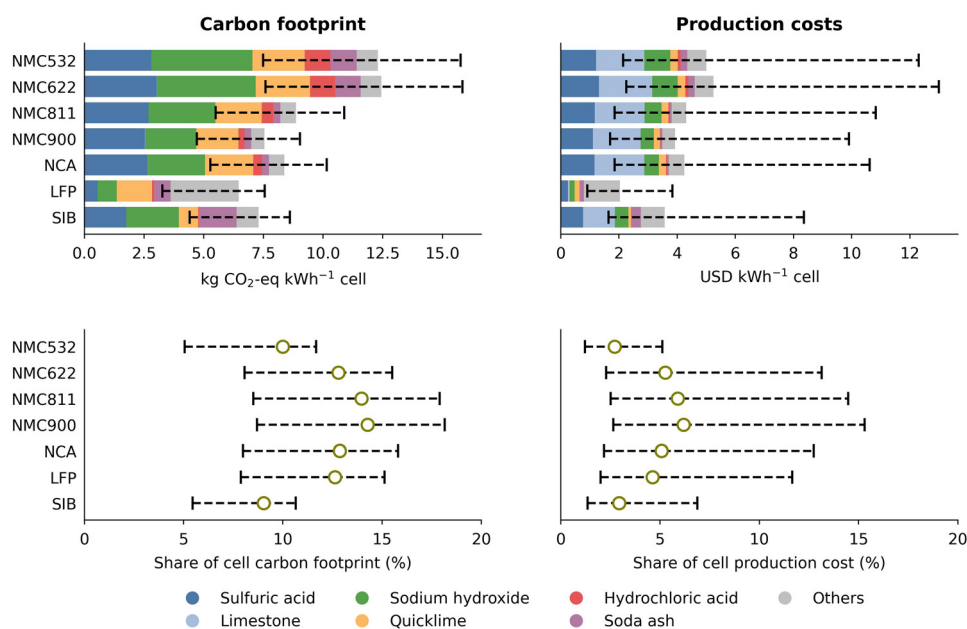


Fig. 4 Contribution of chemical reagents to the carbon footprint and production costs of battery cells. Horizontal bars show the carbon footprint based on average values from the literature and costs based on median market spot prices in China, USA, and Europe (2016–2025). Error bars indicate the range derived from minimum and maximum carbon footprint figures and market prices. For costs, this range reflects the lowest and highest monthly market prices observed between 2018 and 2025 across the three regions. NMC: nickel–manganese–cobalt. NCA: nickel–cobalt–aluminium. LFP: lithium–iron–phosphate. SIB: sodium-ion battery based on nickel–manganese layered oxide (NaNFM442).



reagents ranges from 2 to 5 USD per kWh. As total cell production costs have been reported in the range of 75 and 122 USD per kWh (LFP and SIB cells, respectively),^{41,42} reagents would account for 3–6% of these costs. However, we note that fluctuations in reagent prices can significantly affect cell production costs (error bars in Fig. 4). If the maximum monthly historical prices observed over the last decade are applied simultaneously (see SI Excel S5), the contribution of reagents could rise to 5–15% of these costs. The market prices of some reagents like sodium hydroxide are heavily dependent on electricity prices, making them prone to spike in prices under energy crises such as the one suffered in Europe in 2022. Median costs are closer to the minimum historical market prices due to occasional price spikes. For example, sulfuric acid reached 171 USD per tonne in China in 2021, compared to a median price of 91 USD per tonne, while soda ash rose to 540 USD per tonne in the same year, compared to the median of 269 USD per tonne. We excluded SSB cells from this analysis due to their early development stage and the current lack of carbon footprint and production cost data for this emerging cell chemistry.

Outlook and future work

In this study, we addressed the use of chemical reagents across the supply chain of mainstream EV battery cells, emphasizing the role of securing reagent supplies to enable the large-scale deployment of EVs and realize their expected climate benefits. Satisfying the growing demand for reagents may face challenges from a myriad of factors, including their co-/by-production with other commodities, lack of domestic production, insufficient logistics infrastructure, and competition with other industries whose demand is likewise expected to grow as well.

Our analysis identified sulfuric acid as the most widely used reagent across the battery supply chain, reflecting its central role in leaching processes for both battery materials production and battery cells recycling. Yet its future supply is highly uncertain due to strong dependence on fossil fuels: about 80% of elemental sulfur used in industry (primarily for sulfuric acid production) originates as a by-product from the desulfurization of fossil fuels, mainly during petroleum refining and natural gas processing.⁴³ Metal smelting of sulfidic minerals provides around 20% of sulfur as a by-product.²⁵ Historically, sulfur has been in oversupply,⁴⁴ and large reserves of sulfur in crude oil, natural gas, and sulfide ores could make supply adequate for the foreseeable future.⁴³ However, the global transition away from fossil fuels could significantly constrain future supply.⁴⁵ A previous study estimated that global sulfuric acid production could decline from 258 Mt in 2025 to around 170 Mt by 2040 under a net-zero scenario.²⁴ Our projections indicate that battery cell manufacturing alone could require 21–40% of this future supply. Given competing demand from other sectors such as the production of phosphate fertilizers (accounting for 50% of current sulfur

demand)⁴⁶ or other metals processing,⁴⁷ our findings highlight the risk of constrained sulfuric acid availability, potentially leading to higher battery cost and slower EV deployment.

This risk is further amplified by the current lack of cost-competitive alternatives. Sulfuric acid can be produced on-site using SO₂ from flue gases. For example, the Tenke Fungurume and Mutanda copper-cobalt mines in the Democratic Republic of Congo (DRC) operate with on-site sulfuric acid production.⁴⁸ Yet additional external sulfur is still required to meet the plant's sulfuric acid demand. Other sources include expanding current mining capacity of sulfides and elemental sulfur and increasing mining capacity of low-quality sulfide ores; however, these sources may come at increased costs and environmental impacts that remain largely unassessed (*e.g.*, due to sulfidic tailings).²⁴ Alternative acids such as hydrochloric acid or nitric acid can sometimes be used as substitutes, yet they are generally more expensive and less effective.^{43,46}

Sodium hydroxide and hydrochloric acid are produced almost entirely as co-/by-products in the chlor-alkali process (99% of global sodium hydroxide)⁴⁹ and chlorinated organics production (90% of hydrogen chloride, the basis of hydrochloric acid),⁵⁰ respectively. Their supply therefore depends on chlorine and chlorine-derivative products. Consequently, regional sodium hydroxide and hydrochloric acid supply disruptions have been common in the past due to temporal decline in demand for chlorine.^{50,51}

Soda ash faces fewer long-term availability concerns, but its production is highly concentrated in a handful of countries. Soda ash is primarily produced either from trona and sodium carbonate-rich brines (natural soda ash, accounting for 35% of global production) or from salt brine and limestone *via* the Solvay process (synthetic soda ash, 65% of global production).⁵² Natural soda ash reserves are estimated at 25 000 Mt, with more than 90% located in the USA.⁵² Synthetic soda ash production depends on practically inexhaustible limestone resources. As a result, long-term supply is likely to remain secure. However, current production is highly concentrated: China, Turkey, and the USA together account for 78% of global production.⁵² This geographic concentration can create dependencies for countries lacking domestic production. Lithium producers in Chile and Argentina rely heavily on soda ash imports from China and the USA. The lack of local production combined with insufficient logistic infrastructure to transport the reagents to the mining and refining sites has been highlighted as a bottleneck for the Argentinian lithium industry.²³ In response to the anticipated expansion of lithium projects, Argentina is considering building domestic synthetic soda ash capacity dedicated to meeting lithium-sector demand.⁵³ This illustrates how the growth in demand for batteries and their materials can directly influence investment decisions in upstream chemical reagent industries.

Chemical reagents also make a non-negligible contribution to the carbon footprint of battery cells, with implications for battery manufacturers. The EU Battery Regulation introduces requirements for carbon footprint declarations and aims to



establish carbon footprint threshold values for batteries entering the EU market.⁵⁴ In this context, greener production routes for chemical reagents can contribute to reducing battery carbon footprint and supporting regulatory compliance. Substantial opportunities exist to cut GHG emissions from sodium hydroxide production by using renewable electricity and more efficient production technologies (*i.e.*, complete phase-out of diaphragm and mercury cell technologies in favour of membrane cell technology).⁵⁵ Efforts to mitigate CO₂ emissions from quicklime production focus on reducing fuel combustion emissions by shifting from solid fossil fuels such as hard coal and lignite to higher shares of biomass and natural gas.⁵⁶ For example, phasing out solid fossil fuels and oil in the European lime industry could reduce the carbon footprint of quicklime by 22%.⁵⁶ However, about 65% of quicklime-related emissions come from chemical reactions during limestone calcination.⁵⁷ Addressing direct process emissions requires the deployment of costly carbon capture and storage (CCS) technologies.⁵⁸ Synthetic soda ash is also a hard-to-abate commodity, generating significant process CO₂ emissions from the decomposition of limestone and the combustion of coke.⁵⁹ As with lime production, costly CCS is often the main decarbonization option.⁵⁹ The production of chemical reagents is also associated with environmental issues beyond GHG emissions, such as NO_x and SO_x emissions from calcination of limestone in quicklime production⁵⁸ or water losses from soda ash production.¹⁸ These impacts also contribute to the overall environmental footprint of batteries, although these were not quantified in this work.

Our results are subject to limitations related to data availability and representativeness (temporal, technological, and geographical). Wherever possible, we relied on data representative of the dominant current production routes for battery-grade materials. However, the available data do not fully capture the diversity of the market (*e.g.*, reagent use for cobalt sulfate is based on a specific mine in the Democratic Republic of Congo (DRC) and a refining facility in China). Moreover, data sources correspond to different reference years. For example, reagent use and associated life cycle GHG emissions for lithium carbonate production were obtained from a 2022 study,⁶⁰ whereas the most comprehensive data available for cobalt sulfate production date back to 2018.⁴⁸ This temporal heterogeneity introduces uncertainty, as resource characteristics, technologies, and environmental performance continue to evolve.

Improving the availability, granularity, and transparency of data on battery bill-of-materials (BoM), reagent use in battery-grade materials production and cell recycling, and reagent production is therefore essential to better understand the role and relevance of reagents across the battery supply chain. For example, available life cycle inventories (LCIs) for sodium hydroxide and hydrochloric acid, both linked to the chlor-alkali industry, are not sufficiently regionalized, despite grid electricity accounting for more than 95% of the carbon footprint.⁴⁰ Impacts of quicklime are often modelled using an average fuel mix. However, lime and its derivatives are low-cost

materials, typically produced locally,⁶¹ making regionalization important to capture the specific fuel mixes used in different regions. Soda ash is often modelled in LCA studies based on the synthetic route, overlooking the less impactful trona route.⁶² More regionalized consumption mixes are also needed as, for example, the lithium industry in Chile and Argentina imports soda ash primarily from the USA, where trona ash dominates, whereas production in China mainly follows the synthetic route.⁵²

Moreover, our analysis focused only on the main reagents, omitting minor reagents such as electrolyte additives (*e.g.*, flame retardants such as triphenyl phosphate and tris(2,2,2-trifluoroethyl)phosphate),⁶³ refractory materials (*e.g.*, magnesium oxide), and explosives (ammonium nitrate). These reagents are generally used in relatively small quantities. For example, electrolyte additives typically account for less than 5 wt% of the electrolyte,⁶³ corresponding to approximately 0.02–0.05 kg of additives per kWh of battery cell.

Acknowledging these limitations, our work demonstrates that EV battery supply chains are reagent-intensive, with requirements varying by cell chemistry depending on cathode materials, as their production accounts for most of the reagent demand. While battery cells produced from recycled materials tend to be less reagent-intensive, reagents remain essential in hydrometallurgical recycling processes. Consequently, a highly circular battery economy can reduce reliance on critical minerals, yet significant reagent use would persist. We therefore conclude that, alongside the energy required to power battery manufacturing processes and EVs, chemical reagents play a critical role in the battery supply chain and warrant explicit attention regarding regional availability, cost, and carbon footprint.

Methods

Goal and scope definition

We adopted a life cycle approach to (i) quantify the total amount of reagents consumed across the supply chain to produce one unit of battery cell and (ii) quantify the GHG emissions and costs associated with producing those reagents. The functional unit is defined as either 1 kWh of battery cell capacity (capacity-based reagent intensity) or 1 kg of battery cell (mass-based reagent intensity). The system boundaries include reagent use in the processing of raw materials into battery-grade materials for cathode, anode, electrolyte, and current collectors, the synthesis of pCAM and CAM, and battery cell recycling (Fig. S1). Moreover, cradle-to-gate system boundaries are considered for the quantification of life cycle GHG emissions.

We considered eight battery cell chemistries, including state-of-the-art lithium-ion batteries (LIBs) such as NMC532 (Li₁Ni_{0.5}Mn_{0.3}Co_{0.2}O₂), NMC622 (Li₁Ni_{0.6}Mn_{0.2}Co_{0.2}O₂), NMC811 (Li₁Ni_{0.8}Mn_{0.1}Co_{0.1}O₂), NMC900 (Li₁Ni_{0.9}Mn_{0.05}Co_{0.05}O₂), NCA (Li₁Ni_{0.9}Co_{0.07}Al_{0.03}O₂), and LFP (Li₁Fe₁P₁O₄), and next-generation batteries, such as SIB and SSB.^{1,20} We assumed



NaNFM442 ($\text{Na}_1\text{Ni}_{0.4}\text{Fe}_{0.4}\text{Mn}_{0.2}\text{O}_2$) as a representative cathode chemistry for SIB, and NMC900 cathode combined with an oxide solid electrolyte for SSB. These chemistries are promising candidates in the near future due to favourable energy density, low nickel content, and the possibility of being synthesized with existing equipment.^{20,41} However, we acknowledge that a range of SIB and SSB chemistries may play a role in the future.^{41,64} Graphite (without addition of SiO_2) is the assumed anode active material (AAM) for NMC, NCA, and LFP cells, hard carbon is considered for SIB cells, and lithium metal for SSB cells. The cells' energy density and BoM were obtained from Degen *et al.*²⁰ and are reported in SI Excel S1.

The selection of the reagents studied was based on their overall relevance. Sodium hydroxide, sulfuric acid, and quicklime are the highest-volume bulk inorganic reagents used in metallurgy.¹⁶ Sodium hydroxide is a strong base widely used for pH adjustment, as a neutralising agent, or for metal precipitation. Sulfuric acid also serves pH regulation functions but is primarily employed in leaching operations within hydrometallurgical processes for minerals processing and battery recycling. In some cases, sulfuric acid is produced on-site from sulfur. We estimated the corresponding amount of sulfuric acid using the stoichiometric ratio (0.33 kg sulfur per kg sulfuric acid). Quicklime is commonly applied for pH adjustment, precipitation, or causticization. When hydrated lime (slaked lime) was reported, we estimated the corresponding amount of quicklime considering 0.757 kg of quicklime required per kg hydrated lime. Certain purification processes, such as those for graphite, require stronger acids, including hydrochloric acid, hydrofluoric acid, and nitric acid.⁶⁵ Soda ash is largely used in the precipitation of lithium carbonate and also in the CAM for SIB cells. Ammonia is often used in nickel leaching.¹⁶ Sodium hydroxide and ammonium hydroxide are used in the synthesis of pCAM. For consistency, we converted ammonium hydroxide into the required amount of ammonia. Solvents are used in mineral processing and recycling processes reliant on solvent extraction techniques, such as in the purification of lithium brines.⁶⁰ Often the specific chemical compound used as solvent was not reported and, therefore, we considered a generic category of organic solvents. Finally, the synthesis of the CAM uses large quantities of NMP as a solvent.²⁰

Data on use of reagents per process

We identified and compiled the amount of reagents required to (i) produce the battery-grade materials used in the cathode, anode, electrolyte, and current collectors, (ii) synthesise the pCAM and CAM, and (iii) recycle the cells (SI Excel S2). Below, we summarize the key assumptions and data sources used.

Lithium carbonate. We assumed a production mix of 34% from brines and 66% from spodumene. The brine-based route was modelled as a market-weighted average across five salars located in Chile, Argentina, and China, using data from Schenker *et al.*⁶⁰ The spodumene-based route was modelled as a capacity-weighted average of six supply chains, encompassing spodumene concentrate production at different mines in Australia and subsequent refining in China.⁶⁶ Thus, the pro-

duction of 1 kg of battery-grade lithium carbonate requires approximately 1.42 kg of sulfuric acid, 1.10 kg of soda ash, 0.39 kg of limestone, 0.30 kg of sodium hydroxide, 0.18 kg of quicklime, 0.08 kg of hydrochloric acid, and 0.03 kg of organic solvents.

Lithium hydroxide. Lithium hydroxide is commonly used in high-nickel cell chemistries such as NMC900. We assumed that 20% of lithium hydroxide is produced *via* the conversion of lithium carbonate obtained from brine, while the remaining 80% is produced directly from spodumene concentrate. Reagent requirements for the brine-based route was estimated by combining the data on lithium carbonate production from brine described above with data from Lagos *et al.*⁶² for the conversion process. Reagent requirements for the direct spodumene-based route were sourced from Kelly *et al.*⁶⁷ Based on the assumed production mix, the production of 1 kg of battery-grade lithium hydroxide monohydrate requires 1.22 kg of sulfuric acid, 0.96 kg of sodium hydroxide, 0.48 kg of limestone, 0.43 kg of soda ash, 0.32 kg of quicklime, 0.02 kg of organic solvent, and 0.03 kg of hydrochloric acid.

Cobalt sulfate. We modelled the production of cobalt hydroxide from copper-cobalt ores in the DRC, followed by conversion to cobalt sulfate in China. The DRC is the largest supplier of cobalt, accounting for 76% of global cobalt mined in 2024. Moreover, 77% of global cobalt is extracted as a by-product of copper mining.⁴⁵ Reagent consumption was derived from Dai *et al.*⁴⁸ and Arvidsson *et al.*⁶⁸ Economic allocation was applied to apportion the amount of reagent used during hydrometallurgical processing to each of copper and cobalt. Based on these assumptions, the production of 1 kg of battery-grade cobalt sulfate requires 6.05 kg of sulfuric acid, 3.41 kg of sodium hydroxide, 2.11 kg of limestone, 1.80 kg of hydrochloric acid, 0.59 kg of quicklime, 0.05 kg of ammonia (used in the production of ammonium bicarbonate) and 0.03 kg of soda ash.

Nickel sulfate. We considered the three mainstream production routes, weighted according to their market share in 2023: 65% from laterite ore processed *via* high-pressure acid leaching (HPAL), 20% from laterite ore processed *via* use of rotary kiln electric furnaces (RKEF), and 15% from sulfidic ore processed *via* pyrometallurgy (15%).⁶⁹ Data for the HPAL and RKEF routes were obtained from Roy *et al.*,⁷⁰ while data for the sulfidic route is from Valencia *et al.*³⁹ Since laterite ores contain both nickel and cobalt, cobalt may be recovered as a co-product of nickel. In such cases, reagent consumption should be allocated between the co-products. For the HPAL route, the original reference does not specify whether allocation was considered.⁷⁰ However, previous studies suggest that both mass- and economic-based allocation would assign more than 80% of reagent consumption to nickel.^{71,72} On the other hand, the RKEF route is assumed to result in cobalt losses, and no allocation to co-products is required.⁷¹ The sulfidic route may also involve multiple co-products, including copper, cobalt, platinum, gold, palladium, or sulfuric acid.⁷¹ The original data source omitted these co-products, allocating 100% of reagent consumption to nickel. However, this



assumption has limited impact due to the sulfidic route's relatively small market share. Based on these assumptions, the production of 1 kg of battery-grade nickel sulfate hexahydrate requires 5.78 kg of sulfuric acid, 2.45 kg of limestone, 0.45 kg of quicklime, 0.06 kg of sodium hydroxide, 0.03 kg of soda ash, and 0.03 kg of hydrochloric acid.

Manganese sulfate. Battery-grade manganese sulfate is typically produced *via* two main routes: (1) refining of electrolytic manganese metal (EMM) (predominant production route in China) and (2) through the ore route.⁷³ Here, we assumed that 60% of production is derived from the EMM route and 40% from the ore route.⁷³ The EMM route involves leaching of manganese concentrate followed by electrolysis to produce manganese metal, which is subsequently refined into manganese sulfate. Reagent consumption for this pathway was sourced from Zhang *et al.*⁷⁴ The ore route consists of producing manganese oxide concentrate from ore and reacting it with sulfuric acid to form manganese sulfate. Reagent consumption for this route was based on data from the ecoinvent database v3.10,⁷⁵ which describes the production of industrial-grade manganese sulfate. This can serve as a proxy for battery-grade material, as no additional reagents are required to meet battery-grade specifications.⁷³ Based on these assumptions, the production of 1 kg of battery-grade manganese sulfate requires 0.44 kg of sulfuric acid, 0.01 kg of ammonia, 0.002 kg of limestone, and 2.23×10^{-6} kg of organic chemicals.

Other cathode materials. Additional cathode materials considered in our work include aluminium sulfate, ferrous sulfate, diammonium phosphate (for LFP cells), and magnetite. Producing 1 kg of aluminium sulfate requires 0.21 kg of sulfuric acid, 0.015 kg of sodium hydroxide, and 0.007 kg of quicklime.^{75,76} Ferrous sulfate production involves the use of 0.04 kg of sulfuric acid per kg,⁷⁶ while the production of magnetite requires 0.36 kg of sodium hydroxide per kg.⁷⁵ For diammonium phosphate, producing 1 kg of material requires 1.13 kg of sulfuric acid, 0.26 kg of ammonia, 0.11 kg of quicklime, and 0.02 kg of sodium hydroxide.⁷⁵

Graphite AAM. We assumed that 20% of the graphite AAM is produced from natural graphite and 80% from synthetic graphite.⁸ The production of 1 kg of coated natural graphite through acid leaching processes, assumed to occur in China, uses 0.22 kg of hydrochloric acid, 0.20 kg of hydrofluoric acid, 0.11 kg of nitric acid, and 0.33 kg of quicklime.⁷⁷ The production of synthetic graphite only requires some quicklime (0.13 kg per kg of coated synthetic graphite) in the production of calcined petroleum coke used as feedstock.^{28,78}

Hard carbon AAM. Hard carbon serves as the AAM in SIB cells. While various carbonaceous precursors can be used for synthesizing hard carbon, pitch (petroleum and coal tar) is the standard feedstock due to its wide availability.⁶⁴ The production process involves pre-oxidation of the precursor followed by carbonization, and no reagents are assumed to be used in this process.

Lithium metal AAM. Lithium metal, used as the AAM in SSB cells, is produced by direct electrolysis of lithium chloride, which is obtained from the reaction of lithium carbonate with

hydrochloric acid. Consequently, reagent requirements are based on the average inputs for lithium carbonate production described above, with an additional amount of 5.9 kg of hydrochloric acid per kg of lithium metal for the final reaction, according to the ecoinvent v3.10 database.

Electrolytes. Lithium hexafluorophosphate (LiPF_6) is the liquid electrolyte used in NMC, NCA, and LFP cells. It is produced from lithium chloride, requiring lithium carbonate (see above) and hydrochloric acid, and hydrated lime and hydrogen fluoride. The quantities of additional chemicals were obtained from the ecoinvent v3.10 database.⁷⁵ Sodium hexafluorophosphate (NaPF_6) is the liquid electrolyte used in SIB cells. Its production is very similar to that of LiPF_6 , requiring 0.35 kg of sodium chloride (which in turn requires 0.014 kg of quicklime and 0.013 kg of soda ash per kg) and 1.33 kg of hydrated lime, and 0.77 kg of hydrogen fluoride (considered as hydrofluoric acid).^{75,79}

Current collectors. Aluminium foil and copper foil serve as current collectors. They are produced from aluminium and copper treated with sodium hydroxide (0.33 kg per kg aluminium foil; 0.25 kg per kg copper foil) and sulfuric acid (0.21 kg per kg aluminium foil; 0.15 kg per kg copper foil).⁸⁰ Reagents used upstream in the aluminium and copper supply chains were omitted.

pCAM and CAM synthesis. The synthesis of pCAM and CAM for 1 kWh of battery cell capacity requires, depending on the cell chemistry, between 1.1 and 1.8 kg of sodium hydroxide and 0.08–0.4 kg of ammonia.²⁰ SIB cells also require 1.17 kg of soda ash. Moreover, between 1.42 and 2.65 kg of NMP are used in the process.²⁰ However, we assumed that NMP is recycled and reused due to its toxicity, as is standard practice in modern gigafactories.²⁰ Assuming a 99% recovery rate,⁸¹ the demand for fresh NMP amounts to 0.014–0.027 kg per kWh battery cell capacity.

Hydrometallurgical recycling. Reagent requirements for battery cell recycling can vary widely depending on the cell chemistry, treatment type (pyrometallurgy, hydrometallurgy, or direct recycling), and process configuration. Hydrometallurgy is the dominant recycling option for LIBs, accounting for 90% of global recycling capacity in 2023 and anticipated to remain the same by 2030.³² The process typically consists of pre-treatment to obtain black mass followed by leaching with a strong inorganic acid and separation of metal ions in the leachate through different methods such as solvent extraction, chemical precipitation, electrochemical deposition, or ion exchange.³⁷ We used data from Šimaitis *et al.*,²² who described a hydrometallurgical recycling process with requirements of 0.56 kg of sodium hydroxide per kg of battery cell treated, 0.02 kg of soda ash, 1.08 kg of sulfuric acid, and 0.01 kg of hydrochloric acid. We assumed identical recycling processes for all NMC, NCA, and LFP cells,³⁵ scaling the amount of reagents according to the cell energy capacity. We considered the recovery of lithium (90% recovery rate), cobalt (98%), nickel (98%), and manganese (98%), omitting the recovery of aluminium and copper due to their negligible contribution to reagent use. Moreover, we assumed that graph-



ite and electrolyte are lost and did not consider the recycling of SIB and SSB cells as they remain in the early stages of development and dedicated recycling processes have yet to be established.³⁸

Data on battery cell demand scenarios

To estimate the future global requirement of reagents for battery cell manufacturing, we combined cell-specific reagent intensities with global demand for battery cell capacity. We aligned global battery cell demand with Degen *et al.*,¹ who assumed a growth to 5470 GWh by 2040. Historical global demand from 2018 to 2024 was taken from the IEA.²

Four scenarios were considered reflecting varying market shares of battery chemistries based on Degen *et al.*¹ The MIX scenario assumes a balanced deployment where NCA and NMC cells achieve 33% market share by 2040, LFP 28%, and SIB and SSB 39%. The LFP scenario assumes that LFP cells dominate the market, reaching 60% market share by 2040 with NMC and NCA accounting for the remaining 40%. The NCX scenario describes a future where NMC and NCA cells dominate the market with a combined market share of 95% by 2040 with LFP contributing the remaining 5%. Finally, the NEXT scenario describes a future where next-generation cells (SIB and SSB) achieve 60% market share by 2040, with NMC and NCA cells accounting for the remaining 40%. The associated data can be found in SI Excel S3.

To estimate reagent requirements for recycling, we assumed an average lifespan of 15 years for LFP cells and 12 years for the other chemistries.⁹ We also conducted the calculations considering a minimum of 8 years and a maximum of 15 years. Moreover, we further assumed that all batteries reaching their end-of-life are diverted towards recycling, thus ignoring a fraction that could be repurposed for storage applications. However, according to the IEA, persistent economic challenges may limit this second-life application.³² It should be noted that due to the aforementioned data limitations we did not consider the recycling of SIB and SSB cells.

Data on life cycle GHG emissions

We calculate the GHG emissions associated with the production of reagents needed per unit of battery cell by multiplying the reagent-specific intensity by their average life cycle GHG emission intensity. Life cycle GHG emissions associated with reagent production were obtained from the literature (details provided below). We then compared the GHG emissions associated with reagents with the overall carbon footprint of the corresponding battery cell. We obtained the cell-specific carbon footprint values from Degen *et al.*²⁰ It should be noted that some discrepancies may exist because this study contains implicit assumptions about reagent uses.

Sodium hydroxide. Sodium hydroxide is co-produced with chlorine and hydrogen in the chlor-alkali process *via* electrolysis of sodium chloride brine. The dominant technologies are membrane and diaphragm cells. As the process is multifunctional, impacts must be allocated among chlorine, sodium hydroxide, and hydrogen. According to Garcia-Herrero *et al.* in

2017, both mass and economic allocations result in 70% of impacts being allocated to sodium hydroxide.⁴⁰ According to the ecoinvent v3.10 database, the global average carbon footprint of sodium hydroxide is about 1.5 kg CO₂-eq per kg sodium hydroxide,⁷⁵ whereas Euro Chlor reports an average of 0.66 kg CO₂-eq per kg covering 75% of European production capacity.⁸² We used this range, with an average of 1.1 kg CO₂-eq per kg.

Soda ash (light). We assumed that 35% of soda ash is produced from trona and 65% through the Solvay process (synthetic route).⁵² We assumed that the trona route has a carbon footprint of 0.75 kg CO₂-eq per kg, while the synthetic route reaches about 1.6 kg CO₂-eq per kg.⁶² The carbon footprint weighted by production shares is equal to 1.3 kg CO₂-eq per kg.⁶² We used these data for each route to represent the minimum and maximum range.

Sulfuric acid. About 80% of the elemental sulfur used in industry, mostly for sulfuric acid production, is a by-product of the fossil fuel industry. Metal smelting of sulfidic minerals, including copper and zinc, is another important source.^{25,43} The carbon footprint of sulfuric acid varies widely depending on the production route. According to the ecoinvent v3.10 database, the global average is 0.18 kg CO₂-eq per kg sulfuric acid. We used a range from 0.1 to 0.21 kg CO₂-eq per kg corresponding to sulfuric acid production from copper smelting and primary lead production, respectively.

Hydrochloric acid. Industrial-grade hydrochloric acid (30% concentrated) is typically produced by dissolving hydrogen chloride in water. Multiple pathways exist to obtain the hydrogen chloride precursor. According to ecoinvent v3.10, over 95% of hydrochloric acid is produced through four main routes: (i) the Mannheim process (~40%), (ii) combustion of hydrogen with chlorine (~40%), (iii) as a by-product of methylene diphenyl diisocyanate production (<10%), and (iv) as a by-product of toluene diisocyanate production (<10%).⁷⁵ The carbon footprint ranges from 0.4 to 1.8 kg CO₂-eq per kg hydrochloric acid (30% concentrated). We used this range and adopted a weighted average of 0.9 kg CO₂-eq per kg.

Hydrofluoric acid. We used the carbon footprint derived from the ecoinvent v3.10 database.

Nitric acid. We used the carbon footprint derived from the ecoinvent v3.10 database.

Limestone. We obtained the life cycle GHG emissions for a limestone quarry from Kaykov and Petrova.⁸³ These authors provided a range from 0.0013 to 0.0019 kg CO₂-eq per kg, reflecting relatively low emissions associated with activities like drilling, blasting, hauling, crushing and screening, and processing.

Quicklime. Quicklime is produced through calcination of limestone followed by sizing and screening to produce milled quicklime.⁵⁶ We assumed an average carbon footprint of 1.1 kg CO₂-eq per kg, corresponding to parallel flow regenerative kilns (PFRK), the most popular and efficient kiln in the industry.⁵⁸ For the minimum and maximum range, we considered the minimum reported carbon footprint for PFRK (1 kg CO₂-eq per kg) and the average carbon footprint of the long rotary kiln



(1.5 kg CO₂-eq per kg), a less efficient kiln, which, however, offers advantages in robustness and flexibility.⁵⁸

Ammonia. We considered the conventional Haber–Bosch process. The low carbon footprint estimate is based on the use of wind-based electrolytic hydrogen (0.28 kg CO₂-eq per kg), while the high estimate considers the use of natural gas (2.7 kg CO₂-eq per kg).⁸⁴ We assumed the natural gas estimate as the average since this is the main production route currently.

Organic solvents. A variety of solvents are used in industry, with carbon footprints ranging from about 0.5 kg CO₂-eq per kg for kerosene to 3.5 kg CO₂-eq per kg for dichloromethane.⁸⁵ Traditional solvents in minerals processing, such as acetone and ethanol, fall between 1.5 and 2.5 kg CO₂-eq per kg.⁸⁵ Based on these values, we adopted a range of 0.5–3.5 kg CO₂-eq per kg, with an average of 2 kg CO₂-eq per kg.

NMP. We assumed an average carbon footprint of 4.2 kg CO₂-eq per kg NMP based on Pastore *et al.*⁸⁶

Data on economic costs

To calculate the costs of reagents needed per unit of battery cell, we multiplied the reagent-specific intensity by their median market spot price. Spot market prices were sourced from publicly available entries for various regions and time periods at <https://businessanalytiq.com> (see SI Excel S5). We considered median prices over 2016–2025 in China, USA, and Europe. To illustrate the uncertainty associated with fluctuations in market prices, we also reported ranges based on minimum and maximum values corresponding to the lowest and highest monthly market prices observed between 2016 and 2025 across these three regions. We then compared the obtained reagent-specific costs with the production costs of battery cells obtained from the Volta Foundation for NMC cells⁴² and Yao *et al.*⁴¹ for LFP and SIB cells.

Author contributions

RI: conceptualization, formal analysis, investigation, methodology, visualisation, writing – original draft, writing – review and editing; LP: conceptualization, investigation, methodology, writing – review and editing; VS: conceptualization, investigation, methodology, writing – review and editing.

Conflicts of interest

There are no conflicts to declare.

Data availability

The data supporting this article have been included as part of the supplementary information (SI). Supplementary information is available. The SI Excel file contains all the data required to reproduce the results. See DOI: <https://doi.org/10.1039/d5gc05122c>.

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