

Life cycle assessment of battery minerals to 2040: contribution of voluntary sustainability initiatives

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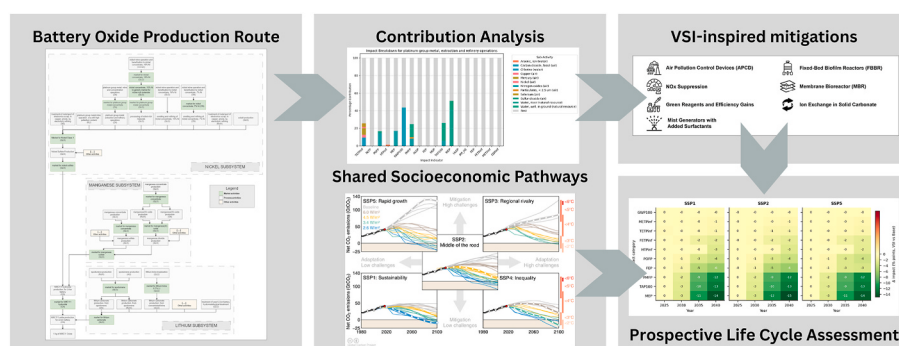
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HIGHLIGHTS

- Prospective LCA of NMC111 oxide production to 2040 under SSP scenarios.
- VSI-inspired process interventions modelled as emission reduction coefficients.
- Framework links sustainability initiatives to process-level engineering strategies.
- Air pollution control devices cut PM formation in selected nickel processing.
- Combined scenarios yield up to ~15% reduction at oxide level.

GRAPHICAL ABSTRACT



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ABSTRACT

The expansion of electric mobility is intensifying demand for lithium, nickel, and manganese, increasing the environmental burdens of mineral extraction and processing. Voluntary sustainability initiatives (VSIs) have emerged to encourage improved environmental management, yet their long-term effectiveness remains uncertain. This study explores a proof-of-concept of how VSI-aligned operational interventions could influence the future environmental performance of battery mineral supply chains, using a scenario-based prospective environmental assessment informed by life cycle modelling. By integrating Shared Socioeconomic Pathways (SSPs) with VSI-aligned process measures such as air pollution control devices (APCDs), we assess midpoint impacts including climate change, particulate matter formation, and human toxicity. Results show that systemic background decarbonization dominates reductions, while VSI-inspired interventions deliver complementary benefits, including up to ~75% reductions in particulate matter formation for nickel beneficiation and localized process-level reductions of up to ~90%. These findings highlight how coupling systemic and operational measures can improve resource efficiency and environmental performance in battery-mineral supply chains.

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1. Introduction

1.1. NMC batteries, oxide production routes, and associated impacts

The decarbonization of the transportation sector is a pivotal strategy in mitigating climate change, necessitating a transition to low-carbon technologies (Habib et al., 2020), driving unprecedented demand for lithium-ion batteries (LIBs) and the critical minerals they rely on, such as lithium, nickel, manganese, and cobalt (Dominish et al., 2019). Among these, nickel-manganese-cobalt (NMC) batteries dominate due to their optimal balance of energy density, safety, and longevity, making them indispensable in electric vehicles (EVs) (Nitta et al., 2015). Demand for NMC batteries is projected to grow exponentially, raising concern over the production of compounds such as nickel sulfate, manganese sulfate, lithium carbonate, and lithium hydroxide, which involve complex, impact-intensive processes with significant environmental impacts and resource supply risks (Chen et al., 2025, 2026; Sadhukhan and Christensen, 2021; Xu et al., 2022). These materials are often sourced from resource-rich regions in the global south, where concerns over environmental, social, and governance (ESG) risks further complicate supply chains and have become a critical consideration in the sustainability of battery materials (Lèbre et al., 2020).

1.2. Voluntary sustainability initiatives and their mitigation potential

Voluntary Sustainability Initiatives (VSIs) have emerged as a response to growing pressure on the mining sector from investors, regulators, and civil society to adopt more sustainable practices (Franken and Schütte, 2022). These initiatives encompass standards and certifications aimed at improving transparency and reducing the environmental and social impacts associated with mining supply chains. Their adoption has been connected with the rise in material demand by industries like EV manufacturers (Amnesty International, 2017). Notable mentions include global schemes aimed towards large-scale mining operations, like the *International Council on Mining and Metals* (ICMM) Sustainable Development Framework (ICMM, 2023), the *Initiative for Responsible Mining Assurance* (IRMA) (IRMA, 2018), and the *Global Reporting Initiative* (GRI) Reporting Principles and Standards (GRI, 2023).

Although a range of VSIs has been implemented, their effectiveness in driving long-term sustainability remains debated. While they can support early adoption, foster cooperative relations with regulators, and bring non-industry stakeholders to the discussion table, criticisms persist regarding their potential to facilitate greenwashing by focusing on short-term impacts. Moreover, the voluntary nature of these initiatives leaves them vulnerable to inconsistencies in enforcement and impact (Tröster and Hiete, 2018). Nevertheless, the growing demand for battery minerals and the expected uptake in VSIs underscore the importance of monitoring VSI adoption to mitigate future environmental risks. We view VSI adoption as part of an adaptive management strategy, where monitoring and transparency are key components. To our knowledge, this is the first study to explicitly link VSI-aligned sustainability commitments to empirically documented mitigation technologies, sourcing emission reduction coefficients from the engineering literature for specific elementary flows and compartments, and integrate them into a prospective LCA framework for battery mineral supply chains. This approach bridges a gap between the policy-oriented literature on voluntary sustainability initiatives and the process-level modelling used in prospective LCA, enabling scenario-based assessment of how operational interventions encouraged by VSIs could influence future environmental performance alongside systemic background changes.

1.3. Structure and scope of this study

We evaluate potential impact mitigation in the LIB supply chain from 2025 to 2040 through a prospective LCA (pLCA) of NMC oxides,

focusing on nickel, manganese, and lithium. The analysis integrates Shared Socioeconomic Pathways (SSP1, SSP2, SSP5) to capture evolving energy systems alongside VSI-inspired interventions. This study builds on a growing body of research employing prospective life cycle assessment (pLCA) to evaluate the environmental impacts associated with material extraction and processing for energy transition technologies (Harpprecht et al., 2024). Previous studies have explored critical factors influencing life cycle impacts, including production location (Ambrose and Kendall, 2020), variations in ore grades (Harpprecht et al., 2021), energy efficiency (Watari et al., 2022), and the role of the background energy mix (van der Meide et al., 2022). However, much of the existing research concentrated on major metals, such as copper and iron, which, while economically significant, are not as central to emerging clean energy technologies (Harpprecht et al., 2024). Moreover, impacts beyond those associated with greenhouse gas (GHG) emissions are often overlooked (Watari et al., 2021), even though the potential for environmental impacts of mining activities has been extensively documented in literature, ranging from land-use change (Sonter et al., 2018), impacts on water quality and access (Kemp et al., 2010), decreased air quality (Franks et al., 2013), and biodiversity loss (Sonter et al., 2018), among others. Given the localized and often severe environmental burdens associated with mining operations at the point of extraction, it is critical to expand the scope of assessments to capture a wider range of environmental impacts. This expansion must also consider mitigation strategies beyond the current status quo to account for innovative and operationally feasible solutions.

In parallel, process innovations are reshaping the environmental profiles of battery mineral supply chains. For lithium, Direct Lithium Extraction (DLE) technologies are emerging as alternatives to conventional evaporation-pond methods, with recent LCA studies examining their environmental footprints across climate change, water use, and land use dimensions (Mousavinezhad et al., 2024). For nickel, the growing role of High-Pressure Acid Leaching (HPAL) of laterite ores, particularly from Indonesia, has prompted cradle-to-gate LCAs revealing significant environmental concerns for this processing route (Bartzas and Komnitsas, 2024). Moreover, disaggregated process-level inventories have highlighted considerable variability across processing pathways (Schenker et al., 2022). However, these studies primarily assess individual process routes under current conditions, rather than evaluating how process-level interventions might interact with evolving background systems over time. Moreover, while DLE and HPAL represent the frontier of new project development, the existing installed base of conventional operations covered in this study, such as evaporation-pond lithium extraction, spodumene processing, and pyrometallurgical nickel refining, will continue to operate. These legacy operations are precisely where VSI-aligned mitigation strategies are most applicable. Our study complements the emerging literature on new process routes by focusing on how targeted interventions can improve the environmental performance of established operations.

It's important to clarify that we do not claim that the mitigation technologies modelled in this study are exclusive products of VSI adoption. Technologies such as APCDs or MBRs exist independently and may be adopted for regulatory compliance, operational efficiency, or risk management reasons. Rather, our framing positions VSIs as enabling mechanisms that can accelerate or incentivise the adoption of these technologies at operations where they would not otherwise be prioritised, particularly at sites where regulatory requirements alone do not mandate their implementation.

This framing is motivated by a gap in the current landscape of prospective environmental modelling. The Integrated Assessment Models (IAMs) that underpin future scenarios such as the Shared Socioeconomic Pathways (SSPs) are primarily designed to capture energy-system decarbonization and its associated effects on climate-related impact categories. They do not, however, systematically incorporate process-level mitigation strategies targeting non-GHG impacts such as particulate matter formation, human toxicity, or ecotoxicity. All being

categories that are disproportionately relevant at the point of mineral extraction and processing. By linking impact mitigation commitments to empirically documented mitigation technologies and integrating them into a prospective LCA framework, this study offers a proof-of-concept for quantifying the environmental consequences of operational interventions that fall outside the scope of IAM-based scenarios. The simplified best-case approach adopted here (applying maximum documented reduction coefficients along a logistic adoption curve) represents an upper-bound estimate but demonstrates that such interventions can be systematically incorporated into pLCA alongside background scenarios.

The following sections outline the methods employed to model these processes and scenarios (section 2), the results obtained (section 3), and their implications for stakeholders and policymakers (section 4). Moreover, the supplementary material contains significant information to replicate this methodology with different compounds, processing routes, and background scenarios.

2. Materials and methods

We modelled the extraction and processing of lithium, nickel, and manganese used in nickel-manganese-cobalt (NMC) oxides, key compounds in the production of lithium-ion battery cells. The selection of these three materials is particularly relevant due to their significant contributions to a wide range of environmental impacts of NMC oxide production and, consequently, battery cell manufacturing (Murdock

et al., 2021).

We employed the stepwise approach of Scenario-based Inventory Modelling for Prospective Life Cycle Assessment (SIMPL) (Langkau et al., 2023) to systematically identify and model relevant factors. The SIMPL approach involves: (a) identifying key inventory parameters and critical factors, (b) establishing assumptions for each identified parameter, and (c) combining these assumptions to generate future scenarios. To identify key factors and parameters, we built on previous works that utilized a group-model building approach rooted in system dynamics, leading to the development of a causal loop diagram (CLD) with inputs from industry stakeholders (Mendonca Severiano et al., 2025). This collaborative process provided valuable insights into the parameters influencing voluntary impact mitigation in the context of battery mineral mining. Results from this exercise were subsequently refined to align with the SIMPL framework. The parameters and factors' definition and modelling involved the following key steps:

Mapping the production route:

- The production route for NMC111 oxide used in lithium-ion batteries was mapped using the ecoinvent 3.8 cut-off database (Wernet et al., 2016) (Fig. 1). Relevant upstream unit processes supplying compounds for NMC111 oxide production, such as lithium hydroxide, lithium carbonate, manganese sulfate, and nickel sulfate, were identified and further explored.
- Processes involved in the supply of the products used in these compounds (e.g., *nickel mine operation and beneficiation to nickel*

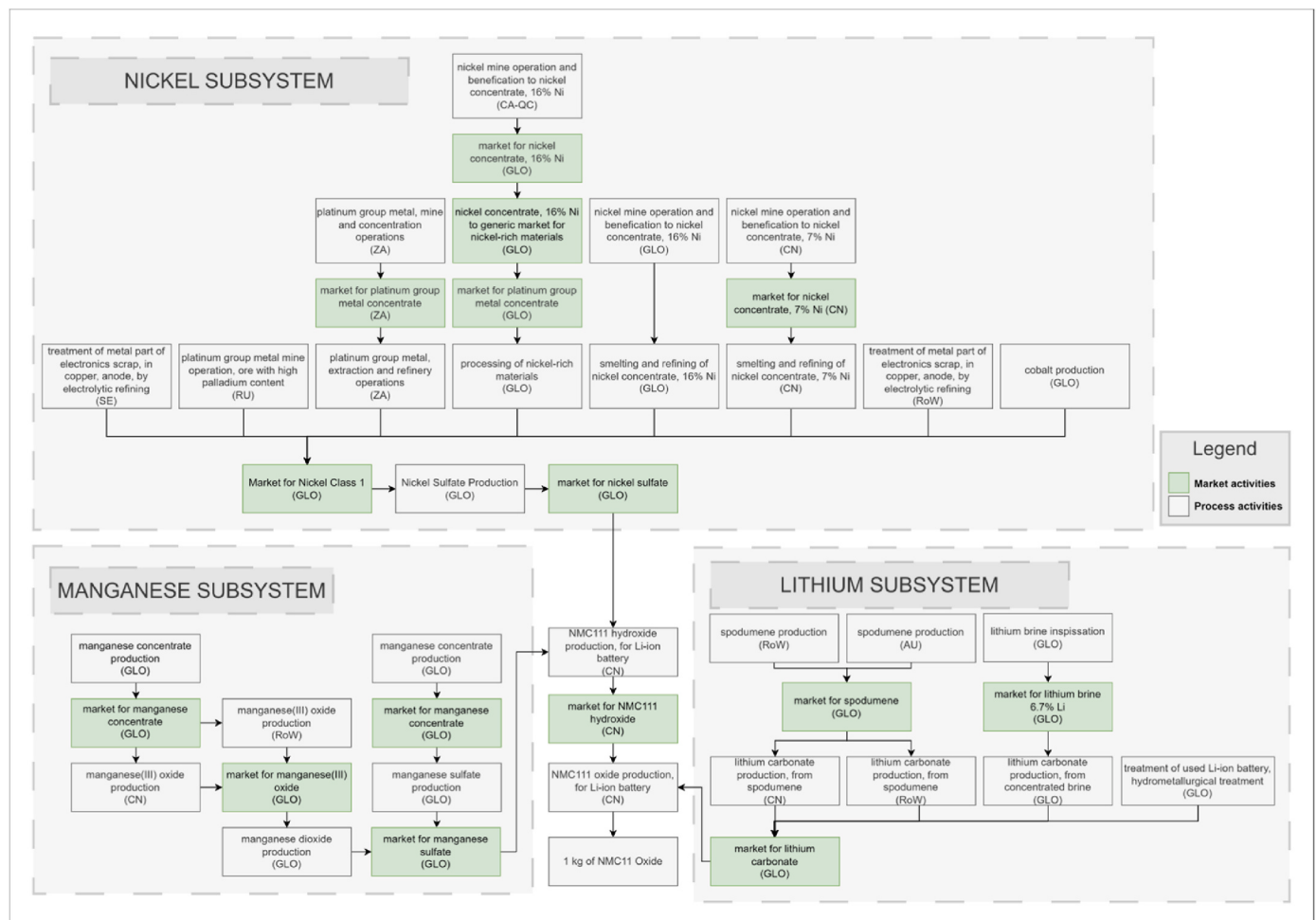


Fig. 1. Cradle-to-gate production route of NMC111 Oxide, with a focus on lithium hydroxide, nickel sulfate, and manganese sulfate production. Subsystems are colour-coded: nickel-related processes (blue), lithium-related processes (green), and manganese-related processes (orange). Production routes are based on processes from ecoinvent 3.8. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

concentrate, and smelting and refining of nickel concentrate to produce nickel class 1) were further identified and selected for a detailed parameter exploration.

Initial inventory modelling, preliminary impact assessment, and parameter selection:

- An initial life cycle inventory and impact assessment were conducted using data from ecoinvent 3.8 (details available in the supplementary material).
- For each unit process (e.g. smelting and refining of nickel concentrate), impacts were disaggregated by impact category, and contributions were analysed at the level of elementary flows to specific compartments (e.g. ecotoxicity impacts of sulfur dioxide emissions to non-urban air).
- A hotspot analysis was performed to identify which elementary flows contributed the most to each impact category, using a threshold of $\geq 1\%$ of relative impact per category.

Foreground inventory modelling:

- Potential strategies for impact mitigation were identified based on the hotspot analysis, with a focus on the elementary flows with the highest contribution per impact category.
- These strategies were incorporated as coefficients of reduction, applied directly to the elementary flows of each unit process to reflect potential voluntary emissions reductions.

Background inventory modelling:

- New inventories were incorporated from results extracted from REMIND for a range of socioeconomic pathways.

Inventory modelling and impact assessments were performed:

- The background and foreground inventories were combined, and prospective impact assessments were performed to evaluate the cumulative effects across various scenarios.

The environmental impacts were quantified through a cradle-to-gate approach. The functional unit is defined as 1 kg of NMC111 oxide at the factory gate. Intermediate reference flows (e.g., 1 kg of nickel class 1, lithium carbonate, or manganese sulfate) are modelled as internal accounting units within the production system and are not treated as separate functional units. The assessment is conducted for four discrete time slices (2025, 2030, 2035, and 2040), rather than as a continuous dynamic simulation. All inventory and impact assessment calculations have been performed using Brightway2.5, an open source framework for life cycle assessment (Mutel, 2017). Further details about the Python code used in the different steps of the process can be found in the supplementary material. Additionally, we used *premise*, an open-source Python library (Sacchi et al., 2022), to incorporate climate mitigation scenarios from the Integrated Assessment Model (IAM) REgional Model of INvestments and Development (REMIND) into the background system (Baumstark et al., 2021). The following sections provide the scenario definitions and describe the steps taken for our systematic scenario modelling approach (sections 2.1 – 2.5).

2.1. Mapping the production route: Battery cell production, NMC oxide, and upstream unit processes

The initial focus of our process modelling was on the production of NMC111 oxide for Li-ion battery (CN). From this processing route, the markets for NMC111 hydroxide and Lithium carbonate were disaggregated (Fig. 1). For these two unit processes, the supporting unit processes involved in the production of lithium carbonate, nickel

sulfate, and manganese sulfate were identified and listed. Similar to previous studies that explored the prospective life cycle assessment of lithium-ion batteries (Xu et al., 2022), we analysed the cradle-to-gate production of battery cell compounds based on the inventories available on ecoinvent 3.8. We included raw materials' extraction, materials' production, and materials' upgrading. When incorporating potential environmental impact, voluntary mitigation strategies associated with modifications to specific unit processes, exchanges within these processing routes were modified by applying mitigation coefficients over time.

2.2. Initial inventory modelling, preliminary impact assessment, and parameter selection

We employed a group model-building approach to integrate diverse perspectives into a cohesive causal loop diagram (CLD), previously introduced in Mendonca Severiano et al. (2025) and now expanded to include key parameters relevant to our modelling framework. To quantify environmental impacts, we conducted a life cycle inventory and impact assessment for each identified processing route utilizing the inventories available in ecoinvent 3.8, with detailed results for all impact categories provided in Supplementary Material 1, Section 2. The assessment utilized the ReCiPe 1.6 Midpoint (H) (Huijbregts et al., 2017), and the Python code used for the analysis, along with the impact results, is available in the Supplementary Material.

To identify the most significant emissions, we performed a contribution analysis across all impact categories, examining the percentage contribution of individual emissions from each processing step. These emissions were categorized by compartment (e.g., air, water, soil) and sub-compartment (e.g., low population density, long-term), as detailed in Supplementary Material 1, Section 3. For example, when evaluating the particulate matter formation (PMFP) impact category to produce 1 kg of nickel class 1 through *platinum group metal, mine and concentration operations* (ZA), the analysis revealed that sulfur dioxide (SO₂), nitrogen oxides (NO_x), and particulate matter (<2.5 µm) emissions to air were the primary contributors, as exemplified in Fig. 2. These findings informed our selection of mitigation strategies, ensuring that efficiency gains, technological advancements, and process optimizations (Fig. 3) directly targeted the most impactful emissions, thereby reducing the overall environmental impact.

2.3. Background modelling

The background system of our analysis is built based on the ecoinvent 3.8 database (Frischknecht et al., 2005). We consider future changes in energy scenarios affecting the supply of battery materials previously described as being part of our foreground scenario. We used the open-source library *premise* to generate future-scenario versions of ecoinvent 3.8 cut-off, expanding the background inventory to reflect changes related to Shared Socioeconomic Pathway (SSP) scenarios, using scenarios from the integrated assessment model REMIND (Sacchi et al., 2022). By using *premise* v2.0.1, the original database (ecoinvent) is systematically transformed and expanded by emerging and future technologies not originally available in the database. REMIND models the energy system by integrating a variety of energy conversion technologies and energy services (such as the ones used by industry sectors) (Baumstark et al., 2021). When using *premise*, the created background inventories are modified according to the selected SSP and henceforth referred to as 'SSP-Base'. SSPs are scenarios used in climate modelling to explore different pathways for global socioeconomic development. A key driver of changes in environmental impacts is the transformation of the electricity mix, particularly the increasing share of renewables, which influences the background emissions of industrial processes. These can be perceived as "directions" of development, taking into consideration climate change impacts, adaptation, and mitigation (O'Neill et al., 2014). SSPs are used across research and feed into the

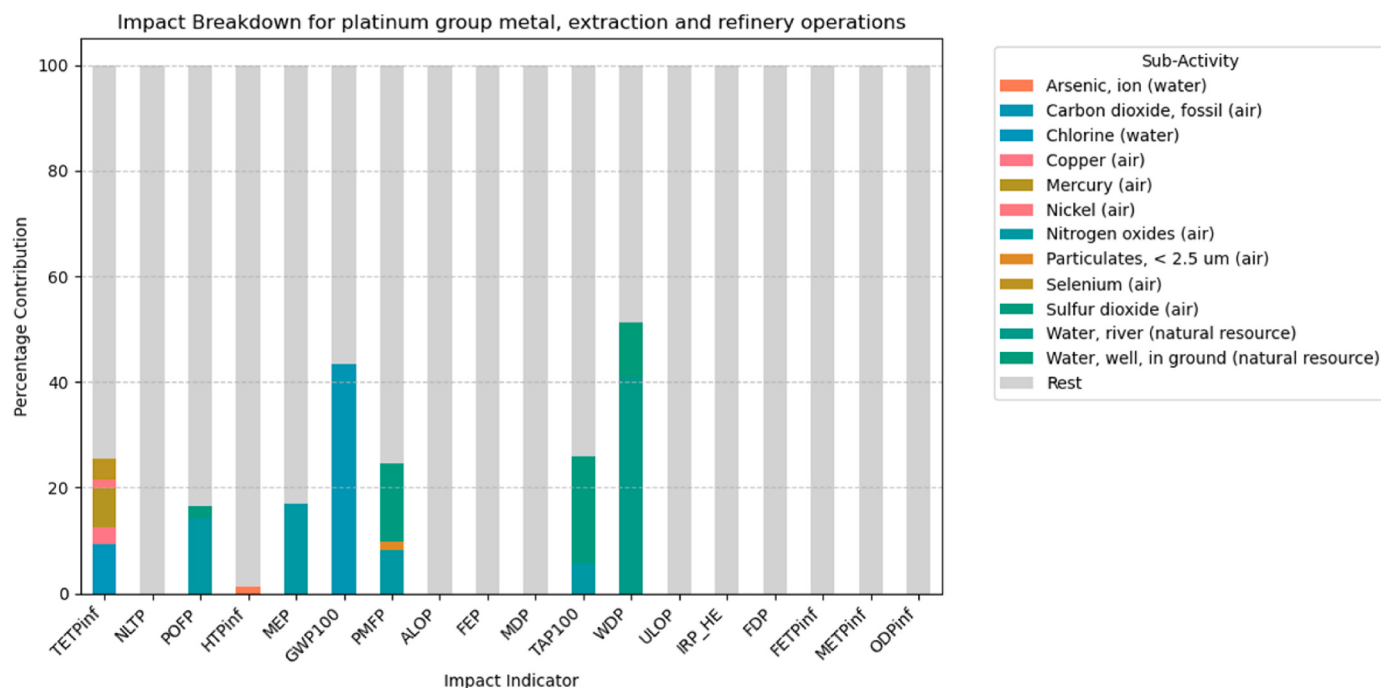


Fig. 2. Contribution analysis for platinum group metal, mine and concentration operations (ZA), producing 1 kg of nickel class 1. The stacked bars represent the percentage contribution of individual emissions, with biosphere exchanges color-coded according to their respective compartments (e.g., air, water, soil). These insights were used to guide the selection of mitigation strategies aimed at reducing key emissions, particularly sulfur dioxide (SO₂), nitrogen oxides (NO_x), and particulate matter (<2.5 μm) emissions to air. TETPinf = terrestrial ecotoxicity; NLTP = Natural land transformation; POFP = photochemical oxidant formation; HTPinf = human toxicity; MEP = Marine eutrophication; GWP100 = Climate change; PMFP = particulate matter formation; ALOP = Agricultural land occupation; FEP = freshwater eutrophication; MDP = Metal depletion; TAP100 = terrestrial acidification; WDP = Water depletion; ULOP = Urban land occupation; IRP_HE = Ionising radiation; FDP = Fossil depletion; FETPinf = freshwater ecotoxicity; METPinf = marine ecotoxicity; ODPinf = Ozone depletion. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

Intergovernmental Panel on Climate Change (IPCC) reports (IPCC, 2023). SSPs reflect future worlds based on their mitigation and adaptation challenges, giving us long-term projections over a range of socioeconomic conditions (Hausfather, 2018). For our analysis, we considered the following background scenarios, informed by (Hausfather, 2018), and the premise documentation (premise, 2025):

- i. **None (Business as usual):** No adaptation or mitigation assumptions applied. Represents a continuation of current trends without policy intervention.
- ii. **SSP1 (“Taking the green road”):** Low challenges to mitigation and adaptation. Characterised by a gradual and widespread shift toward sustainability, inclusive development, and respect for environmental boundaries.
- iii. **SSP2 (“Middle of the road”):** Moderate challenges to mitigation and adaptation. Reflects socioeconomic and technological trends that largely follow historical patterns, with limited shifts in policy or behaviour.
- iv. **SSP5 (“Taking the highway”):** High challenges to mitigation, low challenges to adaptation. Depicts rapid economic and social development driven by fossil-fuel use and resource-intensive lifestyles worldwide.

It's important to note that we used ecoinvent 3.8 to ensure compatibility with the current codebase and libraries used. Later versions (3.9, 3.11) and newer lithium inventories (e.g. (Schenker et al., 2022; Khakmardan et al., 2025)), provide improvements, but incorporation was beyond the scope of this first implementation. The modular design of our framework allows updates as these datasets mature.

2.4. Foreground modelling

To better understand how specific mitigation technologies can translate into mitigated impacts, we modelled their impact mitigation potential through limiting the emissions of a certain pollutant to certain compartments (e.g. emissions of particulate matter to air, which can lead to an increase in respiratory diseases (Huijbregts et al., 2017)). These mitigation technologies include: (i) Air Pollution Control Devices (APCDs) (Wu et al., 2019; Zhang et al., 2022), (ii) Nitrogen Oxides (NO_x) suppression (Rebrov and Gorlov, 2011), (iii) green reagents and efficiency gains (International Finance Corporation, 2023), (iv) fixed-bed biofilm reactors (FBBR) (Zaitsev et al., 2008), (v) membrane bioreactors (MBR) (Dobson and Burgess, 2007; Melin et al., 2006), (vi) ion exchange in solid carbonate (Cueto and Hansen, 2019), and (vii) mist generators with added surfactants (Lee et al., 2022). These technologies were selected based on their demonstrated applicability to the specific process conditions identified in the hotspot analysis (Section 2.2). APCD coefficients derive from non-ferrous metal smelter measurements (Wu et al., 2019; Zhang et al., 2022) and are applied to smelting and refining processes within the nickel, lithium, and manganese subsystems. Where a technology's empirical basis originates from a different but analogous industrial context (e.g., mist generators tested on iron ore piles, applied here to mineral processing dust), this is noted in Supplementary Material 2.

We assessed the emission reduction potential for each technology by elementary flow. Table 1 summarises the key mitigation technologies, their targeted elementary flows, reduction coefficients, and the empirical or analogical basis for each value. Coefficients marked as 'confirmed' are derived directly from empirical measurements reported in the cited source. Those marked as 'assumed' are based on chemical or process analogy where direct measurements were unavailable. The full set of coefficients disaggregated by subsystem (nickel, lithium, manganese),

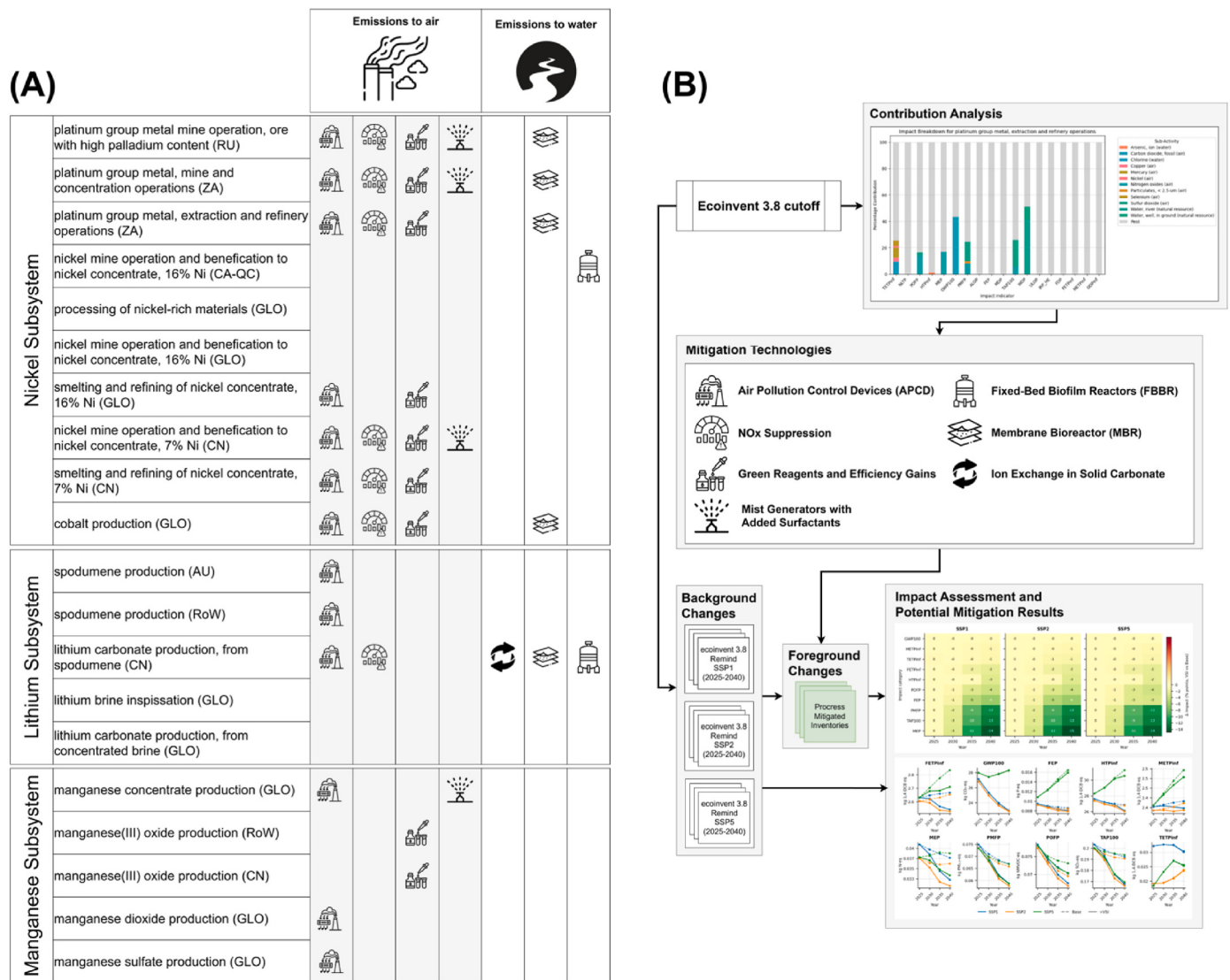


Fig. 3. (A) Mitigation strategies adopted and their mitigation within production subsystems. Unit processes with no mitigation strategies applied to them had only the background inventories modified according to the SSP. (B) Diagram of data generation, transformation, expansion, processing, and expected outputs. SSP = Shared Socioeconomic Pathway.

individual elementary flow, and compartment are provided in [Supplementary Material 2](#).

Additionally, we structured our approach using a time-explicit mitigation strategy, in which we assumed an adaptive management approach that mitigates emissions-to-compartments over time. To reflect this, we assumed that impacts are not mitigated in the starting year (e.g. 2025), achieve the full potential for mitigation in the final year (e.g. 2040), and follow a logistic growth between the starting and final year, represented by equation (1):

$$y = \frac{L}{1 + e^{-k(x-x_0)}}, \quad (1)$$

Where x is the independent variable (e.g., the year for which the interpolated value is required); L represents the upper asymptote (set to the coefficient value of the second known point, y_2); k is the growth rate, calculated as $k = \frac{1}{x_2 - x_1}$; and x_0 is the midpoint between the two known values, calculated as $x_0 = \frac{x_1 + x_2}{2}$.

Our approach represents VSI-inspired mitigation as reductions in elementary flows applied directly to the existing unit process inventories. Importantly, the embodied material and energy burdens of the mitigation technologies themselves (e.g., the manufacturing,

installation, and operation of APCDs, MBRs, and FBBRs) are not included within the LCA system boundary. This means that potential burden-shifting, for example, increased energy demand or chemical consumption associated with operating a flue gas scrubber, is not captured in the current assessment. This simplification was adopted because reliable, generalisable life cycle inventory data for these mitigation technologies in the specific context of mineral processing operations were not available at the time of this study. As a result, our estimates of mitigation potential should be interpreted as upper-bound (best-case) reductions. A full process-based inventory of these technologies would capture trade-offs more comprehensively and is a recommended step for future work. [Fig. 3 \(A\)](#) presents mitigation technologies modelled against respective processes. The individual mitigation factors of each mitigation technology against their respective elementary flow and compartment are provided in [Supplementary Material 2 - Processes and mitigations](#).

This uniform adoption trajectory represents a deliberate simplification. In practice, the uptake of mitigation technologies is likely to vary across regions due to differences in regulatory stringency, enforcement capacity, access to capital, and technical infrastructure (Ediriweera and Wiewiora, 2021; Mendonca Severiano et al., 2024). For instance,

Table 1

Summary of mitigation technologies, targeted elementary flows, reduction coefficients, and their empirical basis. FGS = Flue gas scrubbers; ESD = Electrostatic demisters.

Mitigation technology	Targeted elementary flow(s)	Compartment	Reduction coefficient	Basis	Source
APCD (FGS + ESD)	Cu, Pb, As, Cr, Cd to air	Air	86.3~99.9%	Confirmed (empirical)	Zhang et al. (2022)
APCD (FGS + ESD)	PM2.5, PM10 to air	Air	94.2~99.1%	Confirmed (empirical)	(Wu et al., 2019; Zhang et al., 2022)
APCD (FGS + ESD)	Co, Ni, Zn, Ag, Hg to air	Air	95% (assumed)	Assumed. Analogy to confirmed heavy metals	Zhang et al. (2022)
APCD (FGS + ESD)	SO ₂ , Se to air	Air	97%	Confirmed (SO ₂). Assumed (Se, chemical analogy)	Wu et al. (2019)
NO _x suppression (two-stage non-catalytic)	NO _x to air	Air	96%	Confirmed. Commercial-scale test	Rebrov and Gorlov (2011)
Green reagents & efficiency gains	CO ₂ , CO (fossil) to air	Air	43%	Assumed. Proxy from IFC nickel roadmap	International Finance Corporation (2023)
FBRR	NO ₃ ⁻ , NH ₄ ⁺ to water	Water	95%	Confirmed (nitrate). Assumed (ammonium)	Zaitsev et al. (2008)
MBR	Cl, organic-N, N to water	Water	99%	Assumed. From municipal/industrial wastewater studies	(Dobson and Burgess, 2007; Melin et al., 2006)
Ion exchange (solid carbonate)	Phosphorus to water	Water	92.5%	Confirmed. Lab-scale	Cueto and Hansen (2019)
Mist generators + surfactants	Particulates to air (fugitive)	Air	90%	Assumed. From iron ore pile study	Lee et al. (2022)

operations in jurisdictions with strong ESG-driven supply chain requirements, such as the EU Battery Regulation (European Union (EU), 2023), may adopt these technologies earlier, while operations in regions with limited regulatory oversight or financial constraints may lag significantly (Franken and Schütte, 2022).

2.5. Scenario combination

Following the SIMPL approach, we combined our background scenarios with foreground scenarios. To generate the background datasets, we employed the *premise* tool (Sacchi et al., 2022). Specifically, we utilized the existing implementation of REMIND's projections for different socio-economic pathways (Baumstark et al., 2021). Subsequently, we created additional scenario-specific datasets (combining both background and foreground inventories) to explore the potential impact of VSIs. These datasets were structured into three distinct categories: (i) Background Changes: SSP scenarios only, (ii) Foreground Changes: Process Mitigated Inventories, and (iii) Background + Foreground changes. A graphical representation of this workflow is provided in Fig. 3 (B). This structured methodology allowed for a comparative analysis of the relative contributions of SSP scenarios and VSIs to impact mitigation. The prospective nature of this study means that results are subject to multiple sources of uncertainty. Given the inherent limitations of the generic ecoinvent 3.8 inventories (which do not reflect site-specific conditions, regional regulatory environments, or company-level practices) and absence of data on differentiated adoption rates across geographies, we adopted a uniform logistic adoption trajectory as a baseline assumption. This means that all regions and operations are modelled as adopting mitigation technologies at the same pace, which is a deliberate simplification. As a consequence, the results should not be interpreted as indicative of better or worse environmental performers across geographies, companies, or operations. They reflect what is technologically plausible under idealised, equal-adoption conditions, not what any specific jurisdiction or operator is likely to achieve. The robustness of the adoption timing assumption is assessed through a sensitivity analysis on the logistic curve (Supplementary Material Section 4; Fig. 17), testing early, central, and late adoption trajectories, with qualitative conclusions consistent across all three. Specifying adoption rates at the level of individual geographies or companies would require granular governance, regulatory, and operational data that were beyond the scope of this study, but represents a valuable and tractable direction for future work.

3. Results

3.1. Future impacts and mitigation of NMC111 oxide production

Fig. 4 presents the prospective LCA results for NMC111 oxide production under different SSPs, comparing base and mitigation scenarios informed by the strategies outlined in Fig. 3 (A). Impact categories are shown where foreground operational changes influence results, consistent with the study's focus on VSI-aligned mitigation mechanisms. In general, most impact categories exhibit a downward trend over time, primarily driven by changes in background systems. This trend can be solely attributed to background modifications whenever no variations between the *base* and *VSI* scenarios are present. When differences do arise, such as for marine eutrophication (MEP) in SSP1 for 2040, they are attributed to foreground modifications applied to the unit processes listed in Fig. 3 (A). These results should be interpreted in the context of the chosen modelling assumptions, especially the reliance on the ecoinvent 3.8 inventories, which reflect certain data gaps and baseline process assumptions. The figures illustrate how prospective LCA can incorporate time-varying changes in both the background system (e.g. energy grids) and foreground system (e.g. mitigation measures). This section focuses on the methodological approach of scenario-based prospective LCA, rather than on the accuracy of the absolute values of future impacts.

To highlight the extent of the foreground influence, Fig. 5 illustrates the relative impact variations from the VSI scenario compared to the corresponding SSP scenario. The figure indicates that the introduction of the technologies and processes described in Fig. 3 (A) can lead to varied and meaningful mitigation across a range of impact categories, namely marine eutrophication (MEP), particulate matter formation (PMFP), terrestrial acidification (TAP100), freshwater ecotoxicity (FETPinf), freshwater eutrophication (FEP), photochemical oxidant formation (POFP), and human toxicity (HTPinf). While these improvements may appear modest when viewed through the lenses of producing NMC111 oxide, compound-disaggregated results will provide a more granular perspective in the following sub-section 3.2. Across all categories, the relative mitigation potential presents little variation across SSP scenarios, with freshwater eutrophication (FEP) as the sole exception, displaying a slightly lower mitigation potential in the combined scenario compared to SSP1 and SSP2. Impact categories that are not affected by the VSIs, i.e. have a change rate of 0%, are not displayed.

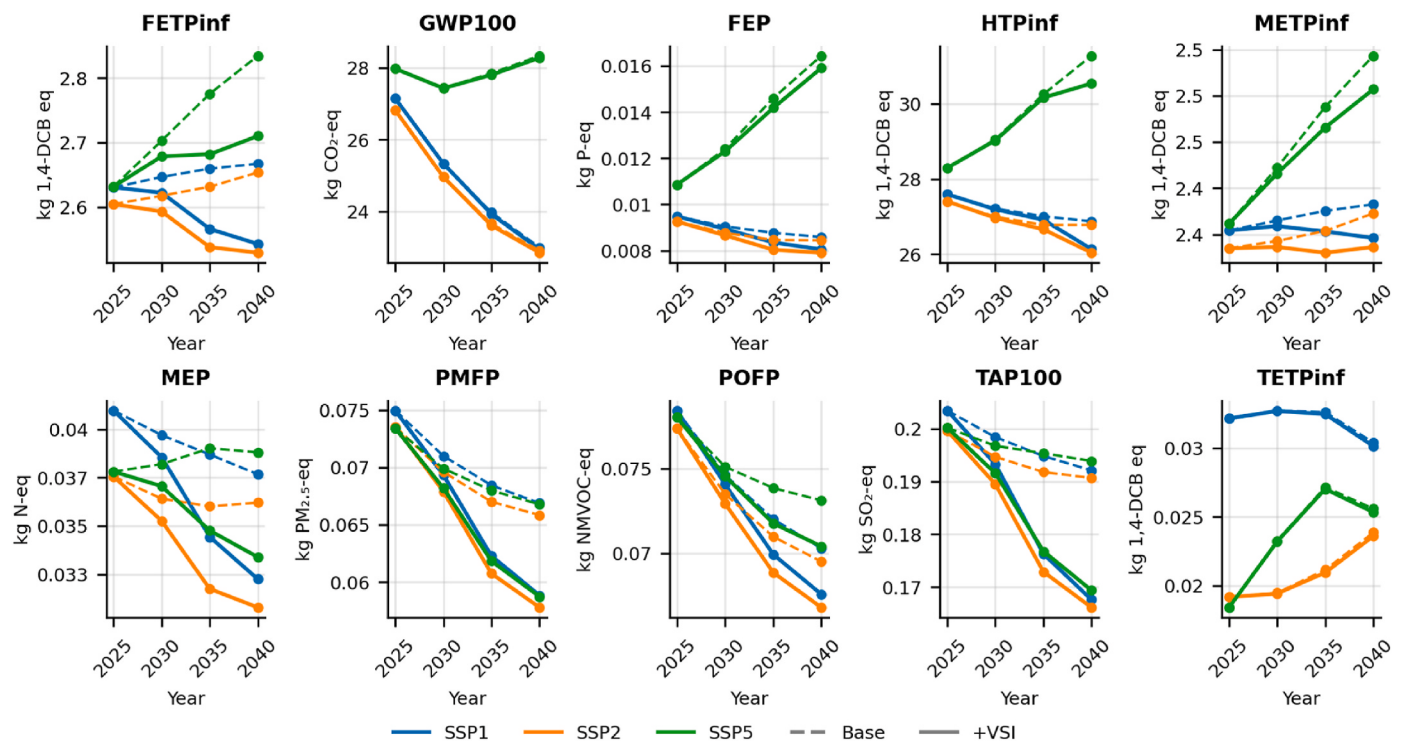


Fig. 4. Prospective LCA results for the production of 1 kg of NMC111 oxide, presented as time series of absolute values per impact category using the ReCiPe 1.6 midpoint (H). Results span 2025 to 2040, disaggregated by SSP scenario, and compare SSP-Base (dashed lines) and SSP + VSI (solid lines). Only impact categories influenced by foreground inventory changes are shown. GWP100 = Climate change (kg CO₂-eq); FETPinf = freshwater ecotoxicity (1,4-DCB eq. emitted to freshwater); FEP = freshwater eutrophication (kg P-eq. to freshwater); HTPinf = human toxicity (1,4-DCB eq. emitted to urban air); METPinf = marine ecotoxicity (1,4-DCB eq. emitted to seawater); MEP = marine eutrophication (kg N-eq to marine water); PMFP = particulate matter formation (kg PM_{2.5}-eq); POFP = photochemical oxidant formation (kg NMVOC-eq); TAP100 = terrestrial acidification (kg SO₂-eq); TETPinf = terrestrial ecotoxicity (1,4-DCB eq. emitted to industrial soil).

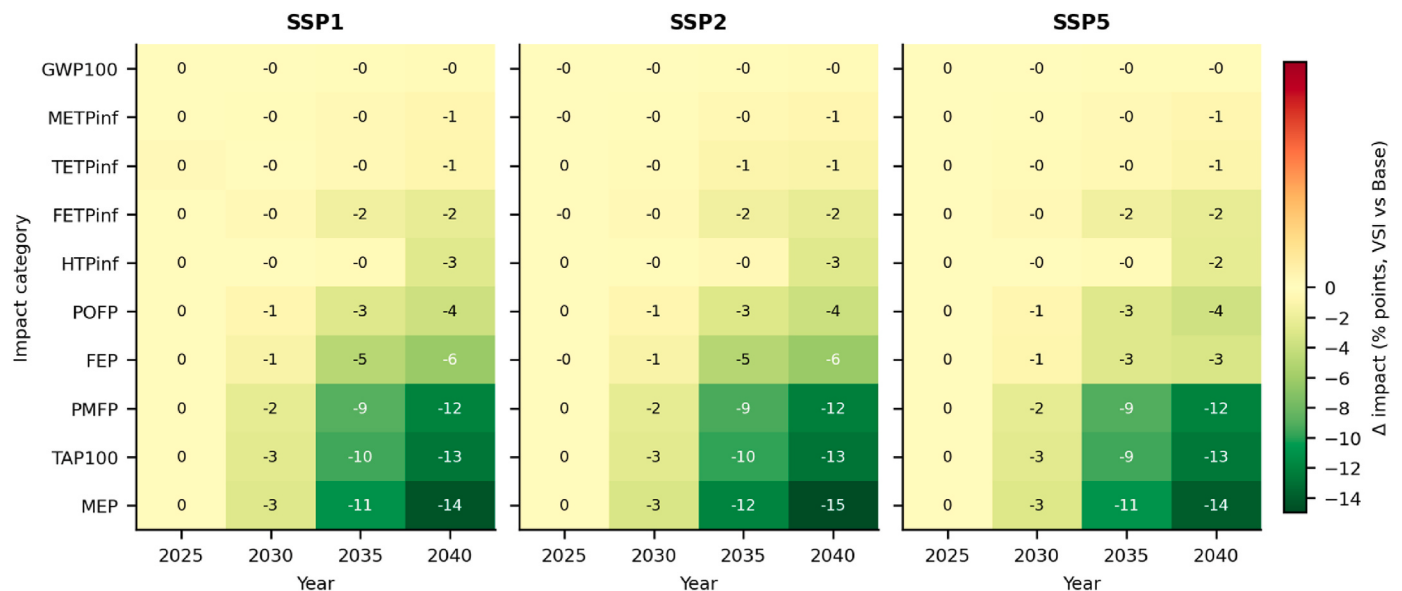


Fig. 5. Relative impact changes attributable to VSI-aligned foreground modifications, expressed as $\Delta\% = \frac{[(SSP + VSI) - (SSP-Base)]}{[SSP-Base]} \times 100$, for the production of 1 kg of NMC111 oxide. Results are presented as a heatmap with impact categories on the vertical axis and years (2025-2040) on the horizontal axis. Each panel represents one SSP scenario. Darker green cells indicate greater mitigation. Impact categories showing no change ($\Delta\% = 0\%$) are omitted. GWP100 = climate change; FETPinf = freshwater ecotoxicity; FEP = freshwater eutrophication; HTPinf = human toxicity; METPinf = marine ecotoxicity; MEP = marine eutrophication; PMFP = particulate matter formation; POFP = photochemical oxidant formation; TAP100 = terrestrial acidification; TETPinf = terrestrial ecotoxicity. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

3.2. Mitigation potential for individual unit processes

As with the aggregated results in Section 3.1, these process-

disaggregated findings serve primarily to illustrate the potential influence of targeted mitigation strategies when combined with time-varying background scenarios. The absolute values should be interpreted

cautiously, given the inherent limitations of the ecoinvent 3.8 data. Among the unit processes analysed, 12 exhibited significant changes in impact scores due to foreground modifications. Fig. 6 presents the mitigation potential for selected mineral extraction and processing unit processes contributing to NMC111 oxide production. This figure compares impact changes under the SSP1, SSP2, and SSP5 background scenarios, both with and without the implementation of previously outlined foreground mitigation strategies. Of the 18 impact categories assessed, 8 remained unaffected by foreground changes: NLTP, ALOP, MDP, WDP, ULOP, IRP_HE, FDP, and ODPinf. Consequently, only the impact categories influenced by foreground interventions are shown in Fig. 6.

Within the nickel subsystem, most processes exhibit a relatively consistent mitigation potential for 10 categories across all scenarios (SSP1, SSP2, SSP5). In some cases, significant mitigation can be observed. For example, “*nickel mine operation and beneficiation to nickel concentrate, 7% Ni (CN)*” can achieve substantial PMFP reductions, up to an additional 75% reduction, through the implementation of APCDs. Terrestrial ecotoxicity (TETPinf) is the category exhibiting higher variability, as exemplified by *platinum group metal mine operation, ore with high palladium content (RU)*, which shows $\Delta\%$ of -24% under SSP1, -45% under SSP2, and -48% under SSP5. Overall, nickel-related processes consistently demonstrate mitigation potential in PMFP, POFP, TETPinf, and TAP100 through APCDs, and in some cases, reduced climate change through the adoption of green reagents and process optimizations.

For lithium-related processes, most mitigation potential arises from background system improvements rather than foreground interventions. Nonetheless, both spodumene production activities examined could further reduce PMFP through APCDs, while phosphorus capture technologies like ion exchange in solid carbonate can mitigate MEP and FEP in lithium carbonate production. Lastly, within the manganese subsystem, the most notable mitigation potential lies in reducing HTPinf via APCDs that capture heavy metals' emissions. These control measures also confer benefits in freshwater and marine ecotoxicity categories. Additionally, the production of manganese (III) oxide can achieve

further climate change mitigation using green reagents and enhanced process efficiencies.

4. Discussion

This study aimed to evaluate the prospective life cycle impacts of NMC111 oxide production and to assess the potential of VSIs in mitigating these impacts across varying SSPs. By integrating VSI-aligned environmental mitigation technologies, such as APCDs, with SSPs (drawing from works from [Mendoza Beltran et al. \(2020\)](#)), our study expands on prior life cycle assessments implemented with premise ([Sacchi et al., 2022](#)) applied to ecoinvent 3.8 (cutoff version) by incorporating dynamic changes in both background and foreground-level systems. Crucially, the numerical results we present are meant as an illustration of how prospective LCA can capture future-oriented changes, rather than as definitive, fixed predictions. Additionally, we explored the individual mining and mineral processing unit processes involved in the production of NMC111 oxide, providing a granular perspective on their environmental impacts and mitigation potential. Given that the inventories extracted from ecoinvent 3.8 rely on processes that may not reflect the most recent industrial changes, our results likely underestimate (or overestimate) the potential of certain emergent technologies. Nonetheless, the strength of the prospective LCA framework is its modular design, allowing future updates as more robust data sources become available.

Our findings demonstrate that while background system improvements, such as decarbonized electricity grids, are critical drivers of impact reductions, the adoption of VSI-aligned mitigation technologies offers complementary benefits. The former results are consistent with previous works that have shown global warming potential reduction for battery cell production (inclusive of anode material such as NMC oxides) ([Xu et al., 2022](#)), and battery-grade nickel ([Harpprecht et al., 2021](#)). The latter results, pertaining to voluntary adoption of mitigation technologies, are novel to the best of our knowledge ([Harpprecht et al., 2024](#)). Our study extends prior work by explicitly modelling VSI-aligned environmental mitigation technologies and quantifying the

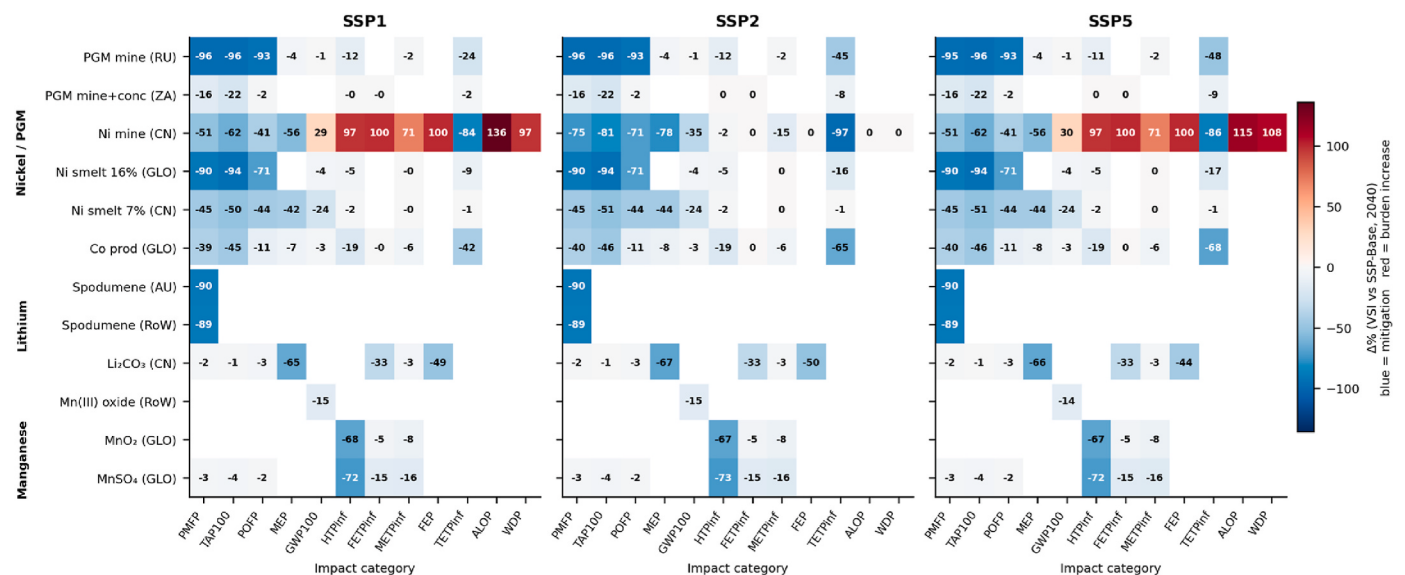


Fig. 6. LCIA results for selected unit processes involved in NMC111 oxide production (see Fig. 1), presented as a three-panel heatmap for the year 2040. Each panel corresponds to one SSP scenario (SSP1, SSP2, SSP5). Rows represent unit processes grouped by mineral subsystem (Nickel, Lithium, Manganese). Columns represent impact categories. Cell values and colour show $\Delta\% = [(SSP + VSI) - (SSP-Base)] / |SSP-Base| \times 100$ at 2040, where blue indicates mitigation (negative $\Delta\%$) and red indicates a burden increase (positive $\Delta\%$). Empty cells indicate no foreground change for that process-impact combination. Subsystem groupings are indicated by labels on the left axis. Due to rounding, displayed differences may vary by up to $\pm 1\%$. GWP100 = climate change; FETPinf = freshwater ecotoxicity; FEP = freshwater eutrophication; HTPinf = human toxicity; METPinf = marine ecotoxicity; MEP = marine eutrophication; PMFP = particulate matter formation; POFP = photochemical oxidant formation; TAP100 = terrestrial acidification; TETPinf = terrestrial ecotoxicity. Categories not shown: NLTP, ALOP, WDP, ULOP, IRP_HE, FDP, ODPinf, MDP. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

contribution of selected mitigation strategies to environmental performance. The selected technologies were evaluated for their potential to mitigate emissions to air and soil at mining operations, focusing on the most impactful elementary flows identified in our hotspot analysis. For instance, APCDs showed significant potential to reduce particulate matter formation (PMFP) and terrestrial acidification (TAP100), while green reagents contributed to reductions in global warming potential (GWP100) in certain unit processes. These findings emphasize the importance of coupling systemic changes in energy supply with targeted operational interventions.

The aggregate results at the NMC111 oxide level confirm that background decarbonization (the progressive reduction in the carbon intensity of electricity and industrial energy systems as modelled within the SSP scenarios) is the dominant driver of impact reduction, particularly for climate change (GWP100), with the other mitigation contributions remaining below 15% across most categories (Fig. 5). However, this apparent imbalance overlooks several important dimensions. First, the relative visibility of VSI contributions is partly a function of the chosen functional unit. When impacts are expressed per kilogram of NMC111 oxide, process-level improvements at individual mining and refining stages are diluted across a complex, multi-stage supply chain. Yet this aggregated perspective does not reflect the environmental reality experienced at the point of extraction. For a community adjacent to a nickel extraction operation, a ~75% reduction in particulate matter formation (Fig. 6) represents a meaningful change in local air quality, regardless of how that improvement appears when normalised to a downstream product such as 1 kg of NMC111 oxide. At the level of individual unit processes, VSI-aligned technologies deliver reductions of up to ~90% for specific elementary flows such as heavy metal emissions to air. The choice of functional unit and system boundary therefore shapes how much "benefit" is perceived from localised mitigation strategies. Second, the scope of what SSP-based background scenarios model must be considered when interpreting the relative contributions. The future inventories generated through premise and REMIND primarily capture the decarbonization of electricity systems and associated energy-intensive sectors. Consequently, they are most influential on impact categories closely linked to energy supply, notably climate change (GWP100). By contrast, several of the mitigation technologies explored in this study, such as APCDs, MBRs, and FBBRs, target impact categories that are largely outside the scope of energy-system transitions such as particulate matter formation (PMFP), and freshwater and marine ecotoxicity. The dominance of SSP-driven reductions therefore reflects, in part, the fact that background scenarios and VSI-aligned interventions operate on different dimensions of environmental performance, rather than indicating that VSIs are ineffective. More specifically, the three SSP scenarios create distinct background conditions under which VSI-aligned interventions operate, though the foreground mitigation coefficients were held constant across scenarios. Under SSP1 ('Taking the green road'), aggressive background decarbonization reduces energy-related impacts substantially, leaving less 'room' for VSI contributions in categories like GWP100 but making process-level emissions a proportionally larger share of the remaining impact. Under SSP5 ('Taking the highway'), fossil-fuel-intensive development maintains higher background impacts, meaning VSI-aligned interventions operate against a larger baseline. SSP2 ('Middle of the road') falls between these extremes. Despite these different background conditions, the relative mitigation attributable to VSI interventions is remarkably consistent across SSPs for most impact categories (Fig. 5). This consistency reinforces the finding that the process-level targeted mitigations are largely independent of the background energy system, given the current way in which these scenarios are devised.

While our results demonstrate the directional potential of VSI-aligned mitigation technologies, their real-world implementation faces significant barriers that merit discussion. In a companion study, Mendonca Severiano et al. conducted a thematic analysis of the drivers and barriers influencing VSI adoption in mining operations for battery

minerals (Mendonca Severiano et al., 2024). That study identified market access and company-community communication as key adoption drivers, while barriers included short-term greenwashing undermining VSI legitimacy, and a lack of comprehensiveness in risk identification and mitigation across supply chains. These findings are directly relevant to interpreting our results. First, technical lock-in may constrain adoption: existing mineral processing facilities are designed around established process configurations, and retrofitting APCDs or MBRs may require substantial capital expenditure and operational redesign, particularly at ageing facilities with limited remaining mine life. Second, compliance costs present an uneven burden across the supply chain. As noted before, battery mineral supply chains span from the Global South (where extraction occurs) to the Global North (where demand originates) (Mendonca Severiano et al., 2024), and the adoption of VSIs by mining companies is shaped by this geography. Companies in jurisdictions with tighter financial margins, weaker institutional support, and limited access to capital face greater obstacles to voluntary adoption (Franken and Schütte, 2022). Furthermore, the extraction phase accounts for a very small fraction of a lithium-ion battery's value-added (Barry et al., 2012), meaning that the economic incentives for upstream operators to invest in mitigation technologies remain limited without external market signals such as green premiums or due diligence requirements. Third, potential rebound effects should be acknowledged. The adoption of end-of-pipe mitigation technologies could reduce the perceived urgency of more fundamental process redesign or demand reduction strategies. While our modelling framework does not capture these socioeconomic and governance dynamics, they represent important considerations for the policy translation of our findings.

Further, the results reveal that nickel production consistently exhibits the highest mitigation potential among the three subsystems examined, with technologies such as APCDs achieving up to 75% reductions in PMFP and TAP100. In contrast, lithium production demonstrated more limited mitigation opportunities at the operational level, with most impact reductions stemming from background system changes, such as a greener electricity supply. Manganese-related processes showed notable potential for reductions in human toxicity impacts through the use of advanced heavy metal capture technologies. These process-specific findings, however, may be caused by data scarcity, exacerbated in prospective LCA. The data constraints of ecoinvent 3.8 were particularly pronounced for lithium and manganese. For lithium, ecoinvent 3.8 contains only a limited number of generic spodumene and brine-based operations, with inventories that do not reflect commercially deployed technologies such as Direct Lithium Extraction (DLE) or recently published site-specific inventories (e.g. (Khakmardan et al., 2025)). Consequently, the limited foreground mitigation potential observed for lithium processes in our results may partly reflect the lack of process granularity in the underlying inventory. For manganese, ecoinvent 3.8 provides only aggregated global-average inventories for manganese dioxide and manganese sulfate production, without differentiation by processing route or geography. The notable human toxicity mitigation potential identified for manganese dioxide and sulfate processes should therefore be interpreted as indicative of the types of impact reductions achievable through heavy metal capture technologies. This is a significant limitation of this study, and was already flagged in several other prospective LCA studies (Arvidsson et al., 2018). The modular design of our framework allows these inventories to be updated as more granular data become available.

These limitations suggest directions for future research. First, efforts should be made to fill foreground data gaps, an effort that is being addressed by generating high-quality inventories (Khakmardan et al., 2023; Schenker et al., 2022), which could be incorporated into LCA databases that can be used in conjunction with premise to generate futurized inventories. Second, prospective LCAs should aim to incorporate the life cycle inventories of the mitigation technologies themselves, as these may introduce new impacts that partially offset the

emission reductions achieved. For instance, APCDs require energy for fan operation and generate secondary waste streams (e.g., scrubber sludge), while MBRs require membrane replacement and chemical inputs. Until these are accounted for, the mitigation potential reported in this study represents an upper bound. Third, while this study focuses on NMC111 oxide production, many of the mitigation strategies explored (e.g., particulate and SO₂ capture, process water treatment) could be adapted to other material supply chains, such as copper. Likewise, reductions in the impacts of nickel, lithium, and manganese production could provide benefits across various sectors, including stainless steel, fuel cells, and alternative battery chemistries. Furthermore, the uniform logistic adoption trajectory used in this study does not capture the geographic, regulatory, and socioeconomic disparities that would influence real-world uptake. Mining operations across the supply chain span diverse jurisdictions, from Australia (spodumene, Processes 9_A in [Supplementary Material 2](#)) to China (nickel concentrate, Process 6_A), Russia (palladium-rich ore, Process 2), and South Africa (PGM concentration, Process 3_A). Each with distinct regulatory environments and institutional capacities. Future work should explore region- and commodity-specific adoption curves, potentially informed by governance indicators, supply chain due diligence frameworks, and empirical case studies of VSI implementation.

5. Conclusion

The decarbonization of the transportation sector is driving unprecedented demand for lithium-ion batteries, necessitating the production of NMC oxides. This, in turn, requires increased mining and processing of battery-grade lithium, nickel, and manganese, often in resource-rich regions of the global south. These operations, while critical for enabling the energy transition, present localized environmental challenges that must be mitigated to ensure sustainable supply chains. In response, this study modelled the future life cycle impacts of NMC111 oxide production and its constituent mineral activities, integrating VSIs taking the form of emission mitigation technologies. By integrating VSI-aligned environmental mitigation technologies, such as APCDs, with expected decarbonization from Shared Socioeconomic Pathways (SSPs), the analysis demonstrates the importance of coupling systemic energy transitions with targeted interventions at mining and mineral processing operations.

Our findings reveal that while improvements at the NMC111 oxide production level can be modest (below 15%) as per [Figs. 4 and 5](#), significant mitigation potential exists at the level of individual mineral extraction and processing unit processes (sometimes as high as 90%) as per [Fig. 6](#). This is achieved through direct reductions in emissions to air and soil, enabled by VSI-aligned technologies such as APCDs and bio-reactors. Our results corroborate that systemic changes in background systems, such as decarbonized electricity grids, provide substantial reductions in categories like global warming potential ([Harpprecht et al., 2021, 2024; Xu et al., 2022](#)), while VSI-aligned technologies effectively address emissions to air and soil, delivering measurable benefits in particulate matter formation, and terrestrial acidification. These findings underscore the relevance of integrating mitigation technologies into broader sustainability frameworks. However, it is critical to view these figures as illustrations of what is technologically plausible given certain assumptions about background decarbonization and operational interventions, rather than fixed forecasts.

Despite our contribution, the study has a range of limitations. First and foremost, by using data from ecoinvent 3.8, our study is constrained by the scarcity of high-quality, first-hand data for the foreground inventory. Also, the mitigation coefficients used are based on available data and assume logistic growth in adoption, which may not fully capture site-specific conditions. A sensitivity analysis testing three alternative logistic adoption trajectories (early, central, and late) is provided in [Supplementary Material 1 Section 4](#) and confirms that the main conclusions are robust to this assumption, with uncertainty confined to

the intermediate years 2030-2035. Moreover, by assuming full mitigation achieved, we modelled a techno-optimistic future, an often common pitfall of prospective LCAs ([Prospective LCA network, 2024](#)). Lastly, our background scenarios rely exclusively on the “Base” variants of SSP1, SSP2 and SSP5. More ambitious trajectories, such as Representative Concentration Pathways (RCPs) RCP 2.6 (<2 °C) or RCP 1.9 (<1.5 °C), would further decarbonise the electricity supply and could shift the relative importance of VSI-driven improvements. Exploring those low-carbon pathways is a logical next step for future prospective LCA studies. To address these challenges and support the refinement of this work, please contact the authors if you wish to receive the LCI data. The full LCI data could not be shared openly here due to the End User Licence Agreement of ecoinvent. If you have an ecoinvent license, the authors can share the entire dataset with you.

Looking ahead, addressing data quality limitations is crucial, both at a background and foreground level. Further research is also needed to explore the socioeconomic dynamics of VSI adoption and its financial scalability across diverse geographic-, commodity-, and operational-contexts. By bridging operational improvements with systemic energy transitions, the battery sector can support the sector-wide decarbonization of the transportation sector, whilst preserving the quality of life of local communities around mining operations. Equally important is advancing the discussion on publicly available inventory data itself. A future in which site-specific data are widely accessible would dramatically enhance transparency and accountability, empowering researchers, policy analysts, and industry stakeholders to apply prospective LCA more rigorously to local contexts.

More broadly, our findings point toward a conceptual framework for understanding the transition from voluntary to mandatory sustainability standards in extractive supply chains. VSIs currently operate as enabling mechanisms that encourage (without guaranteeing) the adoption of mitigation technologies. Our results suggest that when VSI-aligned interventions are modelled as engineering parameters within a prospective LCA framework, their environmental relevance can be quantified, compared, and benchmarked against systemic transitions. This type of evidence base could inform the design of future mandatory standards by identifying which categories of process-level intervention deliver measurable benefits beyond what background decarbonization alone can achieve. By bridging voluntary commitments and quantifiable outcomes, prospective LCA can serve not only as an analytical tool but as a policy instrument for operationalising sustainability standards across mineral supply chains.

CRedit authorship contribution statement

Bernardo Mendonca Severiano: Conceptualization, Data curation, Formal analysis, Methodology, Visualization, Writing – original draft. **Stephen A. Northey:** Conceptualization, Data curation, Supervision, Writing – review & editing. **Carina Harpprecht:** Writing – review & editing. **Damien Giurco:** Supervision, Writing – review & editing.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Bernardo Mendonca Severiano reports financial support was provided by Future Battery Industries CRC. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.jclepro.2026.149037>.

Data availability

The data that support the findings of this study are available on reasonable request from the corresponding author. The codebase is available at: <https://github.com/bernardomendonca/plca-NMC-oxide-BM-PhD/>.

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