Spotlights

Bullet 1: Critical context and background information on the problem addressed

Tracking waste and material flows is essential for developing the circular economy and supply chain resilience

Bullet 2: A brief overview of the key finding of the study (or findings if necessary)

A tool was developed to quantify waste and material footprints of activities in life cycle assessment (LCA) databases

Bullet 3: The most radical, creative, disruptive or innovative aspect of the manuscript

Built to complement the Brightway LCA framework and ActivityBrowser, the tool is customisable and easy to use.

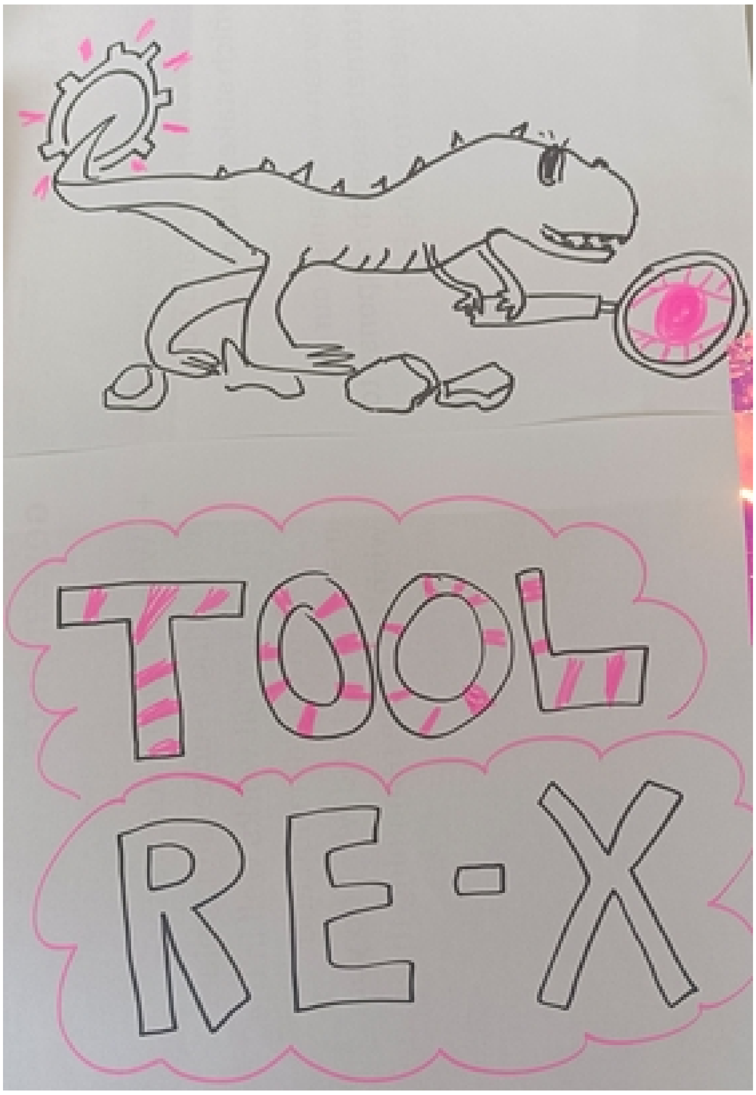
Bullet 4: The significance of the results to the environment, economics or society

The tool can be used to identify pre-consumer waste and material hotspots that are often hidden in supply chains.

Bullet 5: Future vision or the most important implications for continued research

Improved data availability and quality would enable more detailed and accurate waste and material footprinting.

Graphical Abstract



Highlights

- T-reX, a new tool for quantifying waste and material flows in LCA.
- Assesses supply risks by calculating demand for critical materials.
- Simplifies quantification of user-specified waste and material categories.
- Rapidly identifies waste and material demand hotspots.
- Presents a case study of the battery supply chain.

T-reX: A python package to quantify waste and material footprints in current and future LCA databases

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Abstract

Abstract word count: 151, Limit: 150

Minimising material consumption and waste generation is the quintessential principle of the 'circular economy'. Thus, identifying and quantifying waste and material flows are of fundamental importance. Life Cycle Assessment (LCA) is powerful for this end, given its capacity to pinpoint hotspots of environmental impact throughout the life cycle of activities, where the implementation of circular principles could be most effective.

Introducing T-reX, a Python tool extending the brightway ecosystem, allowing facile quantification of user-defined supply-chain demands in current and prospective scenarios. T-reX streamlines database manipulation for LCA practitioners and integrates methods to aggregate and analyse waste and material flows, facilitating rapid hotspot identification.

A case study of 6 Li-ion batteries demonstrated T-reX's utility, quantifying categorised waste and material inventory footprints, and thus, their potential environmental burdens. T-reX can aid sustainable decision-making and contribute to the development of the 'circular economy' by facilitating analysis of material consumption and waste generation in LCA.

Keywords: circular economy, waste, material, life cycle assessment, critical raw material, supply chain

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Total word count: 5000, Limit: 5000

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Table 1: List of abbreviations

CML	Centrum voor Milieuwetenschappen (Centre for Environmental Science)
CRM	Critical Raw Material
CSI	Crustal Scarcity Indicator
CSP	Crustal Scarcity Potential
EDIP	Environmental Design of Industrial Products
EOL	End-of-Life
FOEN	Swiss Federal Office for the Environment
IAM	Integrated Assessment Model
LCA	Life Cycle Assessment
LCIA	Life Cycle Impact Assessment
LFP	Lithium Iron Phosphate
$LiMn_2O_4$	Lithium Manganese Oxide
NCA	Nickel Cobalt Aluminum
NMC	Nickel Manganese Cobalt
PWF	Product Waste Footprint
RCP	Representative Concentration Pathway
ReCiPe	A standard LCIA method set
SSPs	Shared Socioeconomic Pathways
UBP	Umweltbelastungspünkte (Environmental Impact Points)

1. Introduction

Section word count: 1500

To be split into two (sub) sections: Introduction and Background, can be easily condensed by 200 words or so.

The development of a 'circular economy' has become a critical area of focus in the imperative pursuit of achieving sustainability objectives and curtailing our environmental footprint within planetary boundaries (European Commission, 2019, 2020; Government of the Netherlands, 2023, 2016; Pardo and Schweitzer, 2018; Ellen MacArthur Foundation, 2015). Fundamental to this development is a decrease in primary material consumption and a reduction of life cycle waste through the implementation of 're-X' strategies (e.g., refuse, rethink, design for—and implementation of—repair, remanufacturing and recycling) (European Union, 2022; Alfieri et al., 2022; Parker et al., 2015). In addition to circular economy goals, contemporary geo-political tensions in an ever more globalised economy have highlighted the vulnerability of many advanced economies to intentional supply disruptions, wrought as an act of competition or outright hostility (Carrara et al., 2023; Hartley et al., 2024; Berry, 2023).

While some material demands are apparent in the final product and the waste generated may be inferred from knowledge of the use– and end-of-life– (EOL) phases, a significant proportion of these are often 'hidden' in the supply chain and thus not reported directly in the final results (Laurenti et al., 2016; Salviulo et al., 2021). It has been found that these material footprints can be 'highly representative of damage to human health and biodiversity' (Steinmann et al., 2017) and that waste footprints have a 'strong association' with environmental damage (Laurenti et al., 2023). Thus, to reduce the negative externalities of consumption and improve supply chain resilience, it is essential to uncover, disaggregate, and quantify the material and waste footprints of human activities in as much detail as possible.

Life Cycle Assessment (LCA) is a useful method for the holistic estimation of the environmental impacts of products and processes. LCA can comprehensively evaluate these impacts across the entire life cycle—from 'cradle to grave'—, often identifying critical hotspots and guiding prioritisation of actions. The standard approach is to apply Life Cycle Impact Assessment (LCIA) methods (such as ReCiPe (Huijbregts et al., 2016) and CML (Guinée et al., 2002)), which convert the inventory data into a set of impact scores based on the sum of the elementary flows. These scores are then aggregated into a single score for each impact category, which can be compared across products and processes.

Several LCIA methods include, to some extent, waste generation (Swiss Federal Office for the Environment (FOEN), 2021; Hauschild and Potting, 2004; CEN (European Committee for Standardization), 2019) and material consumption (Arvidsson et al., 2020; Swiss Federal Office for the Environment (FOEN), 2021). These methods, however, are generally limited in their scope (especially for waste), do not allow for flexible quantification of specific waste and material types, and often provide results in characterised units that are abstract or difficult to interpret (e.g., Ümweltbelastungspunkte (UBP)).

In the context of a mineral-hungry renewable energy transition and recent geo-political tensions, more attention is being paid to the security of supply of materials, especially those considered 'critical raw materials' (CRMs) (European Commission and Directorate-General for Internal Market, Industry, Entrepreneurship and SMEs and Grohol, M and others, 2023; Hool et al., 2023; Mancini et al., 2013; Carrara et al., 2023; Hartley et al., 2024; Salviulo et al., 2021). While LCA seeks to model the technosphere (a.k.a. the anthroposphere), its focus is often on the environmental impacts of the system—the endpoints— rather than the primary material flows themselves.

A relatively new method, termed the crustal scarcity indicator (CSI) (Arvidsson et al., 2020), was developed to assess long-term global scarcity of minerals in LCA. This method introduced crustal scarcity potentials (CSPs) measured in kg silicon equivalents per kg element, derived from crustal concentrations. CSPs, provided for 76 elements, reflect the long-term global elemental scarcity based on crustal concentration proxies. The CSI, calculated by multiplying CSPs with extracted masses, effectively gauges the impact of elemental extraction.

While useful for its stated purpose, the CSI presents its midpoint results in an abstract unit (kg-Si eq.) that is difficult to interpret and compare with other impact categories. Furthermore, the CSPs are not available for all elements (or more complex materials), and the method does not allow for the quantification of material demands in terms of mass or volume.

1.1. Waste in LCA

Though often described simply as a 'material with a negative economic value' (Guinée et al., 2004), waste is a nebulous concept, and one whose definition is poorly delineated and variable across space and time. Moreover, from a systems perspective, the notion of waste is anathema to the circular economy, and it is far more useful to consider the identity and nature of the specific material flows. Thus, precise and detailed categorisation of these is essential to understand the 'circularity' of an activity and its life cycle externalities. There is a conspicuous gap in the understanding of the waste footprint of human activities and their relationship with environmental damage (Laurenti et al., 2023). Conventional LCAs consider waste as a 'service' (Guinée and Heijungs, 2021) and typically use generic waste processing models (Beylot et al., 2018) that break the causal link between the functional unit and the waste-associated impacts.

In LCA, waste flows are not considered as fundamental biosphere exchanges, but rather as technosphere flows. Waste produced by an activity is transferred to a relevant waste treatment activity where it is accepted 'burden-free' and transformed into a combination of emissions and other waste 'products' (Guinée and Heijungs, 2021). There can be several treatment steps in this pathway leading, ultimately, to a mass of material being deposited in a landfill. In this system of waste accounting, the impacts apportioned to the waste-producing activity are a sum of those incurred by the transport, treatment, and final disposal of the waste into terrestrial or aquatic environments. In particular, the extensive work of Doka (2024) has contributed significantly to understanding the environmental impacts of waste treatment processes and the long-term impacts of disposal.

A significant portion of a product's total waste is generated during earlier stages such as resource extraction, transportation, and manufacturing, often remaining 'invisible' in traditional LCA practices (Laurenti et al., 2016). This oversight in measuring and communicating a cradle-to-grave product waste footprint (PWF) highlights a gap in circular economy indicators. Traditional LCA does not typically view waste as having environmental significance by itself, focusing instead on emissions and resource use resulting from waste treatment. The environmental significance of waste and its correlation with other indicators has been the subject of extensive research. For example, studies have shown that popular resource footprints can cover a significant portion of environmental impact variance in product rankings (Steinmann et al., 2017). However, correlations between various environmental indicators are not always consistent, as seen with the carbon footprint, which often does not correlate with other impact assessment scores (Laurent et al., 2012). The aggregation of waste in PWFs raises concerns among LCA experts, regarding the uncertainties introduced by aggregated measures, as well as the potential misrepresentation of environmental performance due to differences in waste types (Chen et al., 2021; Huijbregts et al., 2010).

Moreover, existing LCA methodologies offer limited direct indicators at the impact assessment level, providing sparse information on the impacts of waste. This limitation becomes particularly evident when attempting to identify waste generation hotspots within a product's life cycle. Addressing these hotspots is crucial for advancing towards circularity, however, there is a lack of a convenient and flexible way to calculate waste flows in LCA and a pressing need for more comprehensive methods that can effectively quantify waste flows and, therefore, contribute to a better understanding of a product's total environmental footprint. Laurenti et al. (2023) developed a method to calculate the waste footprint of a product or service based on solving the demand vectors of the activities, also presenting simple measures to quantify waste hazardousness and circularity. In that study, it was shown that the waste footprint correlates well with other LCIA methods, particularly human health. The method presented, however, is limited in its scope and flexibility, is computationally intensive, difficult to use, is not easily reproducible, and suffers from errors due to double counting. The T-reX tool presented herein provides a more flexible, transparent, and user-friendly approach to quantifying waste flows in LCA. Moreover, the T-reX tool is not limited to waste but can be used to quantify any supply-chain flow, such as water, gas, and critical raw materials.

1.2. The T-reX Tool

To better assess waste and material flows in LCA, we have developed a Python program built on the Brightway framework (Mutel, 2017a) and designed to track these exchanges by translating them into indicators and 'pseudo' LCA impact (LCIA) categories. In this study, we present the T-reX tool that enables LCA practitioners to manipulate their databases to allow them to easily aggregate the mass and volume of any desired exchange, and to create flexible categories that differentiate between material categories, waste types, and EOL handling.

While methods with similar aims exist, they lack customisability and specificity (Swiss Federal Office for the Environment (FOEN), 2021) or can be cumbersome to apply and suffer from errors due to multiple counting (Laurenti et al., 2023).

The purpose of the T-reX tool is not to quantify the environmental impacts of material consumption and waste production, but rather to quantify the material and waste flows themselves, even those that are finally consumed by waste treatment processes. It provides, thus, not an impact assessment in the traditional sense, but an accounting of the material consumed and waste generated by a product or service inside of the technosphere, regardless of the end-of-life fate of these flows. By definition, the development of the 'circular economy' necessitates the reduction and ultimate elimination of waste—though whether this objective is thermodynamically impossible has long been the subject of debate by Ayres (1999), Reuter and van Schaik (2012) and many others. In any case, avoiding material consumption and generation of waste is of paramount importance. By allowing LCA practitioners to easily classify and quantify these exchanges, the T-reX tool provides a practical means to identify hotspots and opportunities for waste reduction and material efficiency.

2. Methodology

Section word count: 1600

This section is divided into two parts. In subsection 2.1, we describe the T-reX tool, in subsection 2.2, we describe the methodology used to calculate the waste and material inventory footprints in a case study of 6 Li-ion batteries.

2.1. The T-reX tool

2.1.1. Computational framework

Developed in the Python programming language, T-reX extends the brightway LCA framework, utilising the components `bw2data`, `bw2calc`, and `bw2io` (Mutel, 2017a). Additionally, the `wurst` package—which can expand entire databases into a list of exchanges—is used to facilitate database searching and data transformation at the exchange level (Mutel, 2017b). Integration with the `premise` package (Sacchi et al., 2022)—which integrates the projections of integrated assessment models (IAMs) into current LCA databases—enables the user to easily create and manipulate prospective LCA databases. T-reX is also compatible with `ActivityBrowser` (Steubing et al., 2020)—an open-source graphical user interface for LCA—after running T-reX, the manipulated databases and the 'pseudo' LCIA methods created by T-reX can be used in the accustomed way. The T-reX tool is installable via the Python Package Index (PyPI) (McDowall and Lanphear, 2023b) and is open source under the CC-0 licence. The full source code for the T-reX tool is indexed on Zenodo (McDowall and Lanphear, 2023a) and under further development in the GitHub repository (McDowall, 2024). T-reX is designed to be used with ecoinvent databases (Wernet et al., 2016), but could be adapted to other databases by changing the search criteria. Currently, it has been tested with all available system models of ecoinvent 3.5–3.10 (Wernet et al., 2016).

T-reX can be used directly from the command line, or imported as a Python module, in which case, the user can access the individual functions and modules. In the simplest case, the user can run the program with the default settings, which will calculate the waste and material footprint of the ecoinvent database. The user can also customise T-reX to calculate the waste and material inventory footprints of a custom database, or a prospective database based on future scenarios by implementing `premise` with an included module.

The supplementary information [ADD LINK] contains the full metadata of T-reX tool, along with a list of the constituent modules of the T-reX tool, a description of their functions and a detailed computational workflow. Further details can be found in the user guide and documentation (McDowall, 2023).

2.1.2. Functionality and purpose

T-reX is a Python package that allows one to produce LCA databases—both current and prospective—that are manipulated to facilitate the calculation of waste and material inventory footprints in the supply chain of any activity in the same was as standard LCIA methods.

If desired, prospective databases can be custom-defined by the user or constructed with the projections of the integrated assessment models such as IMAGE (Stehfest et al., 2014) and REMIND (Aboumahboub et al., 2020), which offer a range of options aligned with the Shared Socioeconomic Pathways (SSPs) (Meinshausen et al., 2020) that can be paired with a variety of mitigation scenarios.

Subsequent expansion of the databases into lists of exchanges allows relevent material and waste flows to be identified and categorised. The search queries are tailored to the specific database and the user can easily modify them to suit their needs. The categories defined in the configuration are used to create T-reX's 'pseudo LCIA' methods that are indicators of aggregated technosphere demand. The exchange editing function of T-reX then takes each list of exchanges and appends to the relevent activity a copy of the technosphere exchange as 'pseudo-biosphere' exchange that matches the 'pseudo LCIA' method.

In the default configuration, there are 10 waste categories which are further divided by their unit of measurement (kilograms and cubic meters) to create a total of 20 waste methods. The waste categories include incineration, recycling, and total waste, and are listed in the supplementary information [ADD LINK]. One advantage of T-reX is that is is able to identify of waste exchanges that would otherwise be 'consumed' by a treatment process and not leave the technosphere. Since 'waste is not a service' (Guinée and Heijungs, 2021), a characterisation factor of -1 is applied to the waste footprint methods (with the exception of CCS exchanges), changing the perspective from 'waste consumed by treatment' to 'waste generated by the activity'.

In addition to the waste categories, the `queries_materials` module defines the material demand categories, which are based on the EU Critical Raw Materials (CRM) list for 2023 (European Commission and Directorate-General for Internal Market, Industry, Entrepreneurship and SMEs and Grohol, M and others, 2023). The CRM list is a list of 30 materials that are considered critical to the EU economy and are at risk of supply disruption. Further materials of interest to the authors were added to the search list, including helium, electricity, petroleum, sand, water, and natural gas. The identity of the materials considered and their categorical groupings are easily customisable by the user. The full list of 59 materials included in the default configuration is provided in the supplementary material [ADD LINK].

The logic for the identification of material exchanges with the T-reX tool differs from that used to identify waste exchanges in that the search queries are based on the names of the so-called relevant 'market activities' for the material of interest. A useful feature of the T-reX tool is that, in cases where there are several markets for one material or material group, the program can easily aggregate these exchanges. For example, exchanges with markets for the rare-earth-elements (REEs) 'market for cerium', 'market for dysprosium', 'market for erbium', etc. can be aggregated into a single indicator category for REEs. Similarly, the total demand for all critical raw materials (CRMs) can be easily calculated in the same manner.

As discussed in the introduction 1 there are some existing material demand methods in the standard LCIA method sets, including the 'crustal scarcity indicator' (which provides only an aggregated, abstracted endpoint) (Arvidsson et al., 2020) and the (deprecated) EDIP 2003 material use indicators (which provide endpoints in fundamental units) (Hauschild and Potting, 2004). In these methods, the material demand is calculated based on the total mass that is extracted from the environment, thus, their focus is essentially solely on the mining-related exchanges that bring these materials from the biosphere into the technosphere. In the T-reX tool, however, the accounting for material demand is based on exchanges solely within the technosphere. This offers a different perspective, allowing for the estimation of overall supply-chain material demands that consider the entire life cycle of an activity, including non-direct impacts on the market such as co-production of other materials. Consider a demand for an activity containing a metal, for example; while the existing material use methods allow one to calculate the total mass of that metal that is extracted from the environment, the T-reX tool can provide insight into the broader supply-chain impacts of the demand for this metal. If the production other materials are attributed to the production of this metal, these would appear as negative material demands in the T-reX results—supply chain pressure for one material can result in lessening of supply chain pressure for another. In the results of the Li-ion battery case study in subsection 3.2, we will see that this is indeed the case for the demand for nickel, which, because of such effects, is counter-intuitively negative despite the presence of nickel in the final products.

2.1.3. T-reX tool workflow

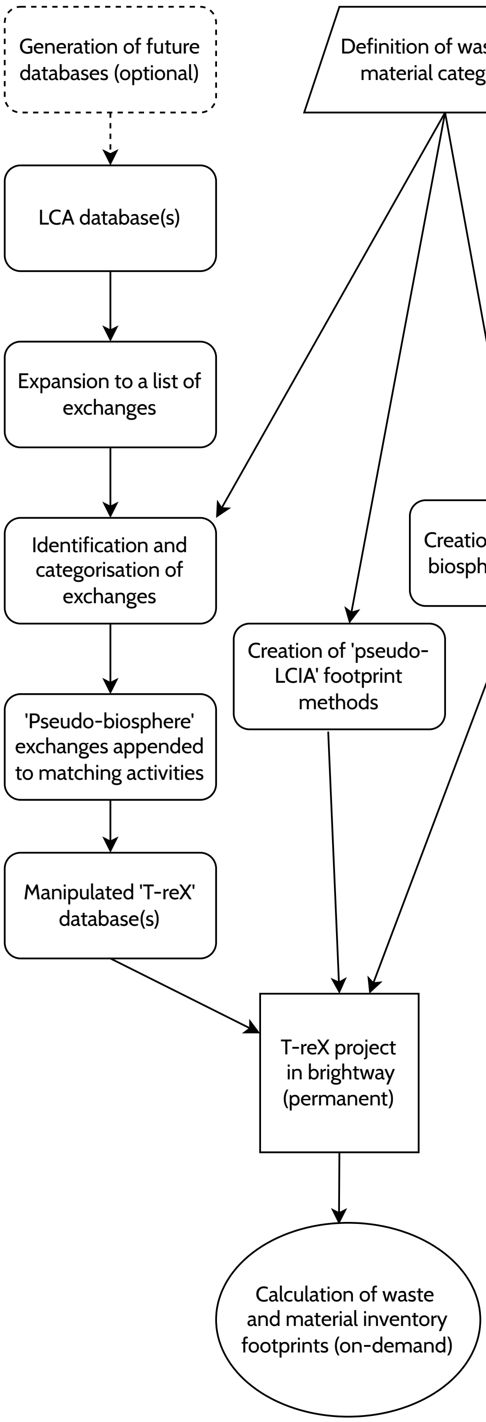
The workflow of the T-reX tool is divided into several modules, each of which performs a specific function. The modules are designed to be used in a specific order, but the user can also use them individually to perform specific tasks. The standard workflow is as follows:

1. Configuration of waste and material exchange categorisation (optional)
2. Generation of prospective LCA databases (optional)
3. Database expansion—to create a list of all exchanges in the database
4. Identification and categorisation of exchanges
5. Creation of 'pseudo-biosphere' databases
6. Creation of 'pseudo-LCIA' methods to calculate waste and material inventory footprints
7. Exchange editing—whereby the technosphere exchange is mirrored as a 'pseudo-biosphere' exchange
8. Database verification

This workflow creates one or more manipulated LCA databases that can then be used to calculate the waste and material inventory footprints of activities in the same way as standard LCIA calculations.

A generic flowchart of the T-reX tool workflow is presented in Figure 1. The supplementary material [ADD LINK] contains a more detailed computational flowchart.

Figure 1: Workflow of the T-reX tool. Application of T-reX to one or more LCA databases creates a brightway project with customised methods and activities that can be used to calculate the waste and material inventory footprints.



2.2. *Case Study Methodology*

We investigated five types of Li-ion batteries, each represented by specific market activities:

- Li-ion, NMC111, rechargeable, prismatic
- Li-ion, LiMn2O4, rechargeable, prismatic
- Li-ion, NCA, rechargeable, prismatic
- Li-ion, NMC811, rechargeable, prismatic
- Li-ion, LFP, rechargeable, prismatic

In addition to the waste and material inventory footprint methods created by the T-reX tool, the following standard LCIA methods were applied for comparison:

- ReCiPe 2016 v1.03, midpoint (I)
- EF v3.0 no LT
- EDIP 2003 no LT
- Crustal Scarcity

The primary source of life cycle inventory data for this case study was ecoinvent 3.9.1 cutoff. Additionally, the T-reX tool was used to create prospective database sets using the REMIND model with the following Representative Concentration Pathways (RCPs):

- SSP2-base: representing an approximate 3.5°C increase in global temperatures to 2100
- SSP2-PkBudg500: representing the achievement of Paris climate goals, ca. 1.3°C increase to 2100

For each pathway, databases were created with textttpremise (Sacchi et al., 2022) and processed with the T-reX tool over the time series: 2020, 2040, 2060, 2080, 2100.

2.2.1. Calculations

For each combination of activity, method, and database, a single score 'LCIA' was calculated along with details of the top contributing processes. Additionally, for the Waste and Material Footprint methods, a contribution analysis was performed. This involved utilizing the `bwa.compare_activities_by_grouped_leaves` function from the `brightway2_analyzer` package (Mutel, 2016), an additional component of the Brightway2 LCA framework. This function performs graph traversal on the impact matrix of the LCA object to a specified cutoff and groups the resulting leaves by their CPC codes. This provides insight into the products and sectors in the supply chain of the activity that carry the most responsibility for the final footprint.

3. Results

Section word count: 1300

3.1. *T-reX tool*

An example of the output from the application of the T-reX tool has been included in the supplementary material. The manipulated ecoinvent databases can be recreated using the code and instructions available in the package documentation (McDowall, 2023).

3.2. *Case study: Li-ion batteries*

As described in subsection 2.2, this case study calculated the waste and material footprints (as well as a variety of other indicators) for the unaltered inventories of five Li-ion batteries with the functional unit being 1 kg of the battery at market. The purpose of this simple case study was to test, verify, and demonstrate the functionality and limitations of the T-reX tool. This section includes some highlights of the results and the full results are available in the supplementary material. Because the T-reX methods are integrated into the brightway project as if they were LCIA methods, the results can be visualised in the same way. In the supplementary material, there are screenshots of selected results obtained using the `ActivityBrowser` software, including contribution analysis and a Sankey diagram that disaggregates the final footprint result over the activities in the supply chain.

3.2.1. *Sankey visualisation of flows in waste and material inventory footprints*

Figure 2 Sankey diagram of the total solid waste footprint flows for the NMC 811 battery in the case study

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[and decide which ones are most interesting (or will fit on a page. The most interesting are the ones that look like the flying spaghetti monster). I would probably make a new sankey (back to coding!), or edit the AB one in inkscape to make it understandable on the page.]

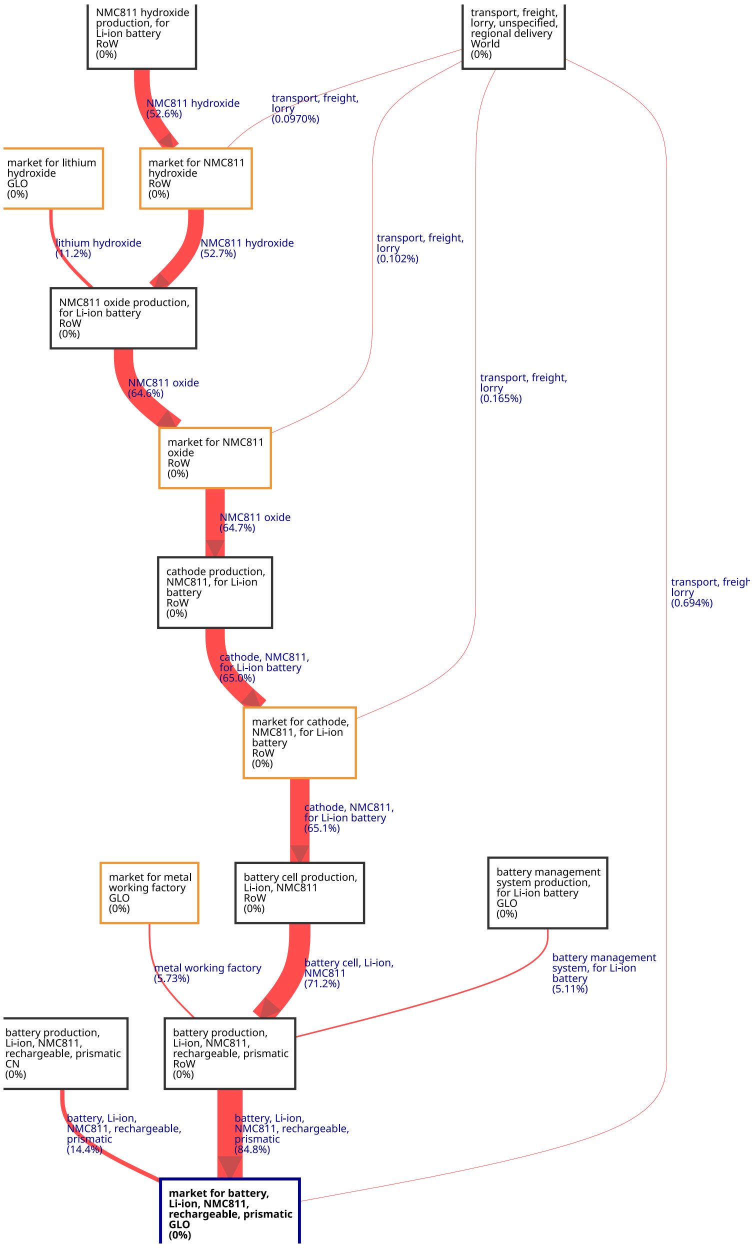


Figure 2: Sankey diagram of the total solid waste footprint flows for the NMC 811 battery in the case study.

Figure 3 shows the Sankey diagram of the chromium inventory demand footprint flows for the LFP battery in the case study.

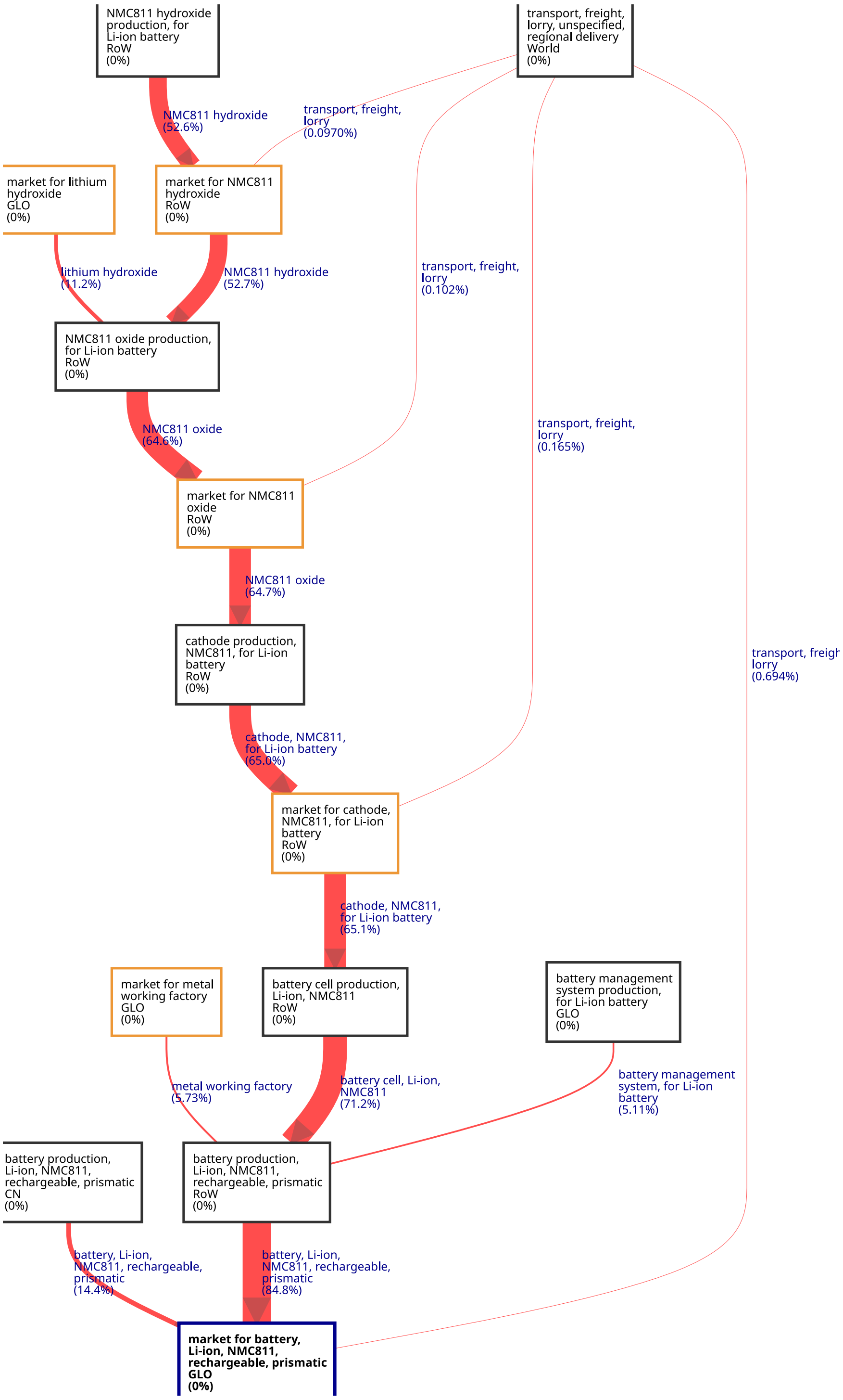


Figure 3: Sankey diagram of the chromium inventory demand footprint flows for the LFP battery in the case study.

3.2.2. *Temporal and scenario variation in waste and material inventory footprints*

Figure 4 shows the total solid waste footprint for the five Li-ion batteries in the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model. The NMC811 battery has the largest footprint, producing over 50 kg of waste per kilogram of battery produced. The LiMn2O4 battery has the smallest footprint, producing less than 4 kg of waste per kilogram of battery. In each case there was a slight downward trend in the waste footprints between 2020 and 2100. This is most notable in the period between 2020 and 2040 and is attributable to the relatively rapid decrease in fossil-fuel use that is included in the models over this time. For the total waste generated by these batteries, there was very little difference observed between the baseline and PkBudg500 RCPs.

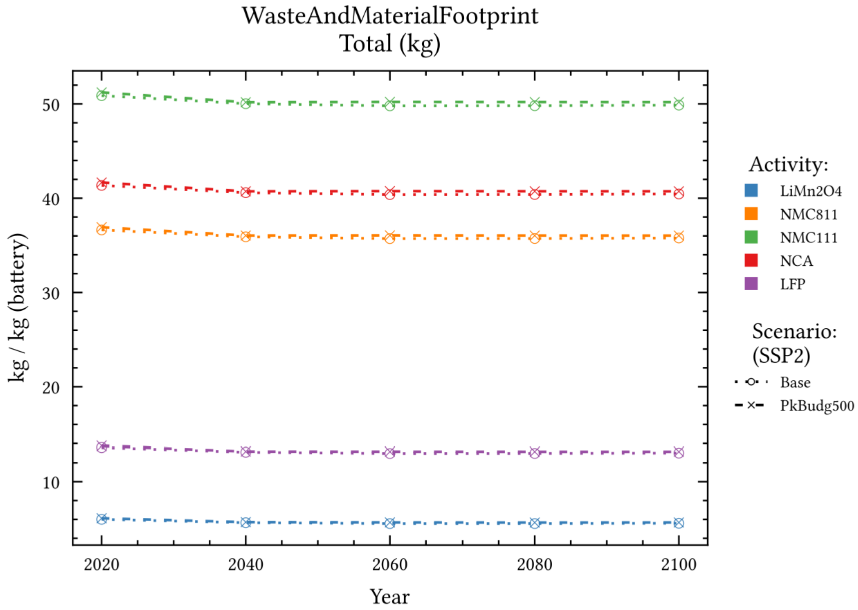


Figure 4: Total solid waste footprints for the five Li-ion batteries in the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model.

The inclusion of carbon capture and storage (CCS) in the prospective databases using the PkBudg500 RCP is evident in Figure 5, which shows a rapid increase in the production of carbon dioxide 'waste' over the period from 2020–2040 that is not seen in the baseline scenario. This result highlights the fact that (frequently) downward trends in global warming impacts calculated with prospective databases using standard LCIA methods are dependent on the assumptions made about the introduction of CCS technology. The actual deployment of these technologies—approximately 37 Mt CO_2/yr as of 2023 (Dziejarski et al., 2023)—falls far short of the levels projected in many of the RCP scenarios (Sacchi et al., 2023).

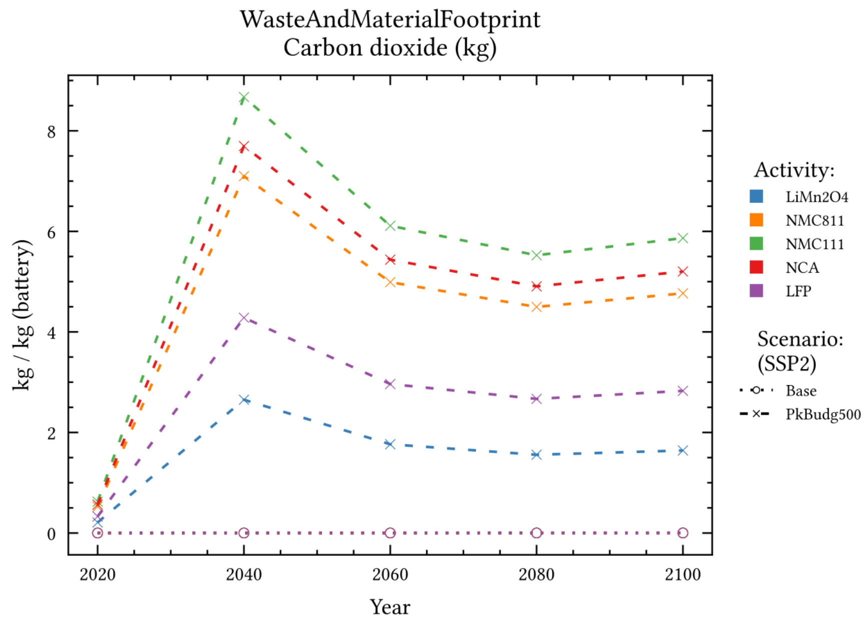


Figure 5: Carbon dioxide waste (from carbon capture and storage) footprints for the five Li-ion batteries in the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model.

For the phosphate demand footprints that are depicted in Figure 6, the LFP (lithium iron phosphate) battery has a much larger footprint than the other batteries, consistent with its composition. In this case, the phosphate footprint of all batteries is shown to decrease over the period from 2020–2100, and the RCP scenarios are seen to converge between 2020 and 2040.

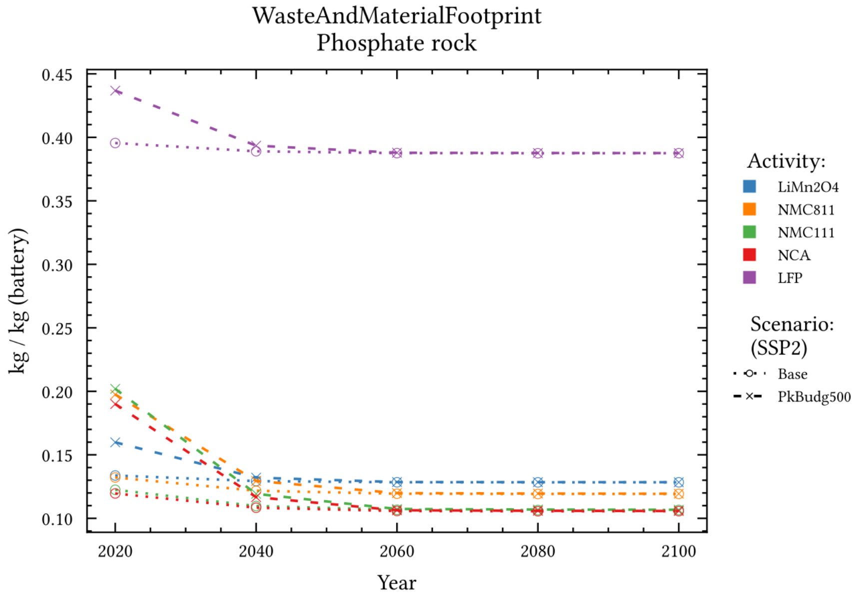


Figure 6: Phosphate material demand footprints for the five Li-ion batteries in the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model.

3.2.3. Contribution of 'top-processes' in the supply chain

Figure 7 shows the contribution of the 'top-processes' to the cobalt footprint of the LiMn2O4 battery under the baseline scenario from 2020–2100. The total footprint is seen to almost triple, from 2.2 kg/kg in 2020 to 6.2 kg/kg in 2100. This result is likely a reflection of the electrification of the transport sector that is included in the REMIND model. The fractional contributions of the top processes remains relatively steady over the coming century in this case.

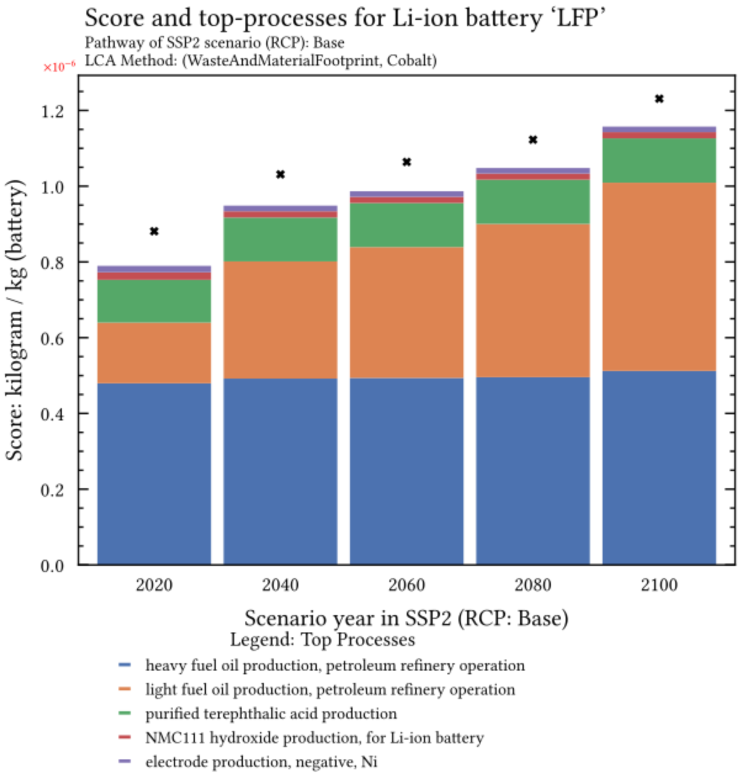


Figure 7: Contribution of 'top-processes' to the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model.

3.2.4. Contribution of sectors in the supply chain

Figure 8 shows the contribution of sectors (grouped by CPC) to the total natural gas footprint of the LFP battery under the PkBudg500 pathway. In this example, the relative contribution of the sector '47160: Electronic integrated circuits' is seen to decrease from 11% in 2020 to 6% in 2100, while over the same period the contribution of the sector '46430: Parts of primary cells, primary batteries and electrodes' increases from 29% to 38%. The method used to calculate these contributions involves traversing the supply chain branches to a certain level (max. 4, in this case), cutting a specified point (5% in this case), and grouping the value of the 'leaves' by their CPC code. The results, therefore, will depend on how deeply the user would like to inspect the supply chain. Additionally, the utility of these results is dependent on how well the CPC codes define the processes in the supply chain for the particular case.

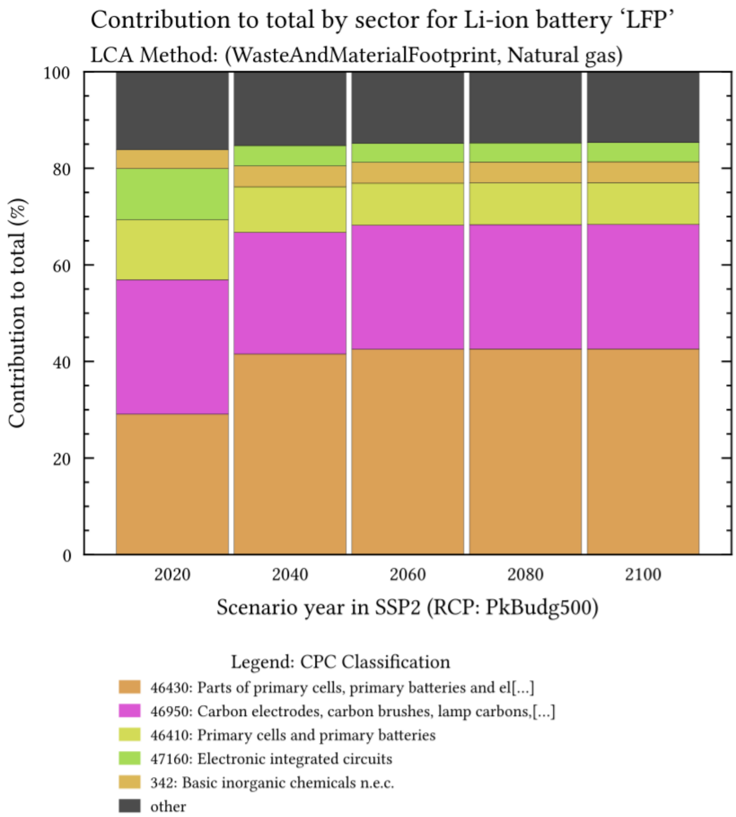
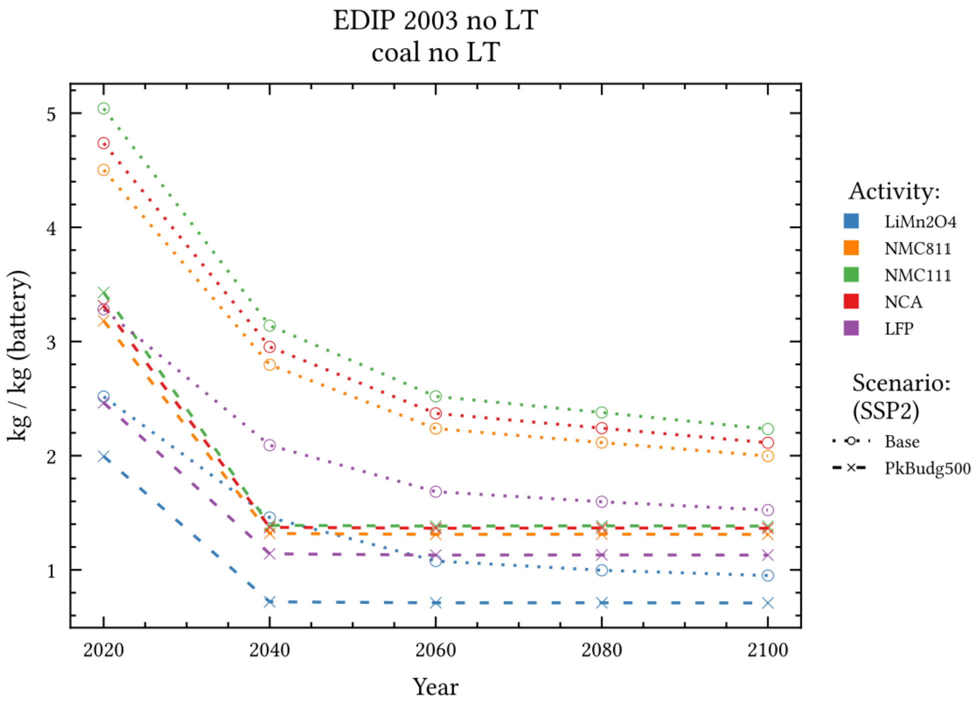


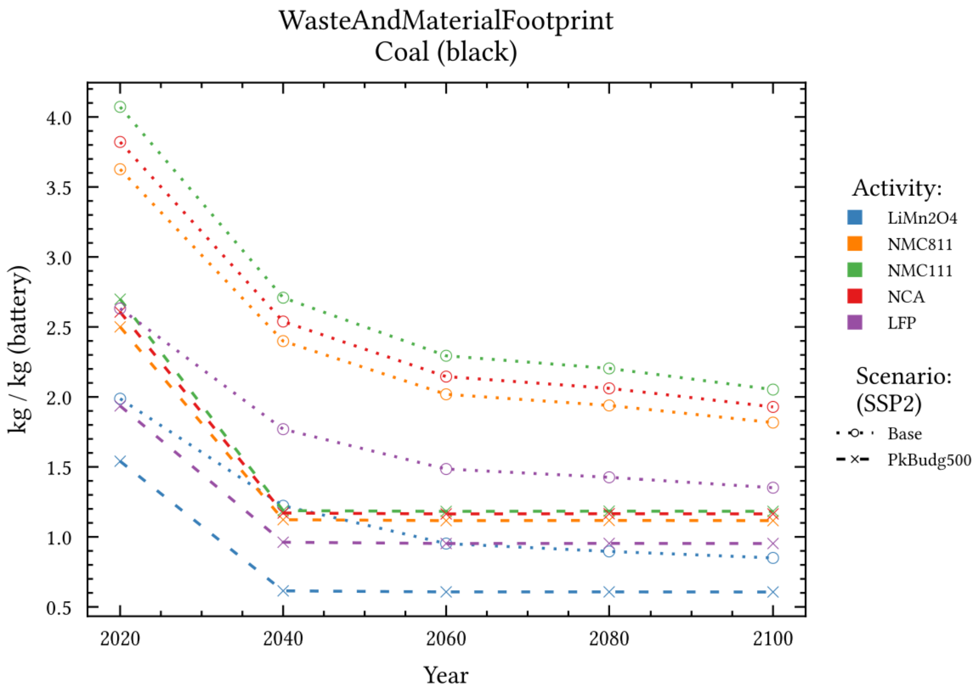
Figure 8: Contribution of industrial sectors to the liquid waste footprint of the NCA battery from 2020 to 2100 under the SSP2 scenario using the PkBudg500 RCP of the REMIND model.

3.2.5. Comparison with 'similar' methods

A comparison of the results from the T-reX tool's 'Coal (black)' demand method with the LCIA method 'EDIP 2003 - coal no LT' is shown in Figure 9. In this case, both the trends and the magnitude of the scores were very similar, both demonstrating a general decrease in the use of coking coal in the battery's footprints. Such comparability was also observed for other fossil-fuel-related methods (e.g., natural gas and petroleum), and to a lesser extent, for some of the metal demand methods (e.g., zinc and cobalt). Correlation between standard LCIA methods and T-reX methods, is not generally to be expected, however, due to fundamental differences in the way that the methods are constructed. In standard LCIA methods, impact scores are derived exclusively from the magnitude of the exchanges between the biosphere and the technosphere, that is, extraction and emission. In the T-reX methods, the footprint scores are based on an accounting of either waste generated or material demand, both of which are technosphere-technosphere exchanges in terms of LCA modelling. For the material demand methods especially, this distinction is critical. For example, application of the EDIP 2003 or the CSP methods for a given metal will provide a score that is proportional to the amount extracted by mining, whereas the T-reX method provides an aggregation of the exchanges with the market for that metal. The T-reX method, therefore, considers cases of co-production, recycling, and substitution, providing a picture of the supply-chain pressures that are not captured by the standard LCIA methods. This makes the T-reX methods more sensitive to the modeling choices (e.g., allocation) that are generally embedded in LCA databases.



(a)



(b)

Figure 9: Comparison of LCIA method 'EDIP 2003 - coal no LT' (a) with the 'T-reX - Coal (black)' (b) in the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model.

3.2.6. Comparison with other studies

Laurenti et al. (2023) used an alternative method for calculating the waste footprint of 1400 activities in ecoinvent version 3.5, which contains only a generic 'market for battery, Li-ion, rechargeable, prismatic'. The inventory of this battery most closely resembles that of the NMC 111 battery in this case study. Table 2 presents a comparison of the results from the two studies, where possible. For liquid, solid, and recycled waste, the results were closely aligned, however for hazardous waste, Laurenti et al. reported 95% of the total waste, whereas the T-reX tool reported only 3%. The reason for this discrepancy is explained by the fact that in the method of Laurenti et al., a "waste flow was regarded as hazardous when the hazardousness was clearly stated in its subsequent waste treatment activity". The authors continue: "It should be noted that the high hazardousness ratios for many products might indicate a weakness in the validity of this measure". In the T-reX method, the source database is exploded into a list of separate exchanges, and only those explicitly defined as hazardous are marked as such.

Table 2: Comparison of the results from the T-reX battery case study (database: ecoinvent 3.9.1 REMIND SSP2 Base 2020, activity: Li-ion NMC 111) with those from Laurenti et al. (2023) (database: ecoinvent 3.5, activity:'Li-ion').

Indicator	T-reX	Laurenti et al.
Total solid waste (kg/kg)	50.9	62.5
Total liquid waste (kg/kg)	3.53	3.63
Hazardous waste (kg/kg)	1.47	62.6
Recycled waste (kg/kg)	1.59	1.98

4. Discussion

Given that both waste generation and material demand are often strongly associated with the environmental impacts of an activity, it is important that they are included in the LCA. While there are numerous examples of existing and proposed methods that attempt to provide endpoint LCIA scores through convoluted formulae or subjective weighting, there is little consensus on their application and their complexity and lack of transparency can make them difficult to use and interpret.

Our contribution advances the state-of-the-art by giving LCA practitioners a simple, flexible, and transparent way to calculate supply chain waste and material footprints, delivering results in standard units and as direct aggregations of the relevant demand inventories. Once the databases have been processed with the T-reX tool, the user can easily apply the T-reX 'pseudo-LCIA' methods to calculate the waste and material inventory footprints in the same way that they would with a conventional LCIA method.

The simple case study of six Li-ion batteries presented in this paper demonstrated the the utility, flexibility and limitations of the T-reX tool.

First, by adjusting the user configuration for future scenarios and waste/material categorisation we easily produced a set of customised versions of the ecoinvent database. Then, by applying the T-reX 'pseudo-LCIA' methods, it was trivial to calculate categorised waste and material inventory footprints for a number of present and future supply chains. Additionally, visual exploration in `ActivityBrowser` was possible because the T-reX 'pseudo-LCIA' methods are integrated in the `brightway` project in the same way as standard LCIA methods.

One limitation of the T-reX tool is that it does not yet provide specific information (in a readily accessible format) on the composition of the waste generated. This is the information would be needed to thoroughly assess the potential environmental impacts of this waste. Currently, the user would need to manually explore the waste footprint inventory produced by the application of the T-reX to determine if, for example, the waste generated represents an actual loss of resources, or is simply a transfer of the 'overburden' in mining activity, which is classified as 'inert waste'. A methodic classification of waste exchanges and the end-of-life fates will be facilitated by the more detailed and disaggregated data that is seen in each successive release of ecoinvent (FitzGerald et al., 2023).

The utility of the T-reX tool in studies of future supply chains is limited by the fact that the currently available prospective databases focus largely on changes in the energy, steel, cement, and transport sectors (Sacchi et al., 2023). As demonstrated in the results of the case study—where there was often very little scenario-temporal change in many waste and material footprint indicators—the utility of prospective LCA is restricted if there is little adaption of the future background inventories. In particular, the inclusion of scenarios with future waste processing technology would greatly improve our predictions of waste and material flows. A strong focus on enhancing these prospective databases is, thus, of critical importance to the future of prospective LCA, and by extension, to the development of the circular economy.

Section word count: 450

5. Conclusions

Section word count: 250

We have created the T-reX tool, an extension to the brightway LCA ecosystem that enables users to calculate the waste and material footprints of a product or service in an LCA database. It explodes the database, identifies upstream waste and material exchanges, edits them, and writes matching custom 'pseudo' LCIA methods. These exchanges become pseudo-biosphere flows and thus, the footprint can be calculated as with the existing LCIA methods. The T-reX tool can be easily customised by the user to calculate the footprints of other supply-chain flows such as water, gas, and critical raw materials.

This paper extends the state of knowledge by exploring the relationship between various waste aggregation methods and environmental damage indicators, contributing to a deeper understanding of life cycle waste inventories and their association with supply-chain risk and potential environmental damage.

Data availability

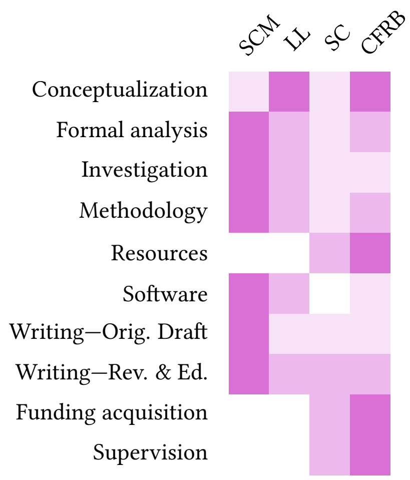
All data used in this analysis are publicly available online under the noted sources. The T-reX tool is installable via the Python Package Index (PyPI) and is available at `https://pypi.org/project/T-reX`. The full source code for the T-reX tool is available at `https://www.github.com/Stew-McD/T-reX`. A user guide and comprehensive documentation are available at `https://T-reX.readthedocs.io`.

CRediT authorship contribution statement

Co-authors, please check this and change as necessary.

Stewart Charles McDowall: Methodology, Software, Validation, Formal analysis, Investigation, Data curation, Writing - original draft, Writing - review & editing, Visualization. **Elizabeth Lanphear:** Conceptualization, Methodology, Software, Validation, Writing - review & editing. **Stefano Cucurachi:** Conceptualization, Writing - review & editing, Supervision, Project administration, Funding acquisition. **Carlos Felipe Blanco:** Conceptualization, Writing - review & editing, Supervision, Project administration, Funding acquisition.

Alternative CRediT statement



Declaration of competing interest

The authors 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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Supplementary material

The supplementary material contains the following:

1. Metadata of the T-reX python package
2. Details of the modules and user configuration
3. Description of the computational workflow
4. Modular flowchart of the T-reX tool
5. Example of the terminal output of the T-reX tool
6. Complete tabulated results of the case study
7. Complete visualisations of the case study

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