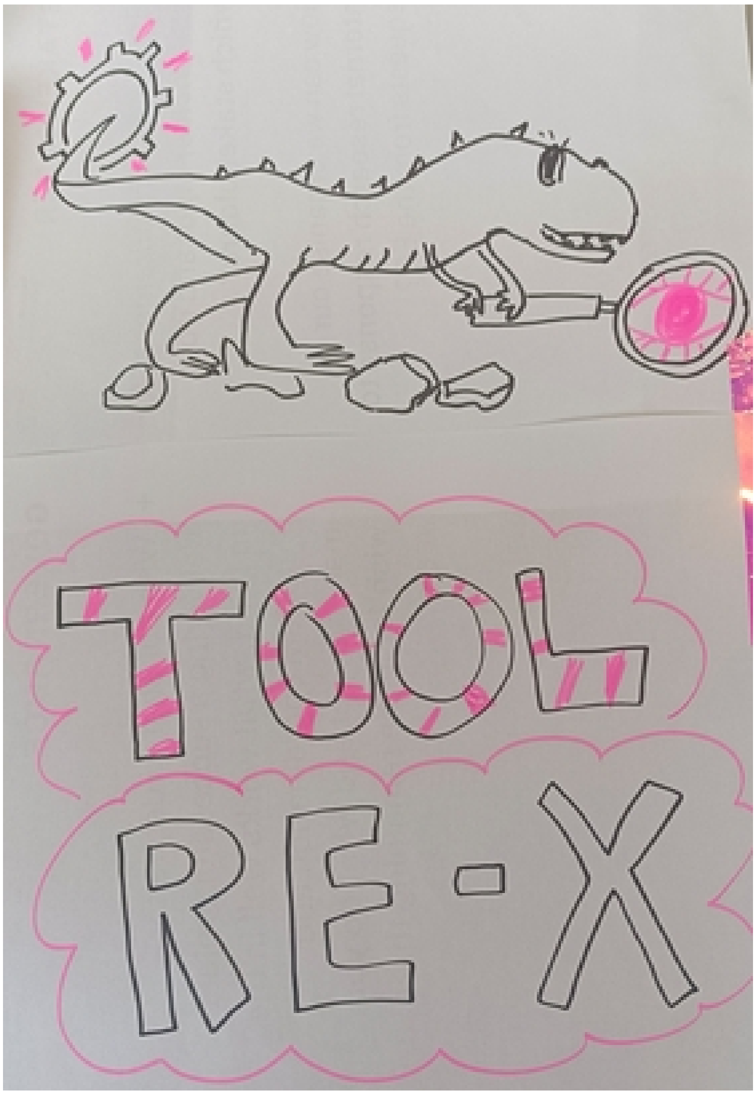
Spotlights

- Tracking waste and material flows is essential for developing the circular economy and supply chain resilience
- A tool was developed to quantify waste and material footprints of activities in life cycle assessment (LCA) databases
- Built to complement the Brightway LCA framework and ActivityBrowser, the tool is customisable and easy to use
- The tool can be used to identify pre-consumer waste and material hotspots that are often hidden in supply chains
- Improved data availability and quality would enable more detailed and accurate waste and material footprinting

Graphical Abstract



Highlights

- T-reX, a new software 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 five Li-ion battery supply chains

T-reX: A tool to quantify waste and material footprints in current and future Life Cycle Assessment (LCA) databases

Stewart Charles McDowall[a,*], Elizabeth Lanphear[a], Stefano Cucurachi[a], Carlos Felipe Blanco[a]

[a]*Institute of Environmental Sciences (CML), Leiden University, P.O. Box 9518, Leiden, 2300 RA, South Holland, The Netherlands*

Abstract

The quintessential principle of the 'circular economy' is to minimise material consumption and waste generation. Thus, identifying and quantifying waste and material flows are of fundamental importance. Life Cycle Assessment (LCA) is a powerful method for this, 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 five lithium ion batteries demonstrates 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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*Corresponding author:
Email address: s.c.mcdowall@cml.leidenuniv.nl (Stewart Charles McDowall)

Table 1: List of abbreviations

CF	Carbon Footprint
EF	Ecological Footprint
CML	Centrum voor Milieuwetenschappen (Centre for Environmental Science)
CRM	Critical Raw Material
CPC	Cooperative Patent Classification
CSI	Crustal Scarcity Indicator
CSP	Crustal Scarcity Potential
EDIP	Environmental Design of Industrial Products
EEIOA	Environmentally Extended Input-Output Analysis
EOL	End-of-Life
FOEN	Swiss Federal Office for the Environment
IAM	Integrated Assessment Model
IE	Industrial Ecology
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LFP	Lithium Iron Phosphate
Li-ion	Lithium ion
$LiMn_2O_4$	Lithium Manganese Oxide
MF	Material Footprint
MFA	Material Flow Analysis
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
T-reX	Tool for re-X in LCA
UBP	Umweltbelastungspünkte (Environmental Impact Points)
UN	United Nations
WF	Waste Footprint

1. Introduction

1.1. Background

The development of a 'circular economy' has become a critical area of focus in the imperative pursuit of sustainability objectives and curtailment of 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) (Reike et al., 2018; European Commission, 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 even outright hostility (Carrara et al., 2023; Hartley et al., 2024; Berry, 2023).

The concept of the 'footprint' as an environmental sustainability indicator began with the Ecological Footprint (EF) (Wackernagel, 1994) and after being popularised by the Carbon Footprint (CF) (Čuček et al., 2015) the 'footprint family' developed strongly and has adopted many additional metrics—albeit without yet coalescing into a coherent or consistent framework (Giampietro and Saltelli, 2014; Vanham et al., 2019; Ridoutt and Pfister, 2013). More recently, the footprint collection has been extended to include the Material Footprint (MF) (Wiedmann et al., 2013), which is more often encountered in the 'macro methods' of Industrial Ecology (IE), such as environmentally Extended Input-Output Analysis (EEIOA) (Lenzen et al., 2021) and Material Flow Analysis (MFA) (Schaffartzik et al., 2013). Whether at the level of products, entire industries, nations or even continents, the material footprint aims to quantify the total material consumed in supply chains. It has been shown that MF can be 'highly representative of damage to human health and biodiversity' (Steinmann et al., 2017) and indeed, this metric was recently beatified by the United Nations (UN), becoming the 'core official indicator' for targets 8.4 and 12.2 of the Sustainable Development Goals (SDGs) (Lenzen et al., 2021).

The incipient Waste Footprint (WF) metric, in contrast, though emerging steadily, has yet to enjoy such noble recognition for its attempts to measure and classify the waste generated by human activities (Laurenti et al., 2016). Despite the fact that reducing life cycle waste is clearly critical to the development of the circular economy Towa et al. (2020); Ellen MacArthur Foundation (2015), the WF remains largely overlooked—especially in LCA models where waste itself is seldom apportioned any inherent evironmental significance aside from the emissions related to its treatment (Laurenti et al., 2023). Such ignominious neglect strikes the authors as unjustified, given that it has been repeatedly demonstrated that waste footprints can have a strong association with environmental damage (Laurenti et al., 2023; Doka, 2024; Ridoutt et al., 2010; Jiao et al., 2013). Alas, in frequent, tragic, failures of evironmental justice, it is often the most vunerable communities who suffer disproportionately from the social and ecological impacts that can be created by wasteful behaviours and sub-standard end-of-life treatment practices (N. Pellow, 2023; Akese and Little, 2018).

WF and MF, the two metrics of focus in the study, can provide a comprehensive assessment of potential environmental impacts across the supply chain, encapsulating both resource use and pollution/waste generation, while offering insights at diverse scales, from individual activities to global systems, facilitating communication with a diverse range of stakeholders. Thus, to reduce the negative externalities of human 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 (Bisinella et al., 2024; Towa et al., 2020).

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 (Guinée et al., 2010). 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 (those between the technosphere and biosphere). These scores can then be aggregated into a single score for each impact category, that can be compared across products and processes. Extending on standard LCA is *ex-ante* LCA, which employs future scenarios to construct prospective background databases in an effort to predict the impacts of supply chains that have not yet been (and may never be) realised (Cucurachi et al., 2018; Blanco et al., 2020).

Several LCIA methods include, to some extent, waste generation (Swiss Eco-Factors, EDIP and EN15804) (Swiss Federal Office for the Environment (FOEN), 2021; Hauschild and Potting, 2004; CEN (European Committee for Standardization), 2019) and material consumption (Crustal Scarcity Indicator (CSI) and Swiss Eco-Factors (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 case of the Swiss Eco-Factors) (Su, 2020).

1.1.1. *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 highly variable across space and time. Moreover, from a systems perspective, the notion of waste is anathema to the 'circular economy', they cannot co-exist. Returning from the abstract and etherial to the economic viability of the waste processing sector. While critical here are energy costs and the relative prices of virgin and secondary materials, the viability of an extensive waste processing system is highly dependent on precise knowledge (or at least, reasonable predictions) of material and waste flows. Thus, as Bisinella et al. (2024) argues, waste must be 'thoroughly characterised' and that 'modelling [of its management] must be physically based'. The reliable, robust models needed to guide the development of the circular economy can be built only on a foundation of high-quality data.

Accurate and detailed information about waste and waste systems is, by definition, essential for understanding the 'circularity' of a human activity and predicting its life cycle externalities, but there remains a conspicuous knowledge gap regarding the waste footprints of human activities and their environmental impacts (Laurenti et al., 2023).

Conventional LCA database models consider waste as a 'service' (accounting for the treatment, not the material) (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 (almost exclusively) not considered as fundamental biosphere exchanges, but rather, as technosphere flows within the human economy. 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 modelling the long-term impacts of disposal.

A considerable portion of a product's total waste is generated during earlier stages of its supply chain such as resource extraction, transportation, and manufacturing, thus, often remaining 'invisible' to conventional LCA accounting 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 *per se*, considering instead only emissions and resource use resulting from waste treatment (Bisinella et al., 2024; Laurenti et al., 2023). The environmental significance of waste and its correlation with other indicators has been the subject of extensive research and studies have shown that popular resource footprints can cover a significant portion of environmental impact variance between activities (Steinmann et al., 2017; Laurenti et al., 2023). Correlations between various environmental indicators are not always consistent, however, as seen with the carbon footprint, which often does not correlate well 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).

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 'circularity', but there is a lack of convenient and flexible ways 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 greater 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 (as the authors themselves acknowledge). The 'T-reX' Python software tool presented herein provides a more flexible, transparent, and user-friendly approach to quantifying waste flows in LCA. Moreover, the utility of T-reX is not limited to waste, it can be used to categorise and aggregate any technosphere exchange of interest (or customised grouping thereof), such as water, gas, and critical raw materials.

1.1.2. Material demand in LCA

In the context of a mineral-hungry renewable energy transition and constant 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 DG-GROW, 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) and its exchanges with the biosphere, its focus is often on the environmental impacts of the system—the endpoints—rather than the primary material flows themselves.

A relatively new (2020) LCIA method, the Crustal Scarcity (CSI), was developed in order to introduce an assessment of the long-term global scarcity of minerals in LCA (Arvidsson et al., 2020). The CSI introduced crustal scarcity potentials (CSPs), which are measured in kg silicon equivalents per kg element and 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 intended purpose, the CSI presents its 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.

1.2. Introduction to T-reX

To facilitate the quantification of waste and material flows in LCA, we developed a Python package to extend the `brightway` LCA framework (Mutel, 2017a) and designed to track these exchanges by translating them into inventory indicators and 'pseudo' LCA impact (LCIA) categories. T-reX, in full, stands for 'Tool for re-X' (reduce, reuse, recycle, etc.) and enables LCA practitioners to manipulate their databases such as 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 some 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).

Integration with the `premise` Python package (Sacchi et al., 2022)—which connects the projections of integrated assessment models (IAMs) with current LCA databases—enables the user to create and manipulate prospective LCA databases. Frustratingly, the current utility of prospective databases—in general, and in particular for the waste sector—is constrained by the fact that, to date, the sectoral coverage of future life cycle inventories (LCIs) is largely confined to energy, steel, cement, and transport (Sacchi et al., 2023). Indeed, despite the ever more critical need to reliably model and future waste management systems, Bisinella et al. (2024) reports an alarming lack of coherent development in this field.

The purpose of T-reX is not to quantify the environmental impacts of material consumption and waste production (the requsite data and impact modelling remains lacking), 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, minimising primary material consumption and the generation of waste is of paramount importance. By allowing LCA practitioners to easily classify and quantify these exchanges, T-reX provides a practical means to identify hotspots and highlight opportunities for waste reduction and material efficiency.

2. Methodology

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

2.1. T-reX

2.1.1. Computational framework

Developed in the Python programming language, T-reX extends the `brightwayLCAframework`, 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. T-reX 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 T-reX 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 versions 3.5–3.10.

T-reX can be used directly from the command line, or imported as a Python package, 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 adapt the settings of T-reX as desired, to calculate alternative or additional waste and material inventory footprints, use a custom database, or to use a prospective database based on future scenarios by implementing the premise `premise` with one of T-reX's internal modules.

The supplementary materialsection 5 contains metadata of T-reX, along with a list of the constituent modules, a description of their functions, and a detailed computational workflow. Further details can be found in the GitHub repository and package documentation (McDowall, 2024, 2023).

2.1.2. Functionality and purpose

T-reX is a Python package that enables 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 way as one would apply standard LCIA methods. We refer to the T-reX methods as 'pseudo-LCIA' methods, as they represent an accounting of a activity's technosphere inventory without reference to impact modelling, as in standard LCIA.

If desired, prospective databases can be 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) and can be paired with a variety of mitigation scenarios.

The deconstruction of the databases by T-reX into lists of exchanges allows the relevant material and waste flows to be identified and categorised by search functions. The queries facilitating this 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 relevant activity a copy of the technosphere exchange as a '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 material section 5. One advantage of T-reX is that it is able to identify 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, T-reX includes numerous material demand categories, which are based on the EU Critical Raw Materials (CRM) list for 2023 (European Commission and DG-GROW, 2023). The CRM list contains 30 materials that are considered critical to the EU economy and are at risk of supply disruption. Several 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 section 5.

The logic for the identification of material exchanges with T-reX 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 rather than keywords in the exchange's name. A useful feature T-reX is that, in cases where there are several markets for one material or material group, the program can aggregate these flows. 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 calculated in the same manner.

As presented in the introduction of this study subsection 1.1, subsubsection 1.1.1, subsubsection 1.1.2 there are some existing material demand methods in the standard LCIA method sets, including the CSI (which provides only an aggregated, abstracted endpoint in units of kg Si eq) (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.

T-reX, in contrast, uses accounting for material demand (and waste generation) 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, T-reX can provide insight into the broader supply chain impacts of the demand for this metal. If the production of other materials is 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 nickel demand, which, in the final inventory because of such co-production, is counter-intuitively negative (due to co-production and substitution in the LCA system models) despite the presence of nickel in the final products.

2.1.3. Mathematical basis

$\boxed{\text{very nice formulae coming soon}}$

2.1.4. *The workflow of T-reX*

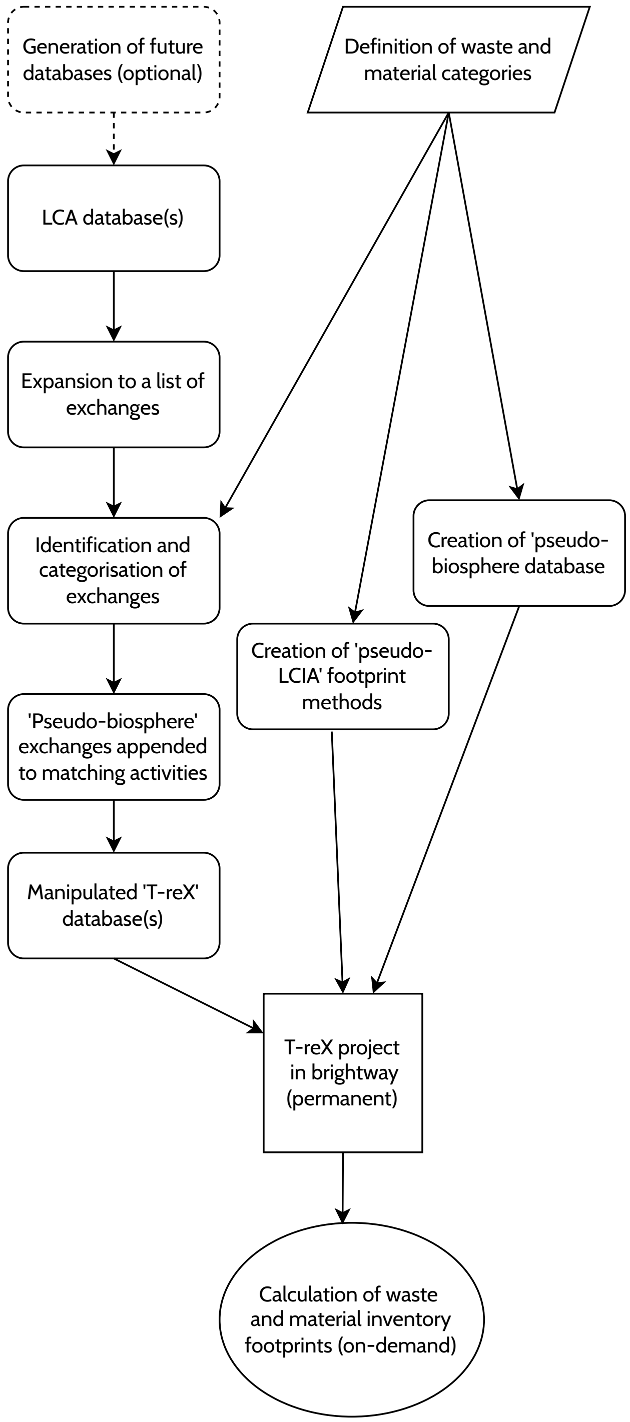
The workflow of T-reX is divided into several modules, each performing a separate function. The modules are designed to be used in a particular order, but the user can also use them individually to perform specific tasks. The standard workflow is as follows:

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—to ensure that T-reX has manipulated the database correctly

This workflow creates a copy of the original `brightway` project containing the original biosphere database, a T-reX 'pseudo-biosphere' database along with one or more manipulated technosphere databases that can 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 workflow is presented in Figure 1. The supplementary materialsection 5 contains a more detailed computational flowchart.

Figure 1: Workflow of T-reX. 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 waste and material inventory footprints of the activity's supply chain.



2.2. Case study methodology

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

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

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

- ReCiPe 2016 v1.03, midpoint (I)
- EF v3.0 no LT
- EDIP 2003 no LT
- CSI 2020

The source of the life cycle inventory data for this case study was the database ecoinvent, version 3.9.1 with the 'cutoff' attributional system model. Additionally, T-reX was used to create prospective database sets using the REMIND model and the baseline scenario SSP2 'middle of the road' 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 (at five year time intervals) were created with `premise` (Sacchi et al., 2022) and processed with T-reX for the period between 2020 and 2100.

2.2.1. *LCA calculations*

For each combination of activity, method, and database, a single score was calculated along with details of the top contributing processes. Additionally, for the T-reX methods, a contribution analysis was performed. This involved utilising the `bwa.compare_activities_by_grouped_leaves` function from the `brightway2_analyzer` package (Mutel, 2016), a component of the `brightway` ecosystem. This function performs graph traversal on the impact matrix of the LCA object to a specified cutoff and groups the resulting leaves by their Cooperative Patent Classification (CPC) codes. This provides insight into the products and sectors in the supply chain of the activity that carry the most substantial responsibility for the final waste generation or material demand.

3. Results

3.1. T-reX tool

An example of the output from the application of T-reX has been included in the supplementary material. The manipulated ecoinvent databases, which are the main product of T-reX can be recreated by following the instructions 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 (with 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 the global market. The purpose of this simple case study was to test, verify, and demonstrate the functionality and limitations of T-reX. This section includes some highlights of the results with full results included in the supplementary materialsection 5. Because the 'pseudo LCIA' T-reX methods are integrated into the brightway project as if they were LCIA methods, the LCA calculations can be performed in the customary 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 presents a Sankey diagram depicting the supply chain flows of 'total solid waste' for the NMC 811 Li-ion battery at the global market in the ecoinvent database version 3.9.1

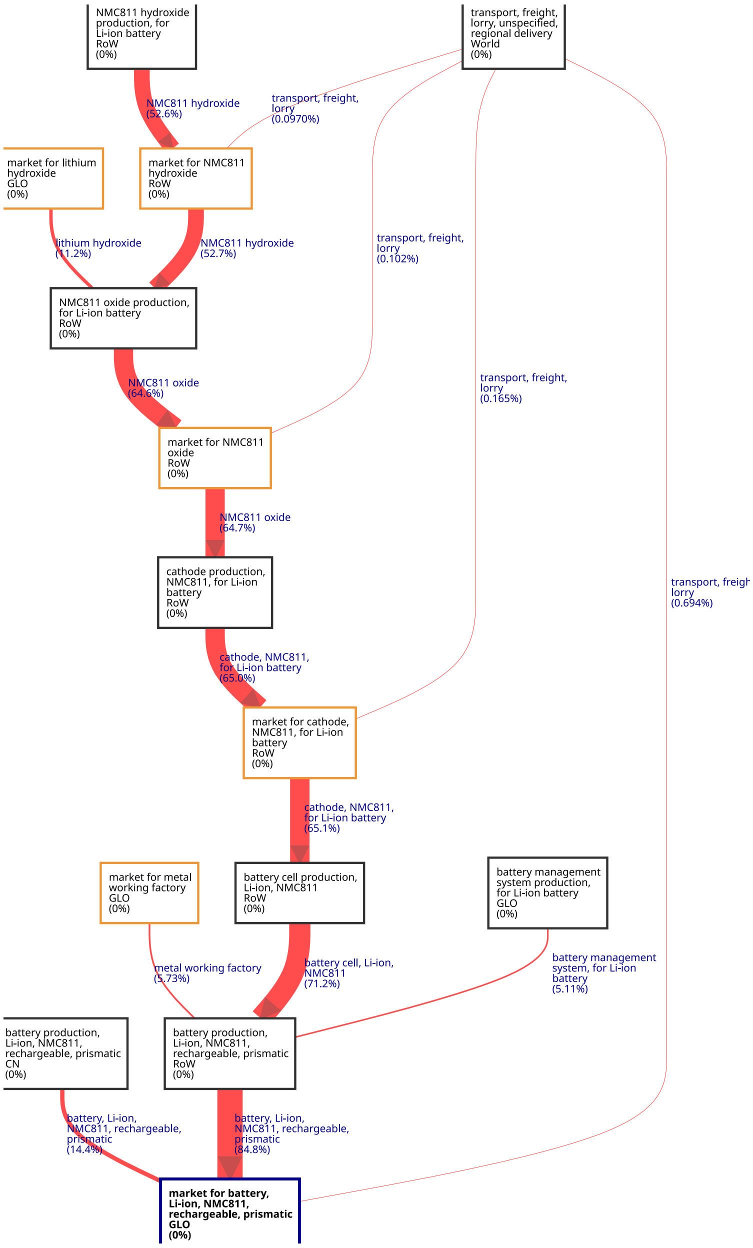


Figure 2: A Sankey diagram of the total solid waste footprint flows for the NMC 811 battery at the global market in the ecoinvent database version 3.9.1 [TO BE IMPROVED!]

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

Figure 3 shows the 'total solid waste' inventory 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 (which can large amounts of waste in its extraction and combustion phases). For the total waste generated by these batteries, there was very little difference observed between the baseline and PkBudg500 RCPs.

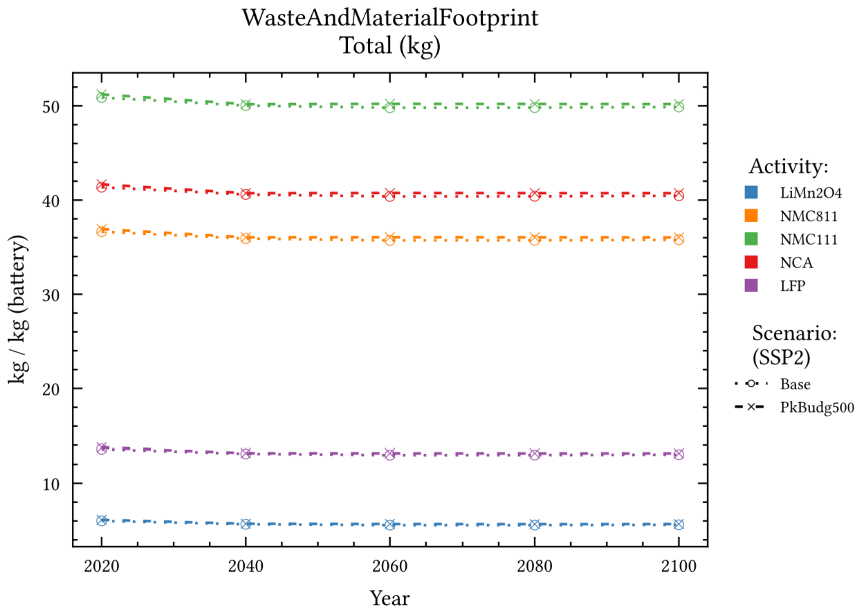


Figure 3: Total solid waste footprints for the five Li-ion batteries in the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model.

The inclusion of carbon capture and storage (CCS) in the prospective databases using the PkBudg500 RCP is evident in Figure 4, 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 the (often) 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 was only around 37 Mt CO_2/yr as of 2023 (Dziejarski et al., 2023), far short of the levels projected in many of the RCP scenarios (Sacchi et al., 2023).

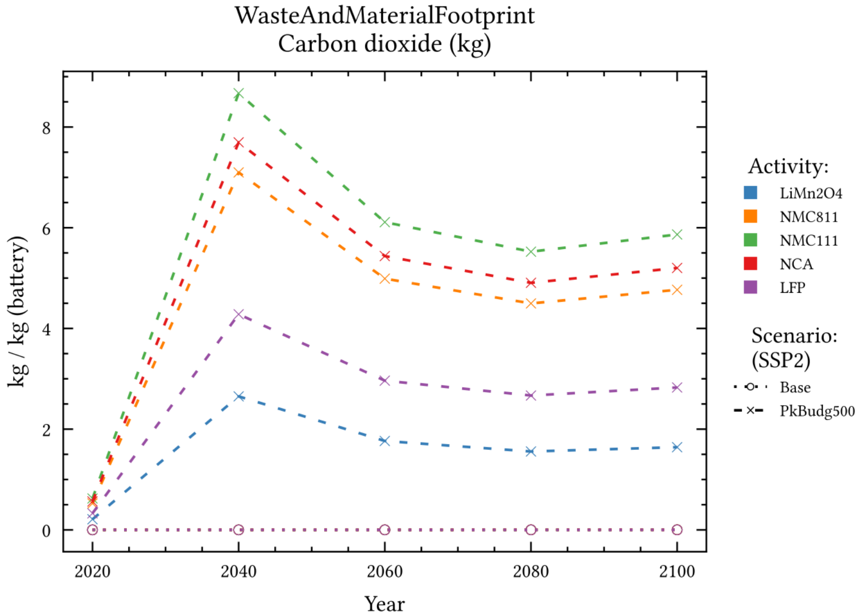


Figure 4: Carbon dioxide waste (from carbon capture and storage) footprints for the five Li-ion batteries in the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model. [TO BE IMPROVED!]

For the phosphate demand footprints that are depicted in Figure 5, 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.

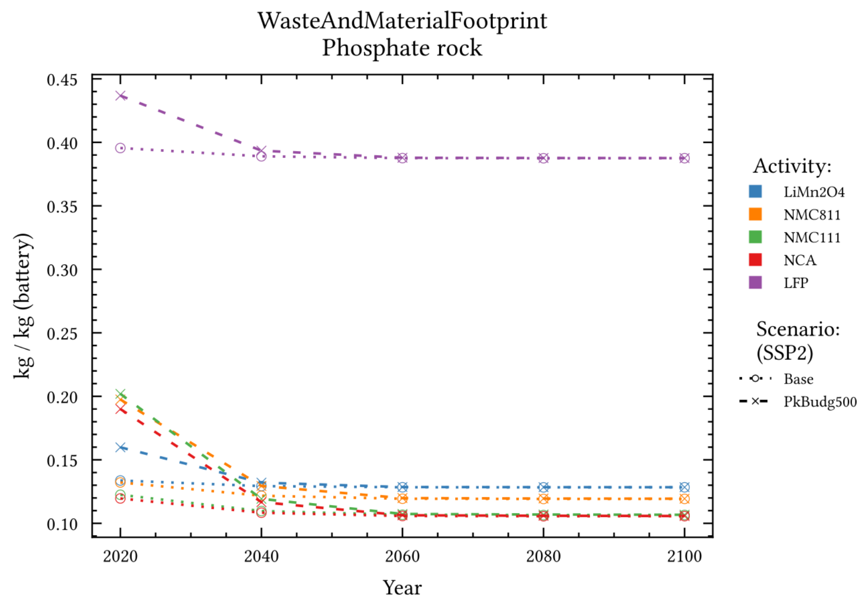


Figure 5: Phosphate material demand footprints for the five Li-ion batteries in the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model. [TO BE IMPROVED!]

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

Figure 6 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.

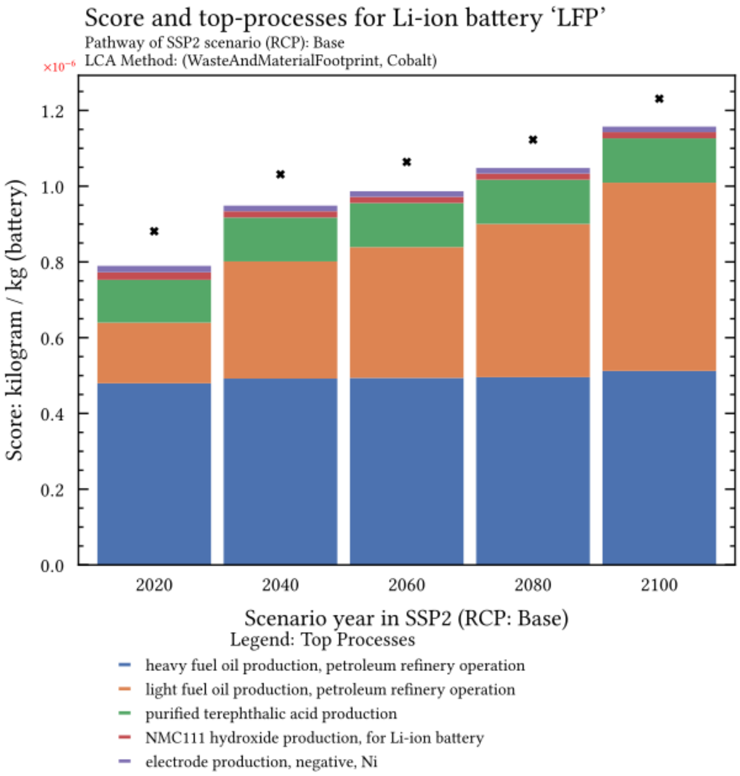


Figure 6: Contribution of 'top-processes' to the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model. [TO BE IMPROVED!]

3.2.4. Contribution of industrial sectors in the supply chain

Figure 7 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.

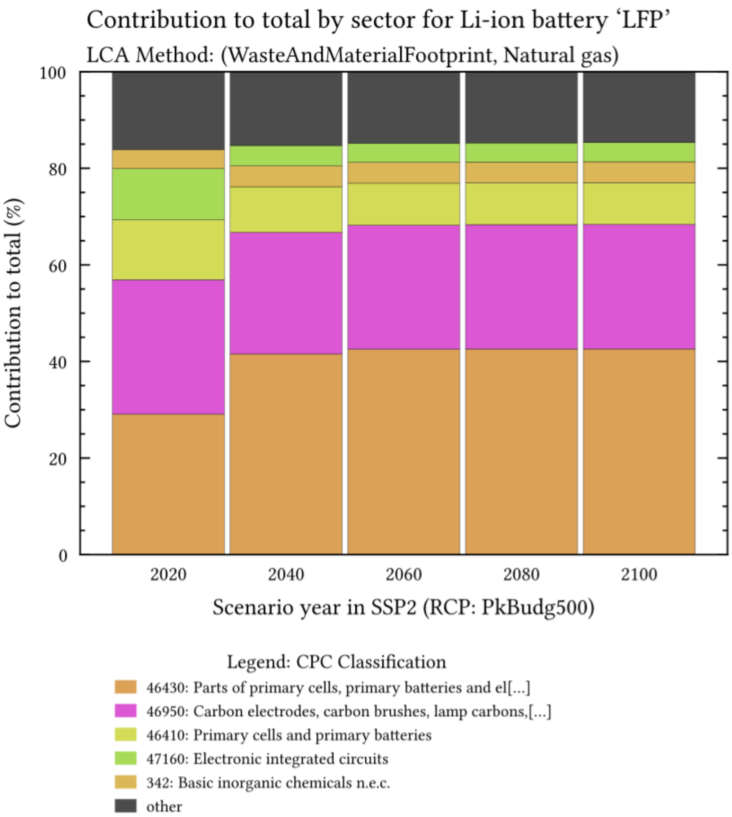
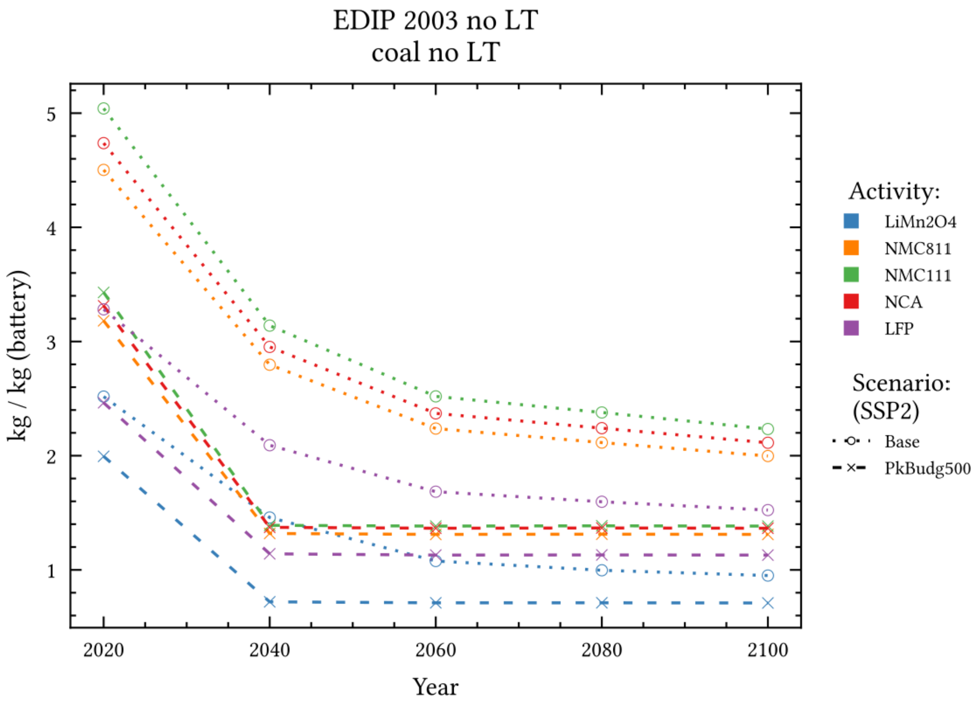


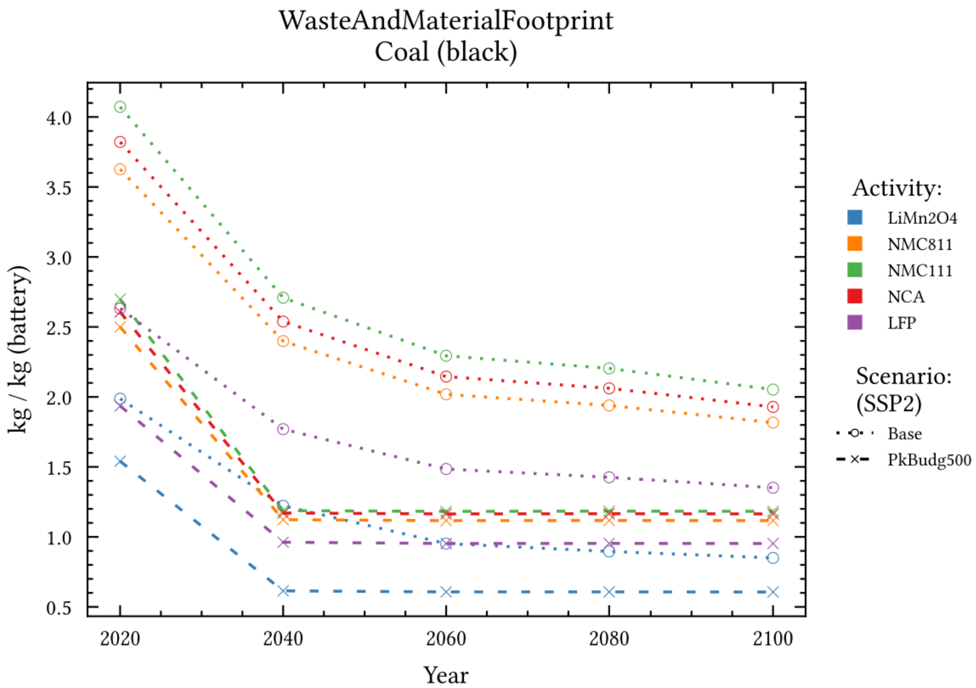
Figure 7: Contribution of industrial sectors to the liquid waste footprint of the NCA battery from 2020 to 2100 under the SSP2 scenario using the PkBudg500 RCP of the REMIND model. [TO BE IMPROVED!]

3.2.5. *Comparison with 'similar' LCIA methods*

A comparison of the results from T-reX's 'Coal (black)' demand method with the LCIA method 'EDIP 2003 - coal no LT' is shown in Figure 8. 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, the 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 8: 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.[TO BE IMPROVED!]

3.2.6. *Comparison with other studies*

Laurenti et al. (2023) used an alternative method for calculating the waste footprint of 1400 activities in the ecoinvent database 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 fraction, Laurenti et al. reported 95%, whereas T-reX 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 T-reX , the source database is deconstructed 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 waste generation and material demand are often strongly associated with the environmental impacts of human activities (Laurenti et al., 2023; Steinmann et al., 2017; Demirer, 2019), we consider it of high importance that they are included LCA accounting. Although there are existing LCIA methods that provide endpoint impact scores related to material demand and waste generation, they generally contain convoluted formulae or subjective weighting, or their complexity and lack of transparency can make them difficult to use and interpret (Swiss Federal Office for the Environment (FOEN), 2021; Hauschild and Potting, 2004; CEN (European Committee for Standardization), 2019; Arvidsson et al., 2020; Swiss Federal Office for the Environment (FOEN), 2021).

T-reX advances the state-of-the-art in LCA providing practitioners with 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 LCA databases in the `brightway` project have been processed with T-reX, 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 five Li-ion batteries presented in this paper demonstrated the utility, flexibility as well as some limitations of T-reX.

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

One current limitation of T-reX 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 that 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 the waste generated represents an actual loss of resources or environmental risk, or, for example, 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 is expected to be facilitated by the ever more detailed and disaggregated data that is seen in each successive release of ecoinvent (FitzGerald et al., 2023).

The utility of T-reX 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 inadequate adaption of the future background inventories. In particular, the inclusion of scenarios with future waste processing technology could greatly improve our predictions of waste and material flows and offer valuable insight into their potential impacts (Bisinella et al., 2024). 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'.

5. Conclusions

We have created 'T-reX', an extension to the `brightway` 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. T-reX can be easily customised by the user to calculate the footprints of other supply chain flows such as water, gas, and critical raw materials.

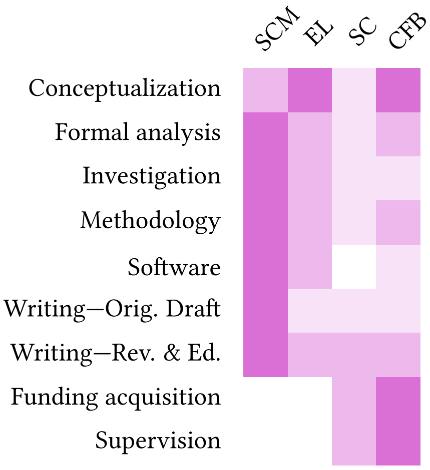
This work extends the state of knowledge by exploring the relationship between various waste aggregation methods and environmental damage indicators, contributing to a deeper understanding of life cycle waste inventories and their association with supply chain risk and potential environmental damage.

Data availability

All data used in this analysis are publicly available online under the noted sources.T-reX is installable via the Python Package Index (PyPI) and is available at https://pypi.org/project/T_reX_LCA. The full source code for T-reX 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

- **SCM**: Stewart Charles McDowall
- **EL**: Elizabeth Lanphear
- **SC**: Stefano Cucurachi
- **CFB**: Carlos Felipe Blanco



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 T-reX
5. Example of the terminal output of T-reX
6. Complete tabulated results of the case study
7. Complete visualisations of the case study

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