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Stew-McD/T-reX

Spotlights

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

- T-reX was developed to quantify waste and material footprints of activities in life cycle assessment (LCA) databases

- T-reX is an adaptable and extensible open-source Python tool complementing the `brightway` LCA framework and `ActivityBrowser`,

- T-reX can be used to identify pre-consumer waste generation and material demand hotspots often hidden in supply chains

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

Highlights

- T-reX, a new open-source program for quantifying waste and material flows in Life Cycle Assessment (LCA)

- Assesses supply risks by calculating demand inventories for critical materials

- Simplifies quantification of user-specified waste and material footprint categories

- Rapidly identifies hotspots of waste generation and material demand in supply chains

- Presents a case study of five lithium-ion batteries to demonstrate T-reX's utility

T-reX: Quantifying waste and material footprints in current and future Life Cycle Assessment (LCA) databases

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Abstract

The quintessential principle of the 'circular economy' is to minimise material consumption and waste generation. Thus, identifying and quantifying waste and material flows is critical. Life Cycle Assessment (LCA) is a powerful method for this, given its capacity to pinpoint hotspots of environmental impact throughout an activity's life cycle, where the implementation of circular principles could be most effective.

We introduce T-reX, a Python tool extending the brightway ecosystem, to allow 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 their potential environmental burdens. T-reX can aid sustainable decision-making and contribute to the development of '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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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
SDG	Sustainable Development Goals
SSPs	Shared Socioeconomic Pathways
T-reX	The Tool for analysing 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 central focus in the frantic pursuit of sustainability objectives and the imperative curtailment of our environmental footprint within planetary boundaries (??????). 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) (????). 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 (???).

The concept of the 'footprint' as an environmental sustainability indicator began with the Ecological Footprint (EF) (?) and after being popularised by the Carbon Footprint (CF) (?) the 'footprint family' has adopted many additional metrics—albeit without yet coalescing into a coherent or consistent framework (???). More recently, the footprint collection has been extended to include the Material Footprint (MF) (?), which is often encountered in the 'macro methods' of Industrial Ecology (IE), such as environmentally Extended Input-Output Analysis (EEIOA) (?) and Material Flow Analysis (MFA) (?). 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 the MF can be 'highly representative of damage to human health and biodiversity' (?) 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) (?).

Though steadily emerging (???), the incipient 'Waste Footprint' (WF) metric, in contrast, has yet to enjoy such noble recognition for its attempts to measure and classify the waste generated by human activities. While it seems obvious that reducing life cycle waste is critical to the development of the circular economy (??), the WF remains largely overlooked—especially in LCA models where waste itself is seldom apportioned any inherent environmental significance aside from the emissions related to its treatment (?). Such ignominious neglect strikes the authors as unjustified, given that it has been repeatedly demonstrated that WFs have a strong association with environmental damage (????). Additionally, it has been shown that the most vulnerable communities suffer disproportionately from the social and ecological impacts created by wasteful behaviours and sub-standard end-of-life treatment (??).

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 (????).

Life Cycle Assessment (LCA) is a useful method for the holistic estimation of the environmental impacts of

products and processes. LCA can comprehensively evaluate 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 (?) and CML (?)), 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' to predict the impacts of supply chains that have not yet been (and may never be) realised (??).

Several LCIA methods include, to some extent, waste generation (Swiss Eco-Factors, EDIP and EN15804) (???) and material consumption (Crustal Scarcity Indicator (CSI) and Swiss Eco-Factors (??)). 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) [English: environmental impact points] in the case of the Swiss Eco-Factors) (?).

1.1.1. Waste in LCA

Though often described simply as a 'material with a negative economic value' (?), waste is a nebulous concept, and one whose definition is poorly delineated and highly variable across space and time. From a systems perspective, the notion of waste is anathema to the 'circular economy', they cannot co-exist. From a practical economic viewpoint, the viability of an extensive waste processing system is highly dependent on precise knowledge (or at least, reasonable predictions) of material and waste flows, in addition to energy costs and the relative prices of virgin and secondary materials. Thus, as ? argues, waste must be 'thoroughly characterised' and '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 for predicting its life cycle externalities. There remains, however, a knowledge gap regarding WFs and their associated environmental impacts (?).

Conventional LCA database models consider waste as a 'service' (accounting for the treatment, not the material) (?) and typically use generic waste processing models (?) 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' (?). 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 ? has contributed significantly to

understanding the environmental impacts of waste treatment processes and the modelling of 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 (?). 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 (??). The environmental significance of waste and its correlation with other indicators has been the subject of extensive research. Studies have shown that popular resource footprints can cover a significant portion of environmental impact variance between activities (??). 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 (?). The aggregation of waste in PWFs raises concerns among LCA experts, regarding the uncertainties introduced, as well as the potential misrepresentation of environmental performance due to differences in waste types (??).

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 methods 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.

? developed a method to calculate the waste footprint of a product or service based on solving the demand vectors of the activities, while also proposing simple measures to quantify waste 'hazardousness' and 'circularity' with this data. The method presented, however, is limited in its scope and flexibility, is computationally intensive, difficult to use, and not easily reproducible. As the authors acknowledge, due to the way that exchanges are identified and 'tagged' this method also suffers from errors due to double counting. 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. 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 geo-political tension and a mineral-hungry 'renewable energy transition', ever greater attention is being given to the security of material supply—especially for those considered 'critical raw materials' (CRMs) (????????). 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.

The Crustal Scarcity (CSI) LCIA method was developed in order to introduce an assessment of the long-term global scarcity of minerals in LCA (?). 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` open-source LCA framework (?) and track these exchanges by translating them into inventory indicators and 'pseudo' LCA impact (LCIA) categories. T-reX is 'T(ool for) re-X' (reduce, reuse, recycle, etc.) and 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.

Integration with the `premise` Python package (?)—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 (?). Indeed, despite the ever more critical need to reliably model and future waste management systems, ? 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 requisite data and impact modelling remain 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 ?, ? 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 **??**, we describe the T-reX program, and in **??**, 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` (**?**). Additionally, the `wurst` package—which can deconstruct databases into a list of exchanges—is used to facilitate searching and data transformation at the exchange level (the individual supply chain flows) (**?**). Integration with the `premise` package (**?**)—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` (**?**)—an open-source graphical user interface for LCA—and after running T-reX, the manipulated databases and the 'pseudo-LCIA' methods created by T-reX can be used in the project in the accustomed way. T-reX is installable via the Python Package Index (PyPI) (**?**) and is fully open-source under the CC-0 licence. The full source code for T-reX is indexed on Zenodo (**?**) and under further development in the GitHub repository (**?**). T-reX is designed to be used with `ecoinvent` databases (**?**), 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 with which 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 a 'prospective' database based on future scenarios by implementing the premise `premise` with one of T-reX's internal modules.

The supplementary material in **??** 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 (**??**).

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 an 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 (?) and REMIND (?), which offer a range of options aligned with the Shared Socioeconomic Pathways (SSPs) (?) 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 flows of material and waste to be identified and categorised by the 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 mirrored '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 in ??. One advantage of T-reX is that it can identify 'hidden' waste exchanges that would otherwise be 'consumed' by a treatment process and not leave the technosphere. Since 'waste is not a service' (?), a characterisation factor of -1 is applied to the waste footprint methods (except CCS exchanges), changing the perspective from 'waste consumed by treatment' to 'waste generated by the activity'.

In addition to the waste categories, T-reX can incorporate any number of material demand categories, the defaults being based on the EU Critical Raw Materials (CRM) list for 2023 (?), which contains 30 materials considered essential to the EU economy and also at risk of supply disruption. Especially valuable in the case of CRMs is T-reX's ability to uncover and quantify these threads of background consumption, which can be inconspicuously embedded in products or consumed in seemingly distant supply chain activities. The identity of the materials considered and their categorical groupings are easily customisable by the user, and in further materials of interest to the authors were added to the example Li-ion case study, including helium, electricity, petroleum, sand, water, and natural gas. The full list of 59 materials included in the default configuration is provided in the supplementary material in ??.

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 relevant 'market activities' for the material of interest rather than keywords in the exchange's name. A useful feature of 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.

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 ??, 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. 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.

An overview of the T-reX workflow is presented in ??. The supplementary material in ?? contains a more detailed computational flowchart.

Figure 1: The workflow of T-reX presented in a generalised (a) and computational (b) format. 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.

The T-reX tool for LCA

a. Generalised method

b. Computational method
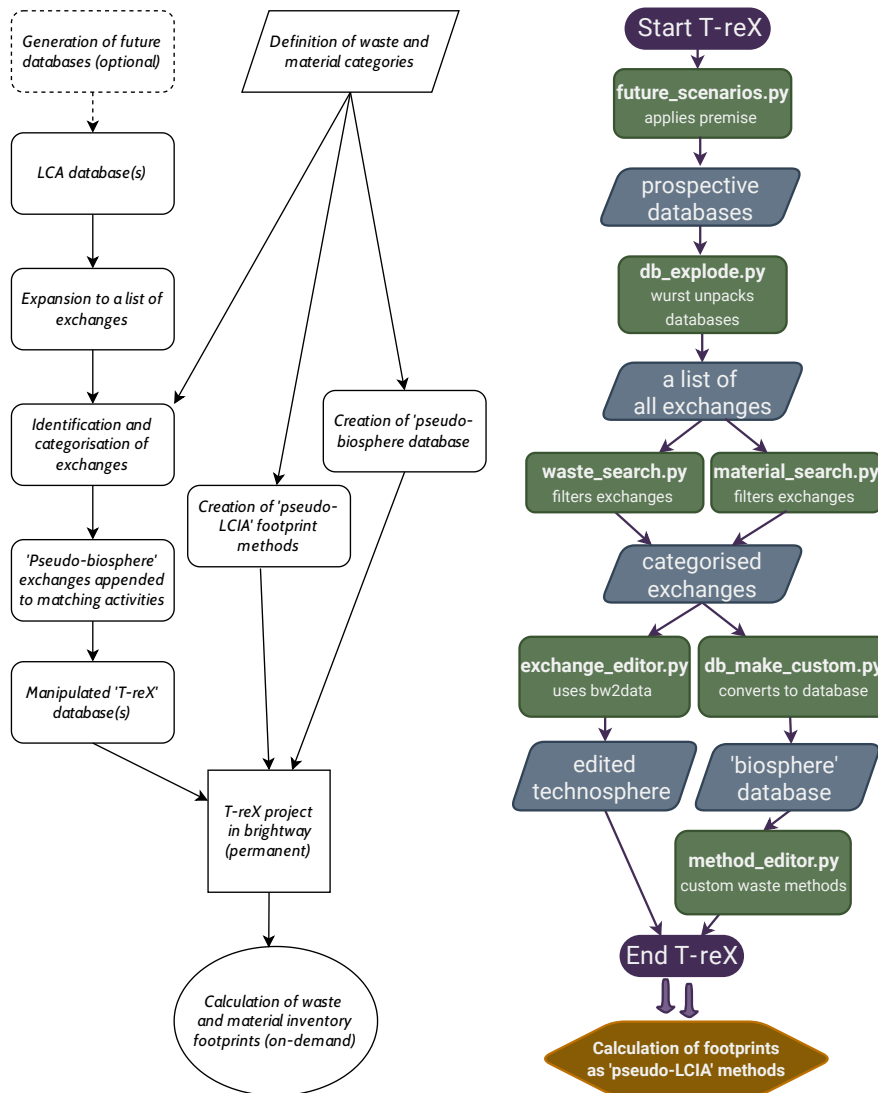
262 *2.2. Case study methodology*

263   We investigated five types of Li-ion batteries in the `ecoinvent` 3.9.1 'cutoff' LCA database (**?**), each represented

264 by their unamended global market inventories:

- Li-ion, LFP, rechargeable, prismatic

- Li-ion, LiMn$_2$O$_4$, 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 (?)

Additional to the present-day databases, T-reX created prospective database sets based on `ecoinvent` 3.9.1 using the functionality of `premise` with 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℃ increase in global temperatures to 2100

- SSP2-PkBudg500: representing the achievement of Paris climate goals, ca. 1.3℃ increase to 2100

For each pathway, databases (at five-year time intervals) were created with `premise` (?) 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 (?), 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 footprints.

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 in ??. The manipulated `ecoinvent` databases, which are the main product of T-reX, can be recreated by following the instructions in the package documentation (?).

3.2. Case study: Li-ion batteries

As described in ??, this case study calculated the waste and material footprints (with a variety of other indicators) for the unaltered background 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 material (??). Because the 'pseudo-LCIA' methods created by T-reX are integrated into the user's `brightway` project as if they were standard LCIA methods, the footprint 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

?? presents a Sankey diagram depicting the supply chain flows of 'total solid waste' attributed to the NMC 811 Li-ion battery at the global market in the `ecoinvent` database version 3.9.1. As the supply chains are expansive, this visualisation has been greatly simplified for print, the full version is included in the supplementary material ??. As is evident in the figure, the largest contributors to the waste footprint are the extraction and processing of the raw materials, with the largest flows coming from the extraction of cobalt, lithium, and nickel. Due to the nature of LCA, the waste flows do not represent the 'real' physical flows directly, but rather an abstraction thereof based on, in this case, economic allocation—the market price of the functional unit produced by the activity (?). If an unallocated database were available, the waste flows could be calculated with T-reX in the same way and be more directly related to the physical flows of the activities.
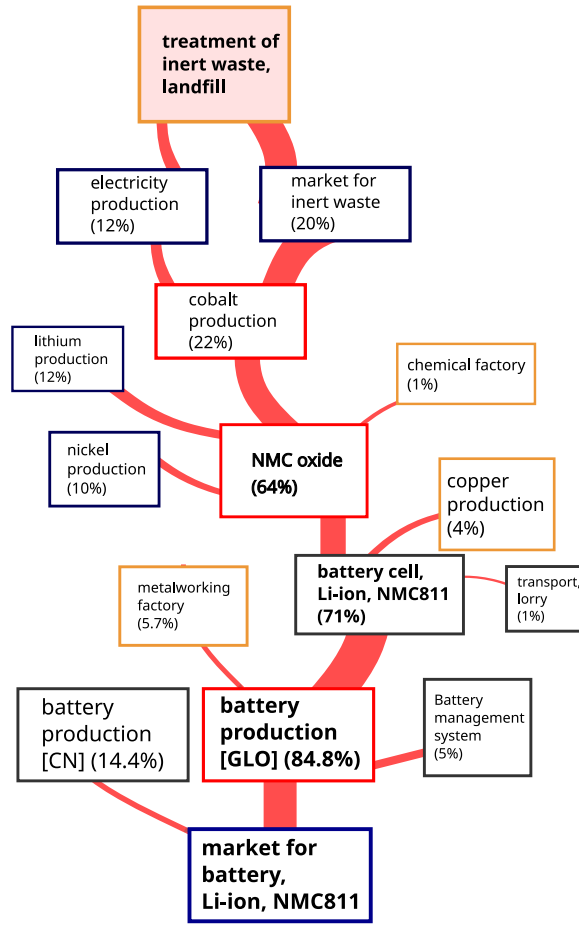
Figure 2: A simplified Sankey diagram showing the total solid waste footprint flows for the NMC 811 battery supply chain at the global market in the `ecoinvent` database version 3.9.1.

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

?? (a) 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 $LiMn_2O_4$ battery has the smallest footprint, producing less than 4 kg of waste per kilogram of battery. In each case, there was only a slight downward trend in the waste footprints between 2020 and 2100. This is mostly in the period between 2020 and 2040 and could be attributable to the relatively rapid decrease in fossil-fuel use that is factored into the models over this time (since many produce relatively large amounts of waste during extraction and combustion). For the total waste generated by these batteries, there was very little difference observed between the baseline and PkBudg500 RCPs.

The inclusion of carbon capture and storage (CCS) in the prospective databases is apparent in ?? (b), with the rapid increase in the production of carbon dioxide 'waste' over the period from 2020–2040 that is not seen in the baseline

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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 (**?**), far short of the levels projected in many of the RCP scenarios (**?**). The authors consider that the over representation of CCS and the under representation of waste processing technologies in the prospective databases is one significant limitation to the validity of prospective LCA databases.
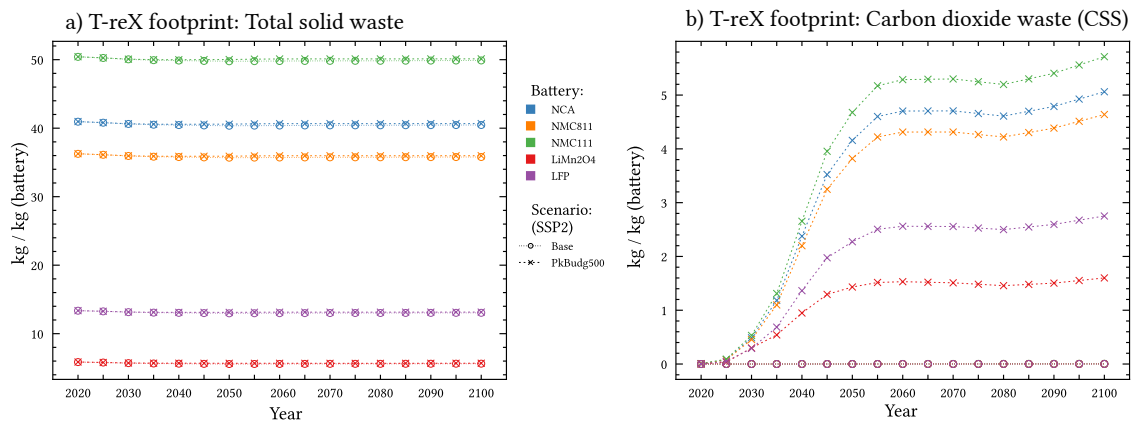

Figure 3: T-reX calculated supply chain inventories for the five Li-ion batteries in the case study, showing their 'footprints' for: (a) total solid waste, and (b) carbon dioxide waste (from carbon capture and storage (CCS) only). The footprints were modelled with prospective LCA databases from 2020 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

?? shows the contribution of the 'top-processes' to the graphite footprint of the $LiMn_2O_4$ battery under the baseline scenario from 2020–2100. The total footprint is seen to more than triple, from 0.16 kg/kg in 2020 to 0.52 kg/kg in 2050 and onward to 2100. The largest contributor is not, in this case, the battery-embedded graphite electrode (which is the second top process), but 'silicon production' from further up in the supply chain. This result is likely a reflection of the electrification of the transport and energy sectors that is included in the REMIND model. The results of this kind of analysis with T-reX can be used to identify the most significant processes in the supply chain and to target interventions to reduce the potential environmental impact of production.
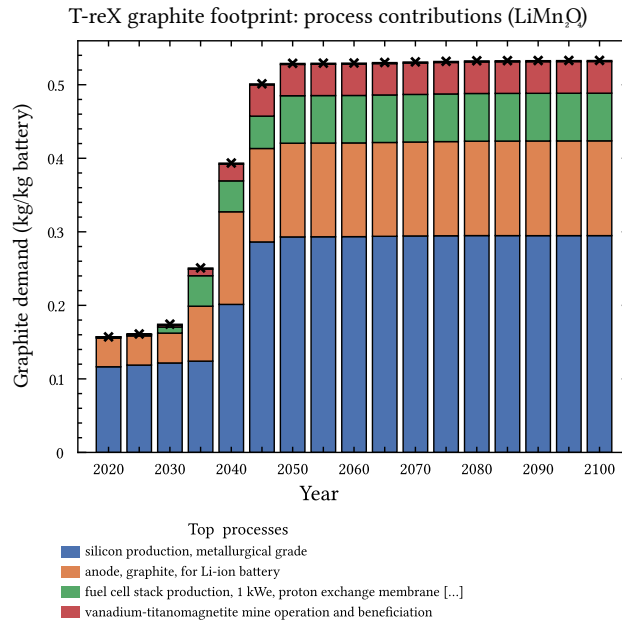
Figure 4: Contribution by the 'top-processes' to graphite demand inventory of the LiMn$_2$O$_4$ battery from 2020 to 2100 under the SSP2 scenario using the baseline RCPs of the REMIND model.

3.2.4. Contribution of industrial sectors in the supply chain

?? shows the contribution of sectors (grouped by CPC codes) 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 8% in 2100, while over the same period the contribution of the sector '46430: Parts of primary cells, primary batteries and electrodes' increases from 32% 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.
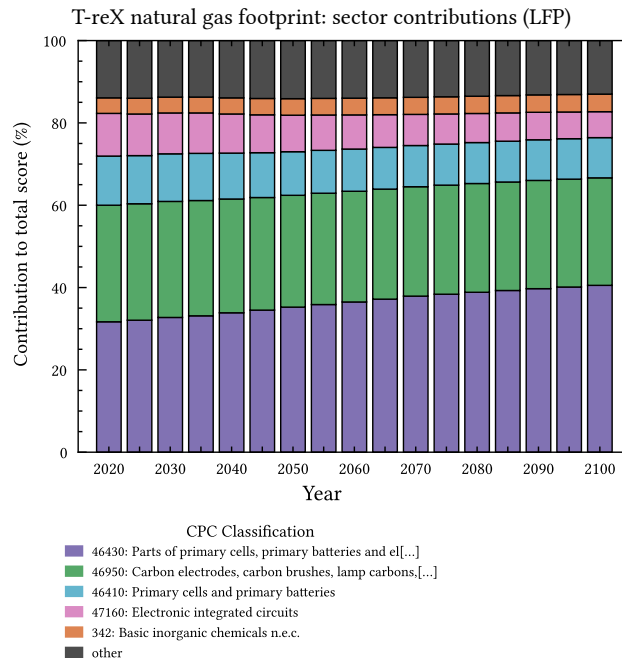
Figure 5: Contribution of industrial sectors to the natural gas footprint of the LFP battery from 2020 to 2100 under the SSP2 scenario using the baseline RCP of the REMIND model.

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 ??. 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.,economic allocation) that are generally embedded in LCA databases.
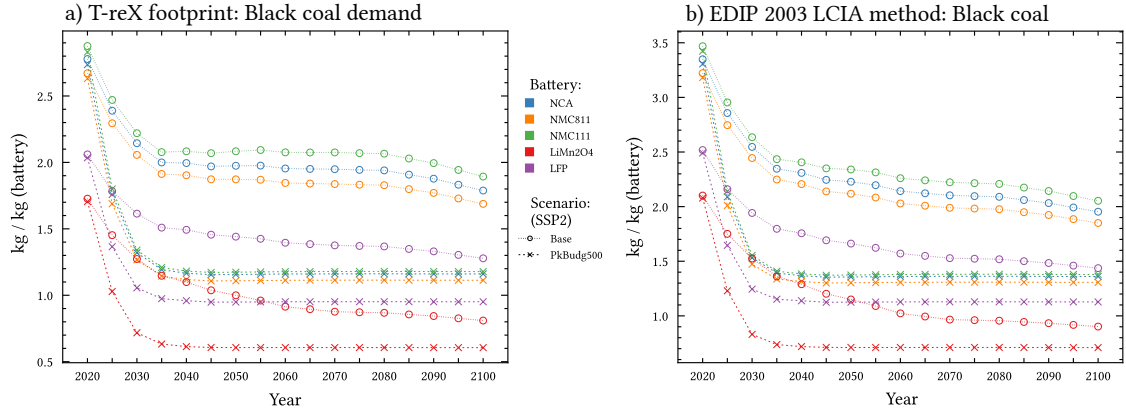
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a) T-reX footprint: Black coal demand

b) EDIP 2003 LCIA method: Black coal

Figure 6: Comparison of the (a) 'T-reX - Coal (black)' demand footprint with the (b) conventional LCIA method 'EDIP 2003 - coal no LT' in the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model for all five batteries.

3.2.6. Comparison with other studies

In the most similar published method, **?** used an alternative procedure for calculating the waste footprint of $\tilde{1}400$ activities in the `ecoinvent` database version 3.5. Direct comparison is not possible, as this database contains only one generic Li-ion battery, '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. **??** 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 the 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 1: 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 **?** (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

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4. Discussion

Waste generation and material demand are strongly associated with the environmental impacts of human activities (???), and thus must be represented in LCA accounting. Although there are existing LCIA methods that provide endpoint impact scores related to material demand and waste generation, they contain convoluted formulae or subjective weighting, or their complexity and lack of transparency can make them difficult to use and interpret (?????).

T-reX advances the state-of-the-art in LCA by 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 (and re-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, and limitations of T-reX.

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 present and future supply chains were trivial to calculate. Additionally, visual exploration in `ActivityBrowser` was possible as the T-reX 'pseudo-LCIA' methods are structurally identical to standard LCIA methods when integrated within the `brightway` project.

One 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 information is required 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 methodical classification of waste exchanges and end-of-life fates is expected to be facilitated by the increasingly detailed and disaggregated data in each successive release of `ecoinvent` (?).

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 (?). As demonstrated in the results of the case study—where there were often very few scenario-temporal changes in many waste and material footprint indicators—the utility of prospective LCA is restricted if there is inadequate adoption of 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 (?). 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

T-reX is an extension to the open-source `brightway` ecosystem that enables users to calculate the waste and material footprints of any product or service in an LCA database. It 'explodes' and reconstructs the database to identify and edit waste and material exchanges and writes matching custom 'pseudo' LCIA methods. These exchanges are mirrored in the `brightway` project as 'pseudo-biosphere' flows and thus, the waste and material footprints of any other supply chain flow of interest, such as water, gas, or critical raw materials, can be calculated similarly to existing LCIA methods.

T-reX elucidates the complex relationships between material demand, waste generation, and environmental impacts. This instrument enables detailed exploration of 'footprints' and life cycle inventories—modelled externalities of human activities—and examines their connections to supply chain risks and potential environmental damage. T-reX is a step towards a better understanding of these interconnections for the practical realisation of 'sustainability' and the 'circular economy'.

Data availability

All data used is publically available online under the noted sources. T-reX is fully open source and dedicated to the public domain under the CC-0 licence. It installable via the Python Package Index (PyPI) under the name 'T_reX_LCA' https://pypi.org/project/T_reX_LCA. The full source code for T-reX is archived by Zenodo at https://zenodo.org/records/10925359 and the development server is hosted by Github at https://www.github.com/Stew-McD/T-reX. A user guide with comprehensive documentation are presented at https://T-reX.readthedocs.io.

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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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6. Supplementary material

The supplementary material supplied with this manuscript 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

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4. Modular flowchart of T-reX

5. Example of the terminal output of T-reX

6. Example of the terminal output of the case study

7. Complete tabulated results of the case study

8. Complete visualisations from the case study