Resources, Conservation & Recycling

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

--Manuscript Draft--

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Abstract:	The circular economy aims to minimise material consumption and waste generation, making the identification and quantification of waste and material flows critical. Life Cycle Assessment (LCA) is a key method for this, as it evaluates an activity's entire life cycle, guiding circular practices effectively. To support these goals, the authors developed *T-reX*, a Python-based LCA tool extending the capabilities of *Brightway* and *Premise*. T-reX quantifies supply chain demands for current and future scenarios, streamlining database manipulation and integrating methods to uncover hotspots of hidden risk. A case study on lithium-ion batteries highlights T-reX's potential, revealing their waste and material footprints. As such footprints often correlate with negative externalities, T-reX provides valuable insights to support sustainable decision-making. By enhancing our understanding of material flows and waste, T-reX contributes to advancing the circular economy.
Response to Reviewers:	I have produced manuscripts from the source .tex in various formats showing changes. There is a preprint, typeset in the journal style, and and a latexdiff. The EM system seems not to be aligned.

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Editors
Resources, Conservation and Recycling
Elsevier

Dear Editors,

We are pleased to submit our original research article titled "T-reX: Quantifying waste and material footprints in current and future Life Cycle Assessment (LCA) databases" for consideration by *Resources, Conservation and Recycling*. This manuscript details the development and application of an innovative tool designed to improve the quantification of waste and material flows, an essential aspect of progressing towards sustainable resource management and circular economy objectives.

Our submission provides a comprehensive description of the tool, which integrates seamlessly with the `brightway` framework to offer a user-friendly and adaptable solution for LCA practitioners. By automating data analysis and aggregation processes, our tool expedites the identification of environmental hotspots within supply chains, thus facilitating more informed decision-making.

We believe our manuscript is an excellent fit for *Resources, Conservation and Recycling* due to its potential contribution to advancing resource conservation and recycling methodologies. The case study presented, focusing on battery supply chains, underlines the tool's practical utility and potential impact on sustainable resource management practices.

The manuscript complies with the journal's requirements for an original research article, having a word count of 4969, including four figures and two tables.

We have no conflicts of interest to declare and have ensured that this work is original, has not been published previously, and is not under consideration by any other publication. All authors have agreed to this submission and are collectively responsible for its content.

We suggest the following reviewers for their expertise relevant to our manuscript's focus:

1. Rafael Laurenti, IVL — Swedish Environmental Research Institute, rafa@kth.se
2. Valentina Bisinella, DTU — Technical University of Denmark, valenb@dtu.dk
3. Chris Mutel, Cauldron Solutions and brightway, cmutel@gmail.com

Thank you for considering our manuscript for publication. We look forward to the opportunity to contribute to *Resources, Conservation and Recycling* and eagerly await your response.

Sincerely,

S McDowall

Stewart Charles McDowall — on behalf of Elizabeth Lanphear, Stefano Cucurachi, and Carlos Felipe Blanco

Declaration of interests

☒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.

☐The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

T-reX manuscript revision

Response to peer review

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  - S.C. McDowall
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Dear reviewers, editor,

We the authors of T-reX would like to thank you for the time and attention that you have generously contributed to the review of our manuscript. We are especially grateful for the extensive and constructive commentary. We have addressed each of your comments in the following text, and have made the necessary changes to the manuscript. We hope that you find the revised manuscript to be satisfactory.

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1. Reviewer One

"I think that this manuscript needs to be ameliorated."

Summary of review

- More detail for case study requested, also sensitivity/uncertainty analysis
- Comment 1.1: system boundary
- Comment 1.2: input-output data
- Comment 1.3: material footprint data (more discussion, and 'overall material footprint')
- Comment 1.4: sensitivity analysis or uncertainty analysis

Author responses

General response As the reviewer points out, the case study could, indeed, benefit from more detail. Additional explanation has been added to the main text and there is detailed discussion in the supplementary information (especially appendices 3 and 4). Furthermore, the complete datasets are publicly available on Github and Zenodo. The case study was included only to demonstrate some potential use cases of T-reX and not to provide a comprehensive waste and material footprint analysis of the Li-ion battery market. This is detailed in the abstract, as well as subsection 2.2 of the methods and 3.2 of the results. The case study is not intended to be intensive or exhaustive and the results are not intended to be used for decision-making purposes. The authors intent is for the focus of the paper to be on the T-reX program itself.

Specific responses

Reviewer comment 1.1 - Case study system boundary "*The system boundary of the case study should define, and it can be shown more clearly by adding diagrams.*"

Author response 1.1 - Case study system boundary A figure could be added to the supplementary information to illustrate the system boundary of the case study. However, given the limitations on space, and that the authors feel it would not add any pertinent information. The system boundary is very simple, as defined in the text (methodology section 2.2). That is, exactly the inventory of the Li-ion battery markets as modelled in ecoinvent version 3.9.1. Essentially, a single market activity for each battery, to serve as a basic example.

Reviewer comment 1.2 - Input-output data "*No input-output table provided for the case studies. Please provide this inventory data in the manuscript.*"

Author response 1.2 - Input-output data As described in the methodology section (subsection 2.2), the inventory data is taken directly from the respective activities in the ecoinvent database (version 3.9.1). The input-output data used in the case study is directly that given by the ecoinvent database, without amendment. Full details are provided in the supplementary information of this manuscript (appendix 3 and 6) and complete data is available in the Github and Zenodo repositories.

Reviewer comment 1.3 - Material footprint data *"Result and Discussion section; this study was present some part of material footprint. I recommend further discussions and interpretation the result. In addition, it is necessary to present the overall material footprint of battery."*

Author Response 1.3 - Material footprint data As is mentioned throughout the manuscript, the material footprint results calculated by T-reX are aggregations of the exchanges in the model system that are targeted by the user's search criteria (in this case, a default selection of 59 materials and their flows as presented by the ecoinvent database and listed in appendix 3, sub section 2 and 3). The authors believe that it would be misleading to present the reader with a 'total material footprint' based on the sum of the material footprints of the individual materials, as the LCA models only represent certain aspects of the system. A 'total material footprint' without respect for the nature of the material is meaningless, and indeed, one of the strengths of T-reX is to allow the user to pinpoint the materials of interest to them.

Reviewer comment 1.4 - Sensitivity analysis and uncertainty analysis *"Authors should also perform the sensitivity analysis or uncertainty analysis."*

Author response 1.4 - Sensitivity analysis and uncertainty analysis Indeed, this is something that also could be done, and may yet make and interesting extension for the next study. However, given that the data for the batteries in this case study is taken directly from the ecoinvent activities and offered as a rudimentary example of the programme's utility, the authors believe that a sensitivity or uncertainty analysis on the case study results is not called for. The authors believe that the presentation of this could be distracting from the message of the paper. For clarity, however, the authors have added further to the discussion on the limitations of the case study results (paragraphs 4-6 and subsection 4) to make this more apparent to the reader.

Reviewer Two

"The manuscript is well-written and presents a clear argument. I had a few minor suggestions."

2. Reviewer Two

Summary of this review

- Expand comparison with existing methods
- Simplify some of the language
- Expand on the future developments and applications of T-reX
- Include higher resolution version of graphical abstract

Specific responses

Reviewer comment 2.1 - To expand on the comparison with existing methods *"To clearly communicate the novelty of this work, the author may* *consider emphasizing explicit Comparison with Existing Methods. Although section 3 has comparisons, it's hard to tell the differences between T-rex with the existing LCIA methods (i.e CO2 emissions/waste). Providing a detailed comparison of T-reX with existing LCA and LCIA methods will be helpful to justify the novelty."*

Author response 2.1 - To expand on the comparison with existing methods As the reviewer correctly points out, there are many similarities between the inventory footprints calculated by T-reX, and that of some exiting LCIA methods. Indeed, the choice of the term 'pseudo-LCIA' is derived from this, because the calculation strategy is very similar to LCIA methods in general. Apart from the added functionality of T-reX, one main difference lies in directness of T-reX aggregations, with comparison to the abstracted methods such as Crustal Scarcity Potential, for example. The authors have expanded the comparison with existing methods by adding more specific details in the relevant sections. In the introduction, this is subsection 1.1 (paragraphs 3-5) and 1.2.1 (paragraph 3). In the methodology, this is 2.1.2, paragraphs 6-7 and section 3.3.2 paragraph 3. In the results section, this is subsection 3.2.5 and 3.2.6. In the discussion, this is first two paragraphs (lines 389-411). Additionally, appendix 3, section 3.3.2, paragraph 3 and 4 cover this in more detail and some of this material has been brought forward to the methods section for more prominence (subsection 2.1.2 paragraph 7-8).

Reviewer comment 2.2 - To simplify some of the language *"There are sections where the language can be simplified for better clarity without losing technical precision. For example, the abstract succinctly summarizes the study. However, consider adding a sentence on the main findings from the case study to give a complete overview. The phrase"frantic pursuit of sustainability objectives" in the introduction could be toned down to "dedicated pursuit of sustainability objectives" for a more neutral tone"*

Author response 2.2 - To simplify some of the language The authors have restructured the abstract to include more reference to the case study (paragraph 3). Additionally, the language in the text has been amended to improve clarity and purvey a more neutral tone, particularly the first sentence of the abstract and the first paragraph of the introduction.

Reviewer comment 2.3 - To expand on the future developments and applications of T-reX *"A discussion on potential future developments and applications of T-reX will be helpful"*

Author response 2.3 - To expand on the future developments and applications of T-reX The authors have expanded the discussion on potential future developments and applications of T-reX in the discussion section (paragraphs 4 and 5). The authors hope that this will provide the reader with a better understanding of the potential of T-reX, as well as its limitations and their relation to some of the challenges in our field, most notably, the need for more comprehensive and reliable data on which to build our models.

Reviewer comment 2.4 - The graphical of abstract *'low resolution figure is hard to read'*

Author response 2.4 - The graphical of abstract The publication portal rendered the resolution of the graphical abstract in this way. It was an unfortunate oversight from the authors not to correct this in the initial submission. The graphical abstract in is now also available in various formats and resolutions in the portal submission as well in the online material that is available with the software.

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3. Reviewer Three

"I think that the paper presents an interesting and novel method to assess waste generation and consumption of material in systems, but some aspects need a more extensive explanation."

Review summary

- Clarification on the difference between T-reX and LCI
- Clarification on the terminology 'pseudo-LCIA'
- Clarification on the single score calculation of T-reX

Major comments

Reviewer comment 3.1 - Clarification on the difference between T-reX and LCI *"Lines 105-106: I can understand the difference between the T-reX method and the results that one can derive from the LCI analysis (i.e. the list of elementary flows associated with the system under analysis) in the case of waste, because, as you said, T-reX considers also waste flows that are treated, but what about material flows? Why should T-reX results be different from those that one can obtain by the LCI analysis? This point remains unclear to me even after reading the entire paper."*

Author response 3.1 - Clarification on the difference between T-reX and LCI One significant difference, and a highlight of the method of the T-reX program is how it makes it easy to identify "hotspots" and perform contribution analysis. Furthermore, the strength of T-reX is to make these calculations simple and easily repeatable (in the way that the databases are manipulated, and the footprints calculated as if they were LCIA methods). The as described in the response to reviewer two, the relevant sections have been refined with the aim of more clearly communicating these differences.

Reviewer comment 3.2 - Clarification/replacement of the terminology 'pseudo-LCIA' *"Line 213: I think that T-reX is a method to perform the interpretation of the LCI results, it does not evaluate impacts; as it is correctly reported in lines 409-410, T-reX method calculates waste and material inventory footprints, so the terminology"pseudo-LCIA" is in my opinion misleading (even if there is the "pseudo") and it should be replaced with e.g. "LCI interpretation" method."*

Author response 3.2 - Clarification/replacement of the terminology 'pseudo-LCIA' Following from the response to the previous comment, the authors agree that the distinction between LCI and LCIA is critical and the text has been refined so as to make this more explicit. The choice of the term 'pseudo-LCIA method' derives from the fact that the T-reX methods are integrated into the code in the same way as LCIA methods. This structure allows for a more user-friendly calculation of these LCI results, being customisable and easy to implement in existing frameworks. The authors have rephrased the relevant sections of the text to make this distinction more clear to the reader.

Reviewer comment 3.3 - Clarification on the single score calculation of T-reX *"Line 300: please say how the single score is calculated for T-reX evaluation. Results section: as in a standard LCA, the results should be reported before starting with their interpretation, so please consider adding here for the analysed systems some of the results in absolute terms. This will really help the reader to understand the type of output that can be achieved with T-reX method."*

Author response 3.3 - Clarification on the single score calculation of T-reX

As the reviewer correctly points out, the phrase "single score" is not clear, and could mislead the reader. T-reX gives a "single score" only in the sense of calculating an aggregate of the particular waste or material streams associated with the production of a given functional unit (in the case study, one kg. of various batteries). The language in subsection 2.2.1 'LCA calculations' was amended to more explicitly convey this point, and further, to better explain the results presented in the case study. The phrase "single score", was replaced with total summation which the authors believe conveys a more specific and appropriate description of the waste and material inventory results. The sentence now reads *"For each combination of activity, method, and database, a total summation was calculated along with details of the top contributing processes."*

Minor comments

Reviewer comment: *"In general, when you refer to the SM section 6, please indicate also the sub-section."*

Author response: The reference to the subsection was incorrect, there is no subsection to appendix 6. This has been corrected in the revised manuscript

Reviewer comment: *"In general, try to avoid putting words in " and use this only when it is strictly necessary (e.g. line 433: why did you write 'circular economy' and not simply circular economy?)"*

Author response: This has been corrected in several places in the revised manuscript.

Reviewer comment: *"Line 128: what do you mean with"generic waste processing models"? e.g. models that do not take into consideration the type of waste? Usually, databases include different treatment processes for the different types of waste, so please explain what you mean."*

Author response: This sentence has been rephrased in the revised manuscript (line X).

Reviewer comment: *"Line 227:"the waste categories include incineration, recycling": do you mean "the waste categories include waste sent to incineration, recycling"?"*

Author response: Yes, that was the intended meaning. This has been corrected in the revised manuscript (2.1.2 paragraph 4).

Reviewer comment: *"Lines 230-231:"a characterisation factor of -1 is applied to the waste footprint methods": what do you mean? Usually, a CF is given to a flow."*

Author response: This sentence has been removed. Being somewhat technical, it has not a general relevance, and could be confusing, perhaps. The previous phrasing stems from the way that methods are constructed in the brightway code, where the characterisation factor is embedded in the method as a parameter. This is then applied to the relevant flow in the LCIA, as you correctly point out. The -1 corrects the perspective to be that of waste produced and not on the treatment services (as in "Waste is not a service", Guinee 2021).

Reviewer comment: *"Line 231: please explain the acronym CCS"*

Author response: Yes. Thank you for pointing out the oversight. The expanded form of CCS has been moved to the first mention of carbon capture and storage in the text and the acronym has been added to the list of abbreviations in the front matter.

Reviewer comment: *"Table 4 of the SM: there is sand but not gravel: why?"*

Author response: There is no reason that gravel could not be included, the user of T-reX can decide on the material and waste streams of interest to them. The list of materials included in the default configuration of T-reX is based on the list of critical raw materials and then expanded to include other materials commonly deemed strategic or important. Some were added solely based on the interest of the authors (thus, sand and not gravel). The list is not supposed to be exhaustive or comprehensive and can be expanded or condensed by the user at their will. Instructions for configuration are included in the documentation of the software in its GitHub repository.

Reviewer comment: *"Line 247: which are the methods are you referring to?"*

Author response: This paragraph has been changed to make a more specific reference to the existing LCA methods (such as the Crustal Scarcity Indicator) that are described initially in the introduction (subsections 1.2.1 and 1.2.2). The textual connection was lost due to restructuring.

Reviewer comment: *"Lines 251-253: T-reX does not calculate impacts, so what do you mean with"including non-direct impacts on the market such as co-production of other materials"?"*

Author response: The word "impacts" has been replaced with "effects" to avoid confusion (subsection 2.1.2, paragraph 8).

Reviewer comment: *"Lines 255-257: are you referring to the cases where the mining of one material is done together with the extraction of another material? Please say more explicitly the situations are you referring to."*

Author response: Covered in the next response.

Reviewer comment: *"Lines 258-260: where exactly can the reader see this aspect in sub-section 3.2?"*

Author response: As the reviewer suggests, co-production is one example of such a situation. It was previously intended to include a more detailed exploration of this through the example of nickle metal production, however, due to space constraints, this data will not be in the main section of the manuscript, but is discussed in more detail in the supplementary material (appendix subsection 3.2.2, paragraph 2).

Reviewer comment: *"Line 260 and line 382:"substitution": substitution of what?"*

Author response: This has been clarified in the text to be more explicit (subsection 3.2.1). The term “substitution” here refers to the subtraction of co-products from the system in question (those which are not the functional unit) using the standard LCA methodology.

Reviewer comment: *“Lines 289 and 290: LT stays for what?”*

Author response: “LT” stands for “long term”. The abbreviation has been replaced by the complete word (subsection 2.2, second list).

Reviewer comment: *“Line 303-305: this sentence is not clear to me. Please consider rephrasing it.”*

Author response: Indeed, the reference to the graph traversal algorithm used in brightway was not clearly explained here. The text has been revised to improve on the description of the calculation methodology (subsection 2.2.1).

Reviewer comment: *“Lines 322 and 332: the title includes both waste and material but then nothing is said about the material inventory footprint in the sub-section.”*

Author response: Yes, only one example was given to illustrate this type of result as the method and the form is identical for both waste and material inventory footprints. This has been made explicit in the text (subsection 3.2.1). The caption now reads *¨Sankey visualisation of flow inventory footprints”*

Reviewer comment: *“Figure 2: if I consider arrows that enter the cobalt production box, I have 12% + 20% that is more than 22% (cobalt box): why?”*

Author response: I have revised this figure (2) and added much more descriptive text. The Sankey diagram shown in is a greatly abridged and simplified version of that produced by using T-reX with the ActivityBrowser software. The full Sankey diagram is far too large and complex to print. Examples of these diagrams are included in their full forms in the supplementary information (appendix 8).

Reviewer comment: *“Figure 2 caption: here you say that the diagram shows the total solid waste footprint but at the top of the diagram I see the box”treatment of inert waste, landfill”, so I do not understand how to read the diagram.”*

Author response: *Figure 2 and its caption have been amended to portray a clearer depiction of the result that the authors are trying to present here. As in the response to the previous comment:*
, the complexity of these flows make it challenging to contain them in a printable figure.

Reviewer comment *"Line 343: what do you mean with"carbon dioxide waste"? Is it not better to call it "waste from CCS"?"*

Author response: *As suggested, the text has been revised to replace "carbon dioxide waste" with "carbon dioxide waste from CCS". And in the caption, to Figure 3(b) "carbon dioxide waste (produced from carbon capture and storage (CCS) only)".*

Reviewer comment: *"Figure 3b: CCS instead of CSS?"*

Author response: Yes, this typographical error has been corrected in the revised manuscript.

Reviewer comment: *"Line 370: I think that"T-reX Coal (black) demand method" should be replaced with "Coal (black) demand of T-reX method". The same consideration is valid for the EDIP method (EDIP is the method, "coal no LT" is one of the results of the method)."*

Author response: This phrasing has been amended as suggested by the reviewer (subsection 3.2.5 and Fig 6)

Reviewer comment: *"Lines 373 and 374: natural gas is given as example of fossil fuel related methods and zinc for metal demand methods, but natural gas and zinc are just elementary flows and not methods. So please use the correct terminology."*

Author response: The terminology has been corrected to be more clear (subsection 3.2.5).

Reviewer comment: *"Lines 422-423: how can a waste represent a loss of resources or an environmental risk? Please explain it better, maybe adding some examples."*

Author response: The message here about the importance of knowing the specific nature and context of what is described as a waste flow in the LCA databases is of fundamental importance in the interpretation of the results obtained from T-reX. This paragraph has been revised to better explain this point (lines X-Y).

Reviewer comment: *"Lines 436-437: I didn't understand the second part of this sentence. Please consider rephrasing it."*

Author response: This sentence has been rephrased in the revised manuscript make the database manipulation process more clear to the reader. "explode" has been replaced with deconstruct. The second sentence of the conclusion now reads *"It deconstructs, manipulates and reconstructs the database to identify and edit waste and material exchanges. . . "*

Reviewer comment: *"Line 443: it does not seem to me that T-reX"examines their connections so supply chain risks and potential environmental damage": T-reX gives simply an overview of waste generated and materials consumed."*

Author response: Agreed. It was intended to convey that T-reX can aid the user in this examination by facilitating the generation of specific inventories.The final paragraph of the conclusion has been amended to soften this language and be more specific about what T-reX can do.

—-

On behalf of all of the authors of T-reX, I would like to extend once our gratitude, the review process was very thorough and I think it has resulted in significant improvement to the manuscript.

All the best,

S.C. McDowall

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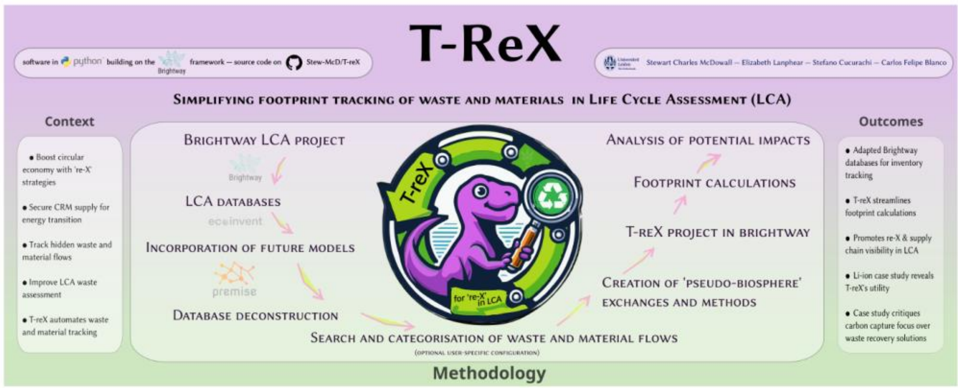
Graphical Abstract

 Click here to view linked References

Graphical Abstract

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

Stewart Charles McDowall, Elizabeth Lanphear, Stefano Cucurachi, Carlos Felipe Blanco



Highlights

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

Stewart Charles McDowall, Elizabeth Lanphear, Stefano Cucurachi, Carlos Felipe Blanco

- T-reX, a new open-source program for waste & material footprints 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 potential

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

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

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ARTICLE INFO

Keywords:
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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 quantitative method for this, especially given its capacity to expose the details of an activity's entire life cycle, often guiding the implementation of circular principles to where they could be most effective.

Pursuant to these goals the authors have developed 'T-reX', an analytical tool for LCA, written in Python. T-reX extends on the existing computational ecosystem centered on `Brightway` and `Premise` and can facilitate the quantification of user-defined supply chain demands for activities in current and prospective scenarios. T-reX streamlines database manipulation for LCA practitioners, integrating methods to aggregate and analyse demand inventories that could expose hotspots of hidden risk.

With a simple case study using lithium-ion batteries, we demonstrate some of T-reX's potential by detailing and exploring aspects of their waste and material footprints. Since such footprints are often linked to negative externalities, T-reX could support sustainable decision-making and contribute to the development of the circular economy by promoting the understanding of our material consumption and waste generation.

1. Introduction

1.1. Introduction to T-reX

The development of a circular economy has become a central focus in the pursuit of sustainability objectives toward 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'v 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 geopolitical tensions in an ever more globalised world have highlighted the vulnerability of many advanced economies to intentional supply disruptions—wrought as an act of competition or even outrighthostility (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' 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 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 the 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).

Though steadily emerging (Laurenti et al., 2016; Demirer, 2019; Guillotreau et al., 2023), the 'Waste Footprint' (WF) metric is less well-developed. While it seems obvious that reducing life cycle waste is 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 environmental significance aside from the emissions related to its treatment (Laurenti et al., 2023). Such neglect strikes the authors as unjustified, given that it has been repeatedly demonstrated that WFs have a strong association with environmental damage (Laurenti et al., 2023; Doka, 2024; Ridoutt et al., 2010; Jiao et al., 2013). Additionally, it has been shown that the most vulnerable communities suffer disproportionately from the social and

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Table 1
List of abbreviations

CCS	Carbon Capture and Storage
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

ecological impacts created by wasteful behaviours and substandard end-of-life treatment (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; Berger et al., 2020; Sonderegger 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 impacts across the entire life cycle—from 'cradle to grave'—often identifying critical hotspots and guiding prioritisation of action (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 one metric 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 (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) [English: environmental impact points] in the case of the SwissEco-Factors) (Su, 2020).

To facilitate the quantification of waste and material flows in LCA, we developed a Python package to extend the `brightway` open-source LCA framework (Mutel, 2017a) 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 treatment or EOL handling.

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). 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. `premise` offers an excellent structure for the integration of future waste and material flow modelling in LCA databases, but its potential contribution to the development of the circular economy cannot be realised if the scientific resources for data collection and validation are not forthcoming. The authors believe that there is an urgent need for research investment in this area.

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 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 potentially highlight opportunities for waste reduction and material efficiency.

With the continual improvement of LCA databases and the development of prospective databases, T-reX can produce ever more realistic estimates, enhancing its actionable utility derived from the exploration of the potential impacts of future waste management systems and the material demands of emerging technologies. The better the data, the more specific and accurate the results of T-reX analysis, and, thus, the more useful the tool becomes. The authors hope that T-reX will be a valuable asset to the LCA community and contribute to the development of a more sustainable and circular economy.

1.2. Background and need

1.2.1. 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. 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 Bisinella et al. (2024) 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 (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 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 (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. 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, as well as the potential misrepresentation of environmental performance due to differences in waste types (Chen et al., 2021; Huijbregts et al., 2010).

Some existing LCA methodologies offer direct indicators at the impact assessment level, but generally, there is little attention given to the impacts of waste in LCA (Oers et al., 2020). 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.

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, while also proposing simple measures to quantify waste 'hazardousness' and 'circularity' with this data. The method presented, as the authors explain, suffers from errors due to double counting due to the way that exchanges are identified and 'tagged'. 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.

1.2.2. *Material demand in LCA*

In the context of geopolitical tension and a mineral-hungry 'renewable energy transition', greater attention is being given to the security of material supply—especially for 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; IEA, 2023a,b). 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 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 (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.

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, highlighting inconsistencies in LCA methodology and probing departures from projections in prospective models.

2.1. T-reX

2.1.1. *Computational framework*

Developed in the Python programming language, T-reX extends the `brightway LCA framework`, utilising especially the components `bw2data`, `bw2calc`, and `bw2io` (Mutel, 2017a). 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) (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—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) (McDowall and Lanphear, 2023b) and is fully 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 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 item 1 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 in the 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 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 (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 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 of T-reX, there are 10 waste categories which are then further divided by their unit of measurement (kilograms and cubic meters) to create a total of 20 waste methods. The waste categories include aggregations such as 'total waste' 'hazardous waste' as well as, those for 'waste sent to treatment' by, for example, incineration or recycling. The full details are listed in the supplementary material in item 3. 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.

In addition to these 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 (European Commission and DG-GROW, 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. The full list of 59 materials included in the default configuration is provided in the supplementary material in item 3.

Following the logic of the standard LCA models Wernet et al. (2016); Guinée et al. (2004), the identification of material exchanges with T-reX differs from that used to identify waste exchanges. That is, 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 grouping, 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, a material basis. 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 effects on the market, such as a 'negative consumption' of other materials due their co-production with the functional unit. 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.

For example, in the results of the Li-ion battery case study, 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 Figure 1. The supplementary material in item 3 provides more detailed information.

2.2. Case study methodology

To provide an example, we investigated five types of Li-ion batteries in the `ecoinvent` 3.9.1 'cutoff' LCA database (Wernet et al., 2016), each represented by their unamended global market inventories. The system boundaries. These following markets were used for the example calculations and unaltered by the authors:

- Li-ion, LFP, rechargeable, prismatic
- Li-ion, $LiMn_2O_4$, 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) (Huijbregts et al., 2016)
- Environmental Footprint (EF) v3.1 (no long-term emissions) (Andreasi Bassi, S and Biganzoli, F and Ferrara, N and others, 2023)
- Spatial differentiation in life cycle impact assessment—the EDIP 2003 no long term emissions method (Hauschild and Potting, 2004)
- The crustal scarcity indicator method—CSI 2020 (Arvidsson et al., 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` (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 total summation was calculated along with details of the top contributing processes. Additionally, for the T-reX methods, a contribution analysis was performed with the `bwa.compare_activities_by_grouped_leaves` function from the `brightway2_analyzer` package (Mutel, 2016), a component of the `brightway` ecosystem. This function performs one subjective method of graph traversal on the impact matrix of the LCA object to a specified cutoff. The groups of the resulting 'leaves' are collected by their Cooperative Patent Classification (CPC) codes [giving a representation of industry sector involvement]. T-reX provides, essentially, a tabulation of internal exchanges and an 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 item 5. 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).

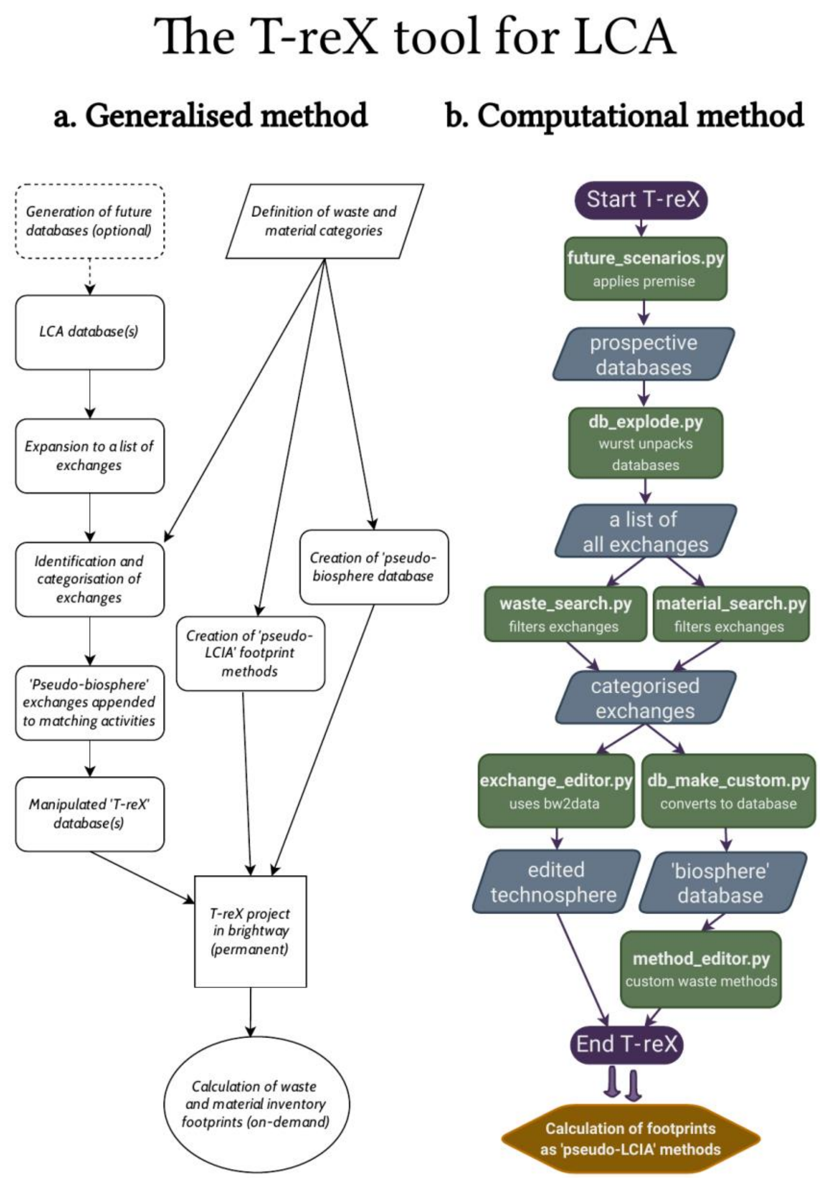

Figure 1: The workflow of T-reX presented in a generalised (a) and computational (b) format. Application of T-reX to one or more LCA databases creates a `brightway` project with customised methods and activities that can be used to calculate waste and material inventory footprints of the activity's supply chain.

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 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 (item 7 and item 8). 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 dis-aggregates the final footprint result over the activities in the supply chain.

3.2.1. Sankey visualisation of flow inventory footprints

Figure 2 presents a heavily abridged 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 to be legible for print, multiple versions are included in the supplementary material in item 8. 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 (Guinée et al., 2004). If an unallocated database were available, the waste flows could be calculated with T-reX in the same way and would be more directly related to the physical flows of the activities.

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

Figure 3 (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.

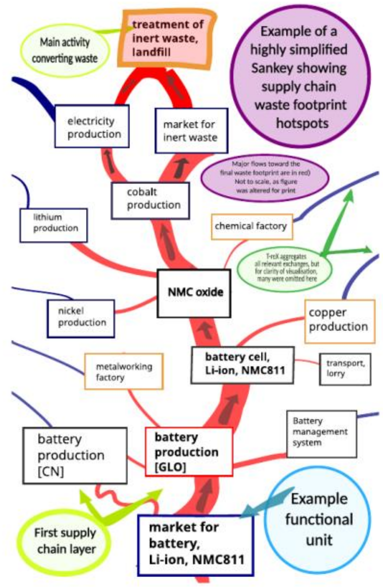

Figure 2: A greatly simplified Sankey diagram from `ActivityBrowser` showing the total solid waste footprint flows for the NMC 811 battery supply chain at the global market in the `ecoinvent` database version 3.9.1

The inclusion of carbon capture and storage (CCS) in the prospective databases is apparent in Figure 3 (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 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). 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. Significant work is needed to improve the representation of these technologies in the databases to ensure that the results are more realistic and useful for decision-making.

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

Figure 4 shows the contribution of the 'top-processes' to the graphite footprint of the $LiMn_2O_4$ battery under

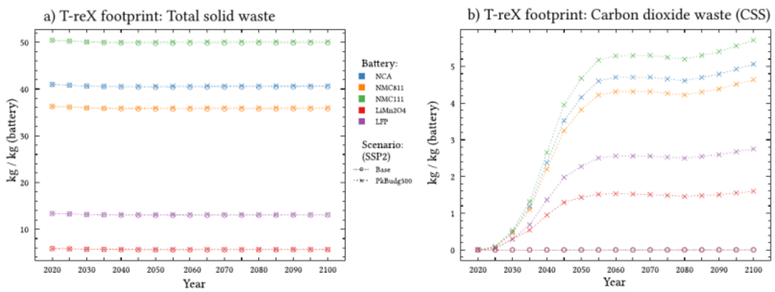

Figure 3: T-reX calculated supply chain inventories for the five Li-ion batteries in the case study, showing their 'footprints' for: (a) total solid waste, and (b) carbon dioxide waste (produced from carbon capture and storage (CCS) only). The footprints were modelled with prospective LCA databases from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model.

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.

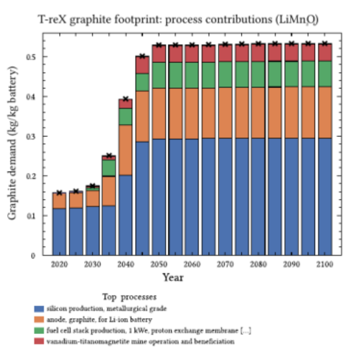

Figure 4: Contribution by the 'top-processes' to graphite demand inventory of the $LiMn_2O_4$ battery from 2020 to 2100 under the SSP2 scenario using the baseline RCPs of the REMIND model

3.2.4. Contribution of industrial sectors in the supply chain

Figure 5 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.

3.2.5. Comparison with 'similar' LCIA methods

A comparison of the results for 'Coal (black)' demand using the T-reX method with the LCIA method 'EDIP 2003 – coal no LT' is shown in Figure 6. 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 demands (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

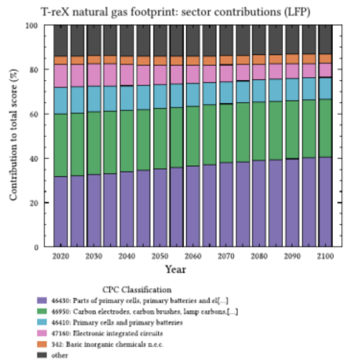

Figure 5: Contribution of industrial sectors to the natural gas footprint of the LFP battery from 2020 to 2100 under the SSP2 scenario using the baseline RCP of the REMIND model

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.

3.2.6. *Comparison with other studies*

In the most similar published method, Laurenti et al. (2023) used an alternative procedure for calculating the waste footprint of 1400 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. 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 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

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

deconstructed into a list of separate exchanges, and only those explicitly defined as hazardous are marked as such.

4. Discussion

Waste generation and material demand are strongly associated with the environmental impacts of human activities (Laurenti et al., 2023; Steinmann et al., 2017; Demirer, 2019), 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 (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 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

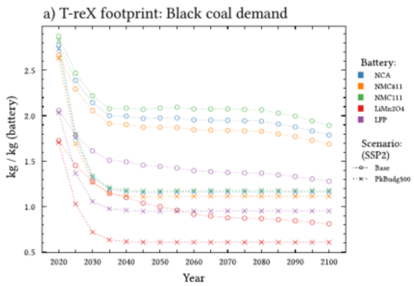

Figure 6: Comparison of the (a) 'T-reX – Coal (black)' demand footprint with the (b) conventional LCIA method 'EDIP 2003 – coal no longterm'. In the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model for all five batteries.

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 the nature of the waste flows. For example, if the waste generated could represent an actual loss of resources or potential environmental risk, or, as is often the case, 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` (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 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 (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

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 deconstructs, manipulates 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.

It is essential that we elucidate the complex relationships between material demand and waste generation and environmental and social harms. The software we present in this article enables detailed exploration of 'footprints' and life cycle inventories—modelled externalities of human activities—and examines their potential connections threats such as supply chain risks and environmental damage. T-reX is a step towards a better understanding of these interconnections for the practical realisation of sustainability and the circular economy.

The supplementary material supplied with this manuscript contains the following sections:

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. Example of the terminal output of the case study
7. Complete tabulated results of the case study
8. Complete visualisations from the case study

Data availability

All data used is publicly available online under the noted sources. T-reX is fully open source and dedicated to the public domain under the CC-1.0 licence. It is 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://ww` w.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.

CRediT authorship contribution statement

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

Figure 7: CRediT authorship visualisation

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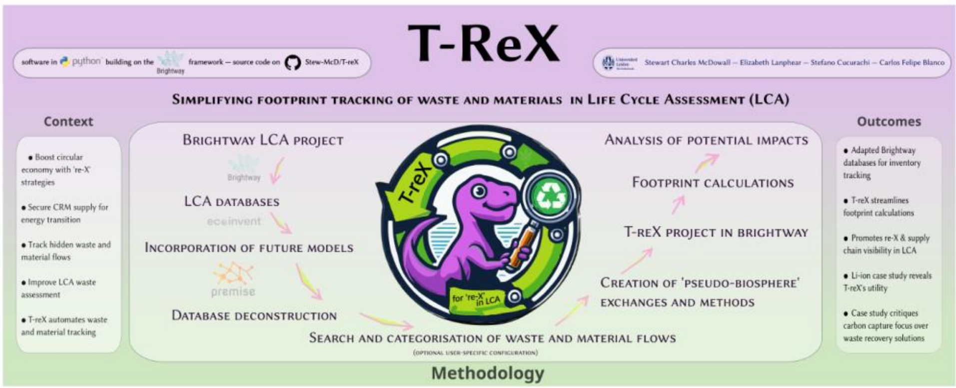
Graphical Abstract

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

Stewart Charles McDowall, Elizabeth Lanphear, Stefano Cucurachi, Carlos Felipe Blanco



Highlights

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

Stewart Charles McDowall, Elizabeth Lanphear, Stefano Cucurachi, Carlos Felipe Blanco

- T-reX, a new open-source program for waste & material footprints 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 potential

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 '~~ 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 quantitative method for this, especially given its capacity to ~~pinpoint hotspots of environmental impact throughout~~ expose the details of an activity's entire life cycle, ~~where~~ often guiding the implementation of circular principles to where they could be most effective.

~~We introduce~~ Pursuant to these goals the authors have developed 'T-reX~~, a Python tool extending the brightway ecosystem , to allow facile~~', an analytical tool for LCA, written in Python. T-reX extends on the existing computational ecosystem centered on `Brightway` and `Premise` and can facilitate the quantification of user-defined supply chain demands for activities in current and prospective scenarios. T-reX streamlines database manipulation for LCA practitioners~~and integrates~~, integrating methods to aggregate and analyse ~~waste and material flows, facilitating rapid hotspot identification~~demand inventories that could expose hotspots of hidden risk.

~~A case study of five~~ With a simple case study using lithium-ion batteries~~demonstrates~~, we demonstrate some of T-reX's ~~utility, quantifying categorised~~ potential by detailing and exploring aspects of their waste and material ~~inventory footprintsand their potential environmental burdens.~~ footprints. Since such footprints are often linked to negative externalities, T-reX ~~can aid~~ could support sustainable decision-making and contribute to the development of ~~'circular economy ' by facilitating analysis of~~ the circular economy by promoting the understanding of our material consumption and waste generation~~in LCA~~.

1. Introduction

1.1. Introduction to T-reX

The development of a ~~'circular economy '~~ circular economy has become a central focus in the ~~frantic~~ pursuit of sustainability objectives ~~and the imperative~~ toward curtailment of our environmental footprint within planetary boundaries ~~(European Commission, 2019, 2020; Government of the Netherlands, 2023, 2016; Pardo and Schweitzer, 2018; Ellen MacArth~~
~~.~~ (European Commission, 2019, 2020; Government of the Netherlands, 2023, 2016; Pardo and Schweitzer, 2018; Ellen MacArthur Founda
.

Fundamental to this development is a decrease in primary material consumption and a reduction of life cycle waste through the implementation of 're-X'v 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~~ geopolitical tensions in an ever more globalised ~~economy~~ world have highlighted the vulnerability of many advanced economies to intentional supply disruptions—wrought as an act of competition or even ~~outright hostility~~outrighthostility (Carrara et al., 2023; Hartley et al., 2024; Berry, 2023).

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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' 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 Pf~~ (Giampietro and Saltelli, 2014; Vanham et al., 2019; Ridoutt and Pfister, . More recently, the footprint collection has been extended to include the Material Footprint (MF) (Wiedmann et al., 2013), which is 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 the 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).

Though steadily emerging (Laurenti et al., 2016; Demirer, 2019; Guillotreau et al., 2023), 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~~is less well-developed. While it seems obvious that reducing life

Table 1
List of abbreviations

CCS	Carbon Capture and Storage
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

cycle waste is 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 environmental 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 WFs have a strong association with environmental damage (Laurenti et al., 2023; Doka, 2024; Ridoutt et al., 2010; Jiao et al., 2013). 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~~ substandard end-of-life treatment (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; Berger et~~ (Bisinella et al., 2024; Towa et al., 2020; Berger et al., 2020; Sonderegger
.

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~~action (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~~ one metric 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 (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) [English: environmental impact points] in the case of the ~~Swiss Eco-Factors~~SwissEco-Factors) (Su, 2020).

To facilitate the quantification of waste and material flows in LCA, we developed a Python package to extend the `brightway` open-source LCA framework (Mutel, 2017a) 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 treatment or EOL handling.

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). 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. `premise` offers an excellent structure for the integration of future waste and material flow modelling in LCA databases, but its potential contribution to the development of the circular economy cannot be realised if the scientific resources for data collection and validation are not forthcoming. The authors believe that there is an urgent need for research investment in this area.

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 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 potentially highlight opportunities for waste reduction and material efficiency.

With the continual improvement of LCA databases and the development of prospective databases, T-reX can produce ever more realistic estimates, enhancing its actionable utility derived from the exploration of the potential impacts of future waste management systems and the material demands of emerging technologies. The better the data, the more specific and accurate the results of T-reX analysis, and, thus, the more useful the tool becomes. The authors hope that T-reX will be a valuable asset to the LCA community and contribute to the development of a more sustainable and circular economy.

1.2. Background and need

1.2.1. *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. 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 Bisinella et al. (2024) 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 (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 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 (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. 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, as well as the potential misrepresentation of environmental performance due to differences in waste types (Chen et al., 2021; Huijbregts et al., 2010).

~~Existing~~ Some existing LCA methodologies offer ~~limited~~ direct indicators at the impact assessment level, ~~providing sparse information on~~ but generally, there is little attention given to the impacts of waste in LCA (Oers et al., 2020) . 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.

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, 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,~~ as the authors explain, suffers from errors due to double counting 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.

1.2.2. *Material demand in LCA*

In the context of ~~geo political~~ geopolitical 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) (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; IEA, 2023a,b). 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~~ system 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 (Arvidsson et al., 2020). The CSI introduced crustal scarcity potentials (CSPs), which are measured in ~~kg–silicon–equivalents per kg–element~~ 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.

1.3. ~~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 (Mutel, 2017a) 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 (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 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 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, highlighting inconsistencies in LCA methodology and probing departures from projections in prospective models.

2.1. T-reX

2.1.1. Computational framework

Developed in the Python programming language, T-reX extends the `brightway LCA framework`, utilising especially the components `bw2data`, `bw2calc`, and `bw2io` (Mutel, 2017a). 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) (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—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) (McDowall and Lanphear, 2023b) and is fully 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 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 item 1 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 in the 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 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 (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 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 of T-reX, there are 10 waste categories which are then 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~~ aggregations such as 'total waste' 'hazardous waste' as well as, those for 'waste sent to treatment' by, for example, incineration or recycling. The full details are listed in the supplementary material in item 3. 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' (Guinée and Heijungs, 2021), 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~~ these 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 (European Commission and DG-GROW, 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 item 3.

~~The logic for~~ Following the logic of the standard LCA models Wernet et al. (2016); Guinée et al. (2004), the identification of material exchanges with T-reX differs from that used to identify waste exchanges~~in that~~. That is, 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~~grouping, 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, a material basis. 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~~ effects on the market~~such as co-production~~, such as a 'negative consumption' of other materials due their co-production with the functional unit. 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~~ For example, 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 Figure 1. The supplementary material in ~~contains a more detailed computational flowchart~~item 3 provides more detailed information.

2.2. Case study methodology

~~We~~ To provide an example, we investigated five types of Li-ion batteries in the `ecoinvent` 3.9.1 'cutoff' LCA database (Wernet et al., 2016), each represented by their unamended global market inventories~~:~~. The system boundaries. These following markets were used for the example calculations and unaltered by the authors:

- Li-ion, LFP, rechargeable, prismatic
- Li-ion, $LiMn_2O_4$, 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) (Huijbregts et al., 2016)
- ~~EF~~ Environmental Footprint (EF) v3~~.0 no LT~~.1 (no long-term emissions) (Andreasi Bassi, S and Biganzoli, F and Ferrara, N and others, 2023)
- Spatial differentiation in life cycle impact assessment—the EDIP 2003 no ~~LT~~long term emissions method (Hauschild and Potting, 2004)
- ~~CSI~~ The crustal scarcity indicator method—CSI 2020 (Arvidsson et al., 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` (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~~ total summation was calculated along with details of the top contributing processes. Additionally, for the T-reX methods, a contribution analysis was performed~~.~~ ~~This involved utilising~~ with the `bwa.compare_activities_by_group` function from the `brightway2_analyzer` package (Mutel, 2016), a component of the `brightway` ecosystem. This function performs one subjective method of graph traversal on the impact matrix of the LCA object to a specified cutoff~~and groups the resulting leaves~~. The groups of the resulting 'leaves' are collected by their Cooperative Patent Classification (CPC) codes ~~. This provides~~[giving a representation of industry sector involvement]. T-reX provides, essentially, a tabulation of internal exchanges and an 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~~ item 5. 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 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 (item 7 and item 8). 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~~ dis-aggregates the final footprint result over the activities in the supply chain.

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

Figure 2 presents a heavily abridged 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 to be legible for print, ~~the full version is~~ multiple versions are included in the supplementary material in item 8. As

~~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.~~

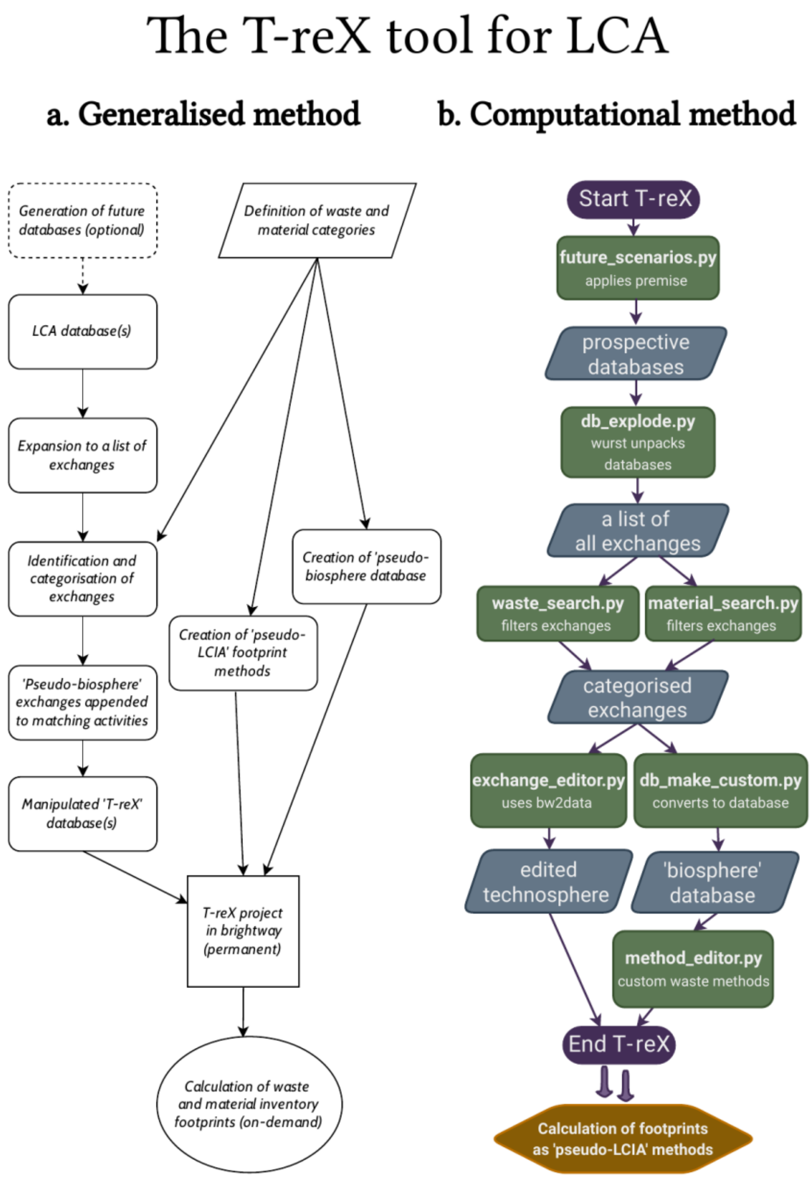

Figure 1: The workflow of T-reX presented in a generalised (a) and computational (b) format. Application of T-reX to one or more LCA databases creates a `brightway` project with customised methods and activities that can be used to calculate waste and material inventory footprints of the activity's supply chain.

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 (Guinée et al., 2004). If an unallocated database were available, the waste flows could be calculated with T-reX in the same way and would be more directly related to the physical flows of the activities.

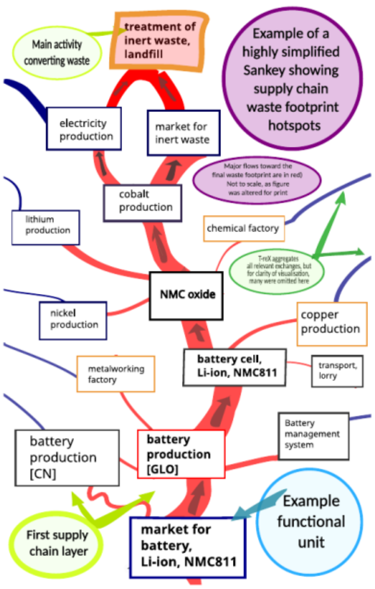

Figure 2: A greatly simplified Sankey diagram from `ActivityBrowser` showing the total solid waste footprint flows for the NMC 811 battery supply chain at the global market in the `ecoinvent` database version 3.9.1~~.~~

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

Figure 3 (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~~ 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 Figure 3 (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 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). The authors consider that the ~~over representation~~ over-representation of CCS and the ~~under representation~~ under-representation of waste processing technologies in the prospective databases is one significant limitation to the validity of prospective LCA databases. Significant work is needed to improve the representation of these technologies in the databases to ensure that the results are more realistic and useful for decision-making.

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

Figure 4 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.

3.2.4. *Contribution of industrial sectors in the supply chain*

Figure 5 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

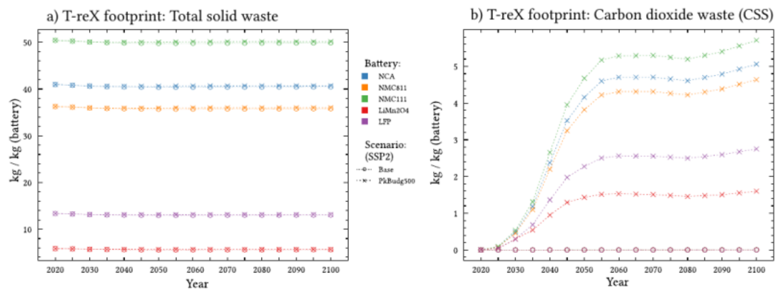

Figure 3: T-reX calculated supply chain inventories for the five Li-ion batteries in the case study, showing their 'footprints' for: (a) total solid waste, and (b) carbon dioxide waste (produced from carbon capture and storage (CCS) only). The footprints were modelled with prospective LCA databases from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model.

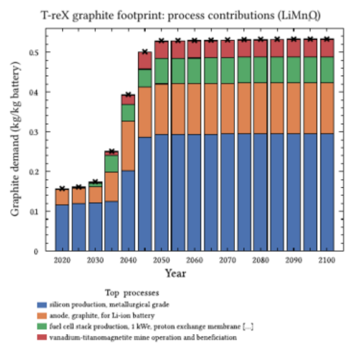

Figure 4: Contribution by the 'top-processes' to graphite demand inventory of the $LiMn_2O_4$ battery from 2020 to 2100 under the SSP2 scenario using the baseline RCPs of the REMIND model~~.~~

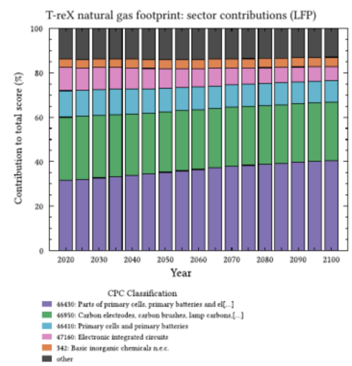

Figure 5: Contribution of industrial sectors to the natural gas footprint of the LFP battery from 2020 to 2100 under the SSP2 scenario using the baseline RCP of the REMIND model~~.~~

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.

3.2.5. Comparison with 'similar' LCIA methods

A comparison of the results ~~from T-reX's~~ for 'Coal (black)' demand using the T-reX method with the LCIA method 'EDIP 2003 ~~—~~ coal no LT' is shown in Figure 6. 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~~ demands (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

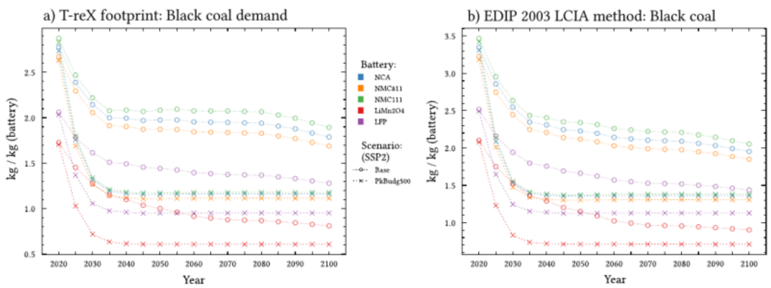

Figure 6: Comparison of the (a) ‘T-reX ~~-~~– Coal (black)’ demand footprint with the (b) conventional LCIA method ‘EDIP 2003 ~~-~~– coal no ~~LT~~longterm’~~in~~. In the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model for all five batteries.

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.

3.2.6. *Comparison with other studies*

In the most similar published method, Laurenti et al. (2023) used an alternative procedure for calculating the waste footprint of 1400 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. 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 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 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

Waste generation and material demand are strongly associated with the environmental impacts of human activities (Laurenti et al., 2023; Steinmann et al., 2017; Demirer, 2019), 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 (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 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 the nature of the waste flows. For example, if the waste generated ~~represents~~ could represent an actual loss of resources or potential environmental risk, or, ~~for example, is~~ as is often the case, 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` (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 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 (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'~~ 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'~~ deconstructs, manipulates 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~~ It is essential that we elucidate the complex relationships between material demand ~~, waste generation , and environmental impacts. This instrument~~ and waste generation and environmental and social harms. The software we present in this article enables detailed exploration of 'footprints' and life cycle inventories—modelled externalities of human activities—and examines their ~~connections to~~ potential connections threats such as 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'~~ sustainability and the circular economy.

The supplementary material supplied with this manuscript contains the following sections:

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. Example of the terminal output of the case study
7. Complete tabulated results of the case study
8. Complete visualisations from the case study

Data availability

All data used is publicly available online under the noted sources. T-reX is fully open source and dedicated to the public domain under the CC-1.0 licence. It is 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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The authors would like to acknowledge those who were part of the futures thinking small group session at the FutuRaM consortium meeting in Berlin in June 2023 in which the term 'T-reX/T(ool)-reX' was coined to name the vision presented by Stewart Charles McDowall of a comprehensive open-source software framework for the study and development of secondary raw material systems. The authors hope to continue the development of T-reX in the service of our shared ideals.

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.

CRediT authorship contribution statement

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

~~CRediT authorship contribution statement~~

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

Figure 7: CRediT authorship visualisation

~~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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~~Part of this research project was financially supported by the European Union's Horizon 2020 research and innovation programme under the grant agreement No. 101058522 (project FutuRaM — futuram.eu). The authors would like to thank the reviewers for their valuable comments and suggestions.~~

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