Spotlights

Bullet 1: Critical context and background information on the problem addressed
Understanding waste and material flows is essential for developing the circular economy and supply chain resilience

Bullet 2: A brief overview of the key finding of the study (or findings if necessary)
A program was developed to quantify waste and material footprints of activities in life cycle assessment (LCA) databases

Bullet 3: The most radical, creative, disruptive or innovative aspect of the manuscript
Built to complement the Brightway LCA framework and ActivityBrowser, the tool is flexible and easy to use.

Bullet 4: The significance of the results to the environment, economics or society
The tool can be used to identify pre-consumer waste and material hotspots that are often hidden in supply chains.

Bullet 5: Future vision or the most important implications for continued research
Improved data availability and quality would enable more detailed and accurate waste and material footprinting.

Highlights

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

WasteAndMaterialFootprint: A python package to quantify supply chain flows of waste and material in LCA databases

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Abstract

Abstract word count: 150, Limit: 150

The 'circular economy' is a concept centered on 're-X' strategies—on the prevention of waste and the reuse of resources. Thus, identifying and quantifying waste and material flows are of fundamental importance. Life Cycle Assessment (LCA) is powerful for this end, given its capacity to pinpoint hotspots of environmental impact throughout the life cycle of products and services, those where the implementation of circular principles could be most effective.

Introducing WasteAndMaterialFootprint, a Python tool extending the Brightway framework for flexible, user-defined quantification of supply-chain demands in current and future scenarios. This tool streamlines database manipulation for LCA practitioners and integrates methods to aggregate and analyse waste and material flows, facilitating rapid hotspot identification.

A case study on battery supply chains demonstrates the tool's utility. WasteAndMaterialFootprint quantifies and compares inventory demands and potential environmental burdens, aiding sustainable decision-making. It contributes to a more sustainable, circular economy by providing detailed material usage and waste generation analysis.

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

Total word count: 6000, Limit: 5000 (can be easily condensed)

1. Introduction

Section word count: 1650

Needs work to make it flow better, also shortened

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

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

Thus, we were motivated to create a flexible and policy-driven approach to understanding a product's demand on the waste management system both now and in the future to ensure that models of circularity and improvements in technology and policy for waste are included in LCA modeling.

1.1. LCA

Life Cycle Assessment (LCA) is a useful method for the holistic estimation of the environmental impacts of products and processes. LCA can comprehensively evaluate these impacts across the entire life cycle—from 'cradle to grave'—, often identifying critical hotspots and guiding prioritisation of actions. The standard approach is to apply Life Cycle Impact Assessment (LCIA) methods (such as ReCiPe (Huijbregts et al., 2016) and CML (Guinée et al., 2002)), which convert the inventory data

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into a set of impact scores based on the sum of the elementary flows. These scores are then aggregated into a single score for each impact category, which can be compared across products and processes.

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

1.2. Material Demand in LCA

In the context of a mineral-hungry renewable energy transition and recent geo-political tensions, more attention is being paid to the security of supply of materials, especially those considered 'critical raw materials' (CRMs) (Commission et al., 2023; Hool et al., 2023; Mancini et al., 2013; Carrara et al., 2023; Hartley et al., 2024; Salviulo et al., 2021). Given the increasing focus placed on this, as well as ideals of improving resource efficiency and developing the circular economy, it is essential to understand the material demands of products and processes. While LCA seeks to model the technosphere (the sum of all supply chains), its focus is often on the environmental impacts of the system—the endpoints— rather than the primary material flows themselves.

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

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

1.3. Waste in LCA

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

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

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

Moreover, existing LCA methodologies offer limited direct indicators at the impact assessment level, providing sparse information on the impacts of waste. This limitation becomes particularly evident when attempting to identify waste generation hotspots within a product's life cycle. Addressing these hotspots is crucial for advancing towards circularity. Thus, there is a pressing need for more comprehensive methods that can effectively quantify waste impacts and contribute to a better understanding of a product's total environmental footprint. There is currently a lack of a convenient and flexible method for calculating waste flows in Life Cycle Assessment (LCA).

Laurenti et al. (2023) developed a method to calculate the waste footprint of a product or service based on solving the demand vectors of the activities, also presenting simple measures to quantify waste hazardousness and circularity. In that study, it was shown that the waste footprint correlates well with other LCIA methods, particularly human health. The method presented, however, is limited in its scope and flexibility, is computationally intensive, difficult to use, is not easily reproducible, and suffers from errors due to double counting. The WMF tool presented in the current work provides a more flexible, transparent, and user-friendly approach to quantifying waste flows in LCA. Moreover, the WMF tool is not limited to waste but can be used to quantify any supply-chain flow, such as water, gas, and critical raw materials.

1.4. The WasteAndMaterialFootprint Tool

To better assess waste and material flows in LCA, the authors have developed a Python program built on the Brightway2 framework and designed to track these exchanges by translating them into indicators and impact categories. In this study, we present the WasteAndMaterialFootprint (WMF) tool that enables LCA practitioners to easily aggregate the mass and volume of any desired exchange, and to creation of flexible categories to differentiate between waste types and End-of-Life (EOL) handling using (in this case) the Ecoinvent 3.9 cutoff database.

The purpose of the WMF tool is not to quantify the environmental impacts of waste treatment, but rather to quantify the 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 waste generated by a product or service, 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 lively debate by Ayres (1999), Reuter and van Schaik (2012) and many others. In any case, waste avoidance is of critical importance and by quantifying and classifying the waste total attributed to a product or service in an LCA database, the WMF tool provides a practical means to identify hotspots and opportunities for waste reduction and efficiency.

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

This tool provides a method for the calculation of waste footprint impact category results, differentiated by the type of waste handling. Furthermore, the tool facilitates rapid investigation and identification of waste hotspots, enabled by standard contribution analysis and Sankey diagram visualization tools. The authors consider this a crucial step in addressing the deficit of Life Cycle Assessment (LCA) methods that consider waste flows in the evaluation of a product or process' circular economy potential.

2. Methodology

Section word count: 2000

This section is divided into two parts. In subsection 2.1, we describe the WasteAndMaterialFootprint (WMF) tool, in subsection 2.3, we describe the methodology used to calculate the waste and material footprints in the case study.

2.1. The WasteAndMaterialFootprint (WMF) tool

The WMF tool is a Python package that allows one to calculate the waste and material footprint of any product or service inside of LCA databases. Metadata of the WMF tool is presented in Table 1.

Table 1: WasteAndMaterialFootprint (WMF) tool metadata

Item	Details
Current version	0.1.21
DOI	`zenodo.org/doi/10.5281/zenodo.10431180`
Code repository	`github.com/Stew-McD/WasteAndMaterialFootp`
License	CC0−1.0 license
Versioning system	git
Language	Python
Documentation	`wasteandmaterialfootprint.readthedocs.io`
Main dependencies	brightway2, premise, wurst
Support email	s.c.mcdowall@cml.leidenuniv.nl

The tool is built on the `Brightway2` LCA framework (Mutel, 2017a) and is also compatible with `ActivityBrowser` (Steubing et al., 2020) an open-source graphical user interface for LCA. The WMF tool is installable via the Python Package Index (PyPI) (McDowall and Lanphear, 2023b) and is open source under the CC-0 licence. The full source code for the WMF tool is indexed on Zenodo (McDowall and Lanphear, 2023a) and under further development in the GitHub repository (McDowall). The tool is designed to be used with ecoinvent databases (Wernet et al., 2016), but could be adapted to other databases as well by changing the search criteria. Currently, it has been tested with all available system models of ecoinvent 3.5–3.10.

The program can be used directly from the command line, or imported as a Python module, in which case, the user can access the individual functions and modules. In the simplest case, the user can run the program with the default settings, which will calculate the waste and material footprint of the ecoinvent database. The user can also customise the program to calculate the waste and material footprint of a custom database, or a prospective database based on future scenarios. The program is designed to be modular so that the user can easily customise the program to their needs.

The following lists outline the constituent modules of the WMF tool, with a brief description of their functions. More extensive details can be found in the user guide and documentation of the program (McDowall, 2023).

2.1.1. Functional modules

- `future_scenarios`: Creates prospective LCA databases based on future scenarios.

- `explode_database`: Responsible for expanding a Brightway2 database into detailed exchange lists.

- `search_waste`: Provides functions for searching and categorising waste generation-related exchange data.
- `search_material`: Provides functions for searching and categorising material demand-related exchange data.
- `make_custom_database`: Facilitates the creation of custom databases based on the waste and material search categories.
- `method_editor`: Manages the custom LCIA methods for waste and material footprint calculations.
- `exchange_editor`: Appends 'pseudo-biosphere' exchanges to activities to match their waste generation and material demand exchanges in the technosphere.
- `verify_database`: Performs verification of the manipulated databases.

2.1.2. *Configuration modules*

- `custom_config`: Provides functions for managing the configuration of the WasteAndMaterialFootprint package.
- `user_settings`: The main configuration file, for defining the project and database settings (user editable).
- `queries_waste`: Defines search parameters and categories for waste generation exchanges (user editable).
- `queries_materials`: Defines search parameters and categories for material demand exchanges (user editable).

Figure 1 shows the flowchart of the WasteAndMaterialFootprint tool. The subsequent subsections describe the computational framework and the modules in more detail.

2.1.3. *Computational framework*

Developed in the Python programming language (version 3), the WMF tool extends the brightway2 LCA framework, utilising the components `bw2data`, `bw2calc`, and `bw2io` (Mutel, 2017a). Additionally, the `wurst` package is used to facilitate database searching and data transformation at the exchange level (Mutel, 2017b). Integration with `premise` package (Sacchi et al., 2022) enables the user to easily create and manipulate prospective LCA databases.

2.1.4. *Generation of prospective LCA databases*

Future waste and material footprints can be projected using the `future_scenarios` module, which uses `premise` to generate prospective scenario databases based on the configuration in `user_settings`. These prospective databases can be custom-defined by the user or can be constructed with the future projections of the integrated assessment models such as IMAGE (Stehfest et al., 2014) and REMIND (Aboumahboub et al., 2020), which offer a range of options aligned with the Shared Socioeconomic Pathways (SSPs) (Meinshausen et al., 2020) that can be paired with a variety of mitigation scenarios.

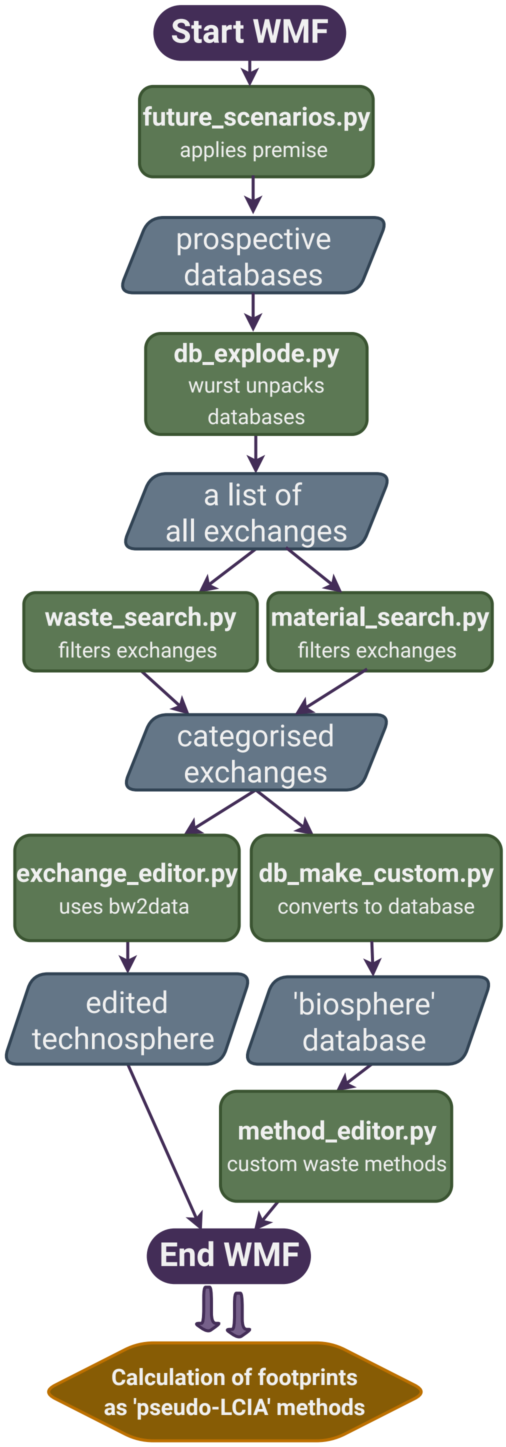


Figure 1: Flowchart of the WasteAndMaterialFootprint (WMF) tool

2.1.5. *Database expansion*

The `explode_database` module uses `wurst` to deconstruct LCA databases into a list of individual exchanges representing all of material and energy flows in the technosphere model. This dataset being converted into a pandas DataFrame and stored as a binary `.pickle` file for subsequent analysis.

2.1.6. *Waste and material flow identification and categorisation*

The `search_waste` and `search_material` modules apply user-defined search parameters from `queries_waste` and `queries_materials` to identify relevant waste and material flows in the list of technosphere exchanges generated by `explode_database` and categorises them accordingly. The results of the search functions are stored in `.csv` files for subsequent use in the WMF tool's workflow.

2.1.7. *Waste exchanges*

In the default configuration, there are 10 waste categories which are further divided by their unit of measurement (kilograms and cubic meters) to create a total of 20 waste methods. The waste categories are:

- digestion
- composting
- open burning
- incineration
- recycling
- landfill
- hazardous
- non-hazardous
- carbon dioxide
- total

The logic of screening for waste exchanges is based on a set of boolean search queries ('AND', 'OR', and 'NOT') that are applied in a list comprehension to the names of every exchange in the LCA database (see 'search_queries.py' for the full list). In this way, the search queries enable classification into categories (such as 'hazardous solid' and 'incineration liquid') and permit the identification of waste exchanges in addition to those directly connected to waste treatment processes. The search queries are tailored to the specific database and the user can easily modify them to suit their needs. In the default settings, there are a total of 18 waste classifications (9 categories, each separated into liquid and solid waste) For example, the identification of 'non-hazardous solid' waste exchanges is based on the following search query; `AND=['waste'],NOT=['hazardous','radioactive'],UNIT=['kilogram']` (this can also be inferred and confirmed by comparison with the difference between the results of 'total solid' and 'hazardous solid'). Table 2 presents a list of waste exchanges identified in the prospective database built from 'ecoinvent 3.9.1' according to the IAM model 'REMIND' with the RCP 'PkBudg500' in the year 2100. Note that the carbon dioxide waste category does not include emissions to the atmosphere. This category is based solely on the accounting of carbon capture and storage (CCS), which is included in many prospective databases as direct sequestration in reservoirs as well as solvent capture.

Table 2: WasteFootprint search results for the database 'ecoinvent cutoff 3.9.1, REMIND, SSP2, PkBudg500, 2100'.

Waste exchanges	Unit	Exchange count
digestion	kilogram	4
composting	kilogram	26
open burning	kilogram	535
incineration	kilogram	2171
recycling	kilogram	137
landfill	kilogram	1530
hazardous	kilogram	1928
carbon dioxide	kilogram	119
total	kilogram	29524
digestion	cubic meter	16
composting	cubic meter	0
open burning	cubic meter	0
incineration	cubic meter	2
recycling	cubic meter	0
landfill	cubic meter	2
hazardous	cubic meter	437
carbon dioxide	cubic meter	0
total	cubic meter	4360

2.1.8. *Material exchanges*

In addition to the waste categories, the `queries_materials` module defines the material demand categories, which are based on the EU Critical Raw Materials (CRM) list for 2023 (Commission et al., 2023). The CRM list is a list of 30 materials that are considered critical to the EU economy and are at risk of supply disruption. Further materials of interest were added to the search list, including helium, electricity, petroleum, sand, water, and natural gas. The identity of the materials considered and their categorical groupings are easily customisable by the user. A full list of 59 materials included in the default configuration is provided in the supplementary material.

The logic for the identification of material exchanges with the WMF tool differs from that used to identify waste exchanges in that the search queries are based on the names of the so-called relevant 'market activities' for the material of interest. That is, for material x, all exchanges with the name 'market for material x' are identified and subsequently apportioned a ('pseudo-biosphere') material demand exchange of the same sign and magnitude as the original exchange. A useful feature of the WMF tool is that, in cases where there are several markets for one material or material group, the program can easily aggregate these exchanges. For example, exchanges with markets for the rare-earth-elements (REEs) 'market for cerium', 'market for dysprosium', 'market for erbium', etc. can be aggregated into a single indicator category for REEs. Similarly, the total demand for all critical raw materials (CRMs) can be easily calculated in the same manner.

As discussed in the introduction 1 there are some existing material demand methods in the standard LCIA method sets, including the 'crustal scarcity indicator' (which provides only an aggregated, abstracted endpoint) (Arvidsson et al., 2020) and the (deprecated) EDIP 2003 material use indicators (which provide endpoints in fundamental units) (Hauschild and Potting, 2004). In these methods, the material demand is calculated based on the total mass that is extracted from the environment, thus, their focus is essentially solely on the mining-related exchanges that bring these materials from the biosphere into the technosphere. In the WMF tool, however, the accounting for material demand is based on exchanges solely within the technosphere. This offers a different perspective, allowing for the estimation of overall supply-chain material demands that consider the entire life cycle of an activity, including non-direct impacts on the market such as co-production of other materials. Consider a demand for an activity containing a metal, for example; while the existing material use methods allow one to calculate the total mass of that metal that is extracted from the environment, the WMF tool can provide insight into the broader supply-chain impacts of the demand for this metal. If the production other materials are attributed to the production of this metal, these would appear as negative material demands in the WMF results—supply chain pressure for one material can result in lessening of supply chain pressure for another. In the results of the Li-ion battery case study in subsection 3.2, we will see that this is indeed the case for the demand for nickel, which, because of such effects, is counter-intuitively negative despite the presence of nickel in the final products.

2.1.9. Creation of custom 'pseudo-biosphere' databases

Custom 'pseudo-biosphere' databases are created by `make_custom_database` module. This module collates the waste and material categories that were present in the databases, producing an `.xlsx` file that is imported back into the Brightway2 project as a biosphere-database named 'WasteAndMaterialFootprint'.

2.1.10. LCIA method management

The `method_editor` module manages the addition, deletion, and verification of the custom LCIA methods used in the WMF tool. This module uses the custom 'pseudo-biosphere' databases created by `make_custom_database` to create these waste and material footprint LCIA methods that have the same unit as the respective technosphere exchange. The methods are stored in the Brightway2 project and can be used for calculating the waste and material footprints of activities in the LCA database in the same way as with other LCIA methods. Since 'waste is not a service' (Guinée and Heijungs, 2021), a characterisation factor of -1 is applied to the waste footprint methods (with the exception of CCS exchanges), changing the perspective from waste consumed by treatment to waste generated by the activity.

2.2. Exchange editing

The `exchange_editor` module loads the `.csv` files created by the search functions and appends 'pseudo-biosphere' exchanges to the matching activities in the LCA database. This is the most computationally intensive part of the WMF tool, as (depending on the search configuration) there are generally more than 100,000 exchanges to be appended to the database.

2.2.1. Database Verification

The `verify_database` module calculates LCA scores for randomly selected activities using Waste Footprint and Material Demand Footprint methods to confirm that the WMF tool has processed the database correctly.

2.3. Case Study Methodology

2.3.1. Activities

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

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

2.3.2. Methods

In addition to the Waste Footprint and Material Demand footprint methods created by the WMF tool, the following standard LCIA methods were applied for comparison:

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

2.3.3. Databases

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

- **SSP2 -base:**
  representing ca. 3.5°C increase in global temperatures to 2100
- **SSP2-PkBudg500:**
  meeting Paris climate goals, ca. 1.3°C increase to 2100

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

2.3.4. Calculations

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

3. Results

Section word count: 1400

3.1. *WasteAndMaterialFootprint tool*

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

3.2. *Case study: Li-ion batteries*

As described in subsection 2.3, this case study calculated the waste and material footprints (as well as a variety of other indicators) for the unaltered inventories of five Li-ion batteries with the functional unit being 1 kg of the battery at market. The purpose of this simple case study was to test, verify, and demonstrate the functionality and limitations of the WMF tool. This section includes some highlights of the results and the full results are available in the supplementary material. Because the WMF methods are integrated into the brightway project as if they were LCIA methods, the results can be visualised in the same way. In the supplementary material, there are screenshots of selected results obtained using the `ActivityBrowser` software, including contribution analysis and a Sankey diagram that disaggregates the final footprint result over the activities in the supply chain.

3.2.1. *Temporal and scenario variation in waste and material footprints*

Figure 2 shows the total solid waste footprint for the five Li-ion batteries in the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model. The NMC811 battery has the largest footprint, producing over 50 kg of waste per kilogram of battery produced. The LiMn2O4 battery has the smallest footprint, producing less than 4 kg of waste per kilogram of battery. In each case there was a slight downward trend in the waste footprints between 2020 and 2100. This is most notable in the period between 2020 and 2040 and is attributable to the relatively rapid decrease in fossil-fuel use that is included in the models over this time. For the total waste generated by these batteries, there was very little difference observed between the baseline and PkBudg500 RCPs.

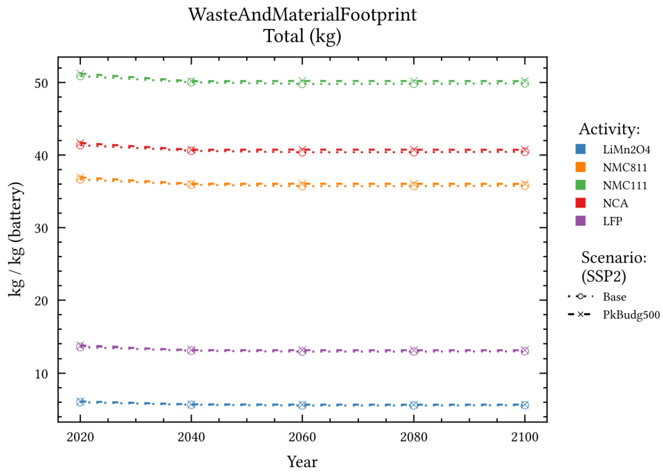


Figure 2: Total solid waste footprints for the five Li-ion batteries in the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model.

The inclusion of carbon capture and storage (CCS) in the prospective databases using the PkBudg500 RCP is evident in Figure 3, which shows a rapid increase in the production of carbon dioxide 'waste' over the period from 2020–2040 that is not seen in the baseline scenario. This result highlights the fact that (frequently) downward trends in global warming impacts calculated with prospective databases using standard LCIA methods are dependent on the assumptions made about the introduction of CCS technology. The actual deployment of these technologies—approximately 37 Mt CO_2/yr as of 2023 (Dziejarski et al., 2023)—falls far short of the levels projected in many of the RCP scenarios (Sacchi et al., 2023).

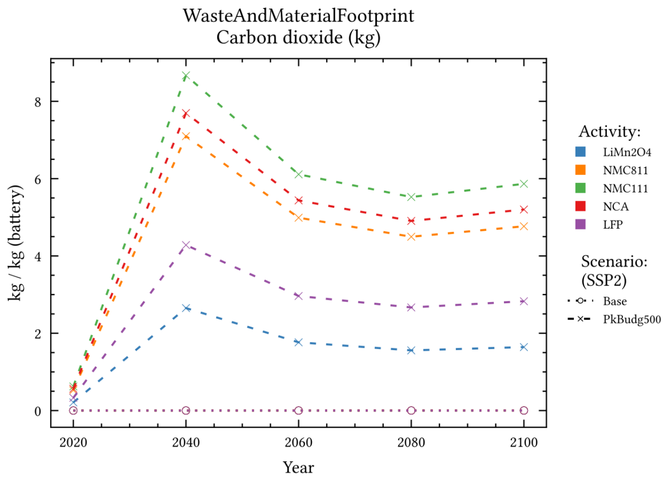


Figure 3: Carbon dioxide waste (from carbon capture and storage) footprints for the five Li-ion batteries in the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model.

For the phosphate demand footprints that are depicted in Figure 4, the LFP (lithium iron phosphate) battery has a much larger footprint than the other batteries, consistent with its composition. In this case, the phosphate footprint of all batteries is shown to decrease over the period from 2020–2100, and the

RCP scenarios are seen to converge between 2020 and 2040.

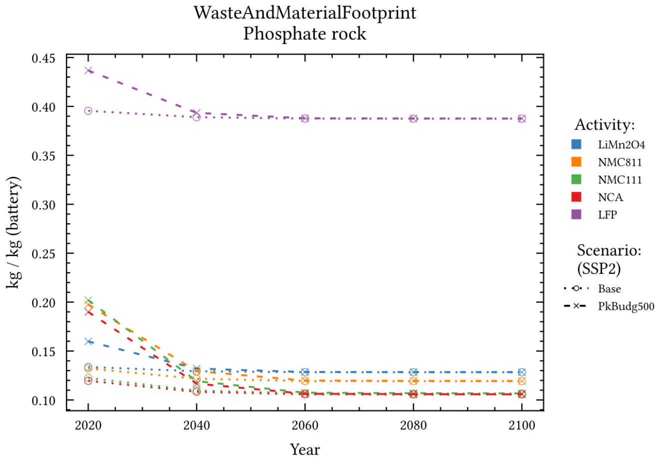


Figure 4: Phosphate material demand footprints for the five Li-ion batteries in the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model.

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

Figure 5 shows the contribution of the 'top-processes' to the cobalt footprint of the LiMn2O4 battery under the baseline scenario from 2020–2100. The total footprint is seen to almost triple, from 2.2 kg/kg in 2020 to 6.2 kg/kg in 2100. This result is likely a reflection of the electrification of the transport sector that is included in the REMIND model. The fractional contributions of the top processes remains relatively steady over the coming century in this case.

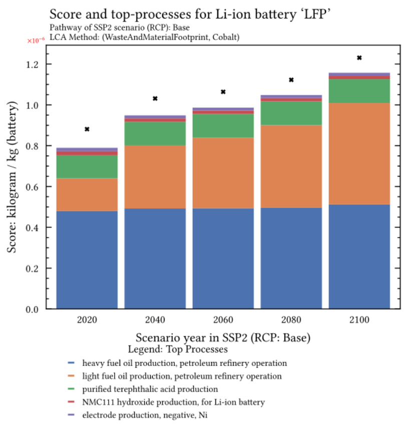


Figure 5: Contribution of 'top-processes' to the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model.

3.2.3. *Contribution of sectors in the supply chain*

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

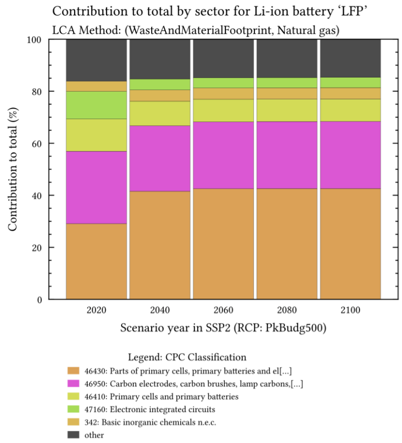


Figure 6: Contribution of industrial sectors to the liquid waste footprint of the NCA battery from 2020 to 2100 under the SSP2 scenario using the PkBudg500 RCP of the REMIND model.

3.2.4. *Comparison with 'similar' methods*

A comparison of the results from the WMF tool's 'Coal (black)' demand method with the LCIA method 'EDIP 2003 - coal no LT' is shown in Figure 7. In this case, both the trends and the magnitude of the scores were very similar, both demonstrating a general decrease in the use of coking coal in the battery's footprints. Such comparability was also observed for other fossil-fuel-related methods (e.g., natural gas and petroleum), and to a lesser extent, for some of the metal demand methods (e.g., zinc and cobalt). Correlation between standard LCIA methods and WMF 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 WMF methods, the footprint scores are based on an accounting of either waste generated or material demand, both of which are technosphere-technosphere exchanges in terms of LCA modelling. For the material demand methods especially, this distinction is critical. For example, application of the EDIP 2003 or the CSP methods for a given metal will provide a score that is proportional to the amount extracted by mining, whereas the WMF method provides an aggregation of the exchanges with the market for that metal. The WMF 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 WMF methods more sensitive to the modeling choices (e.g., allocation) that are generally embedded in LCA databases.

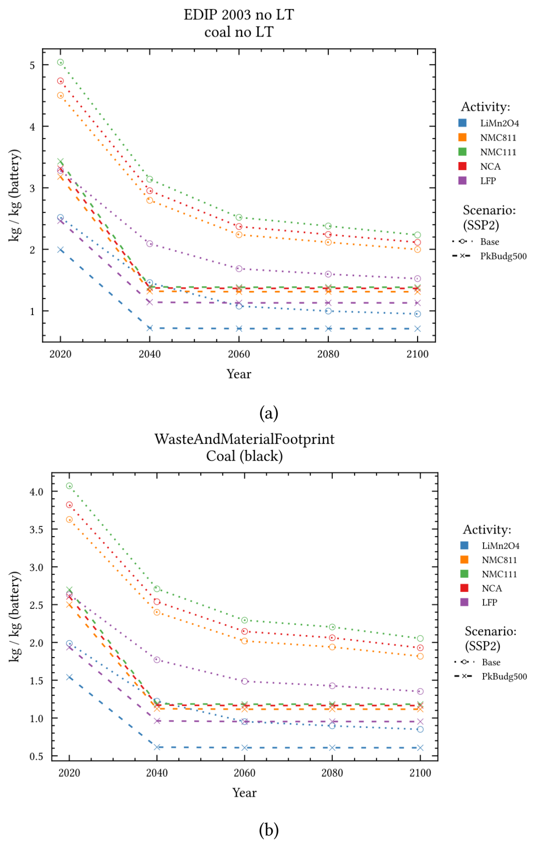


Figure 7: Comparison of LCIA method 'EDIP 2003 - coal no LT' (a) with the 'WMF - Coal (black)' (b) in the case study from 2020 to 2100 under the SSP2 scenario using the baseline and PkBudg500 RCPs of the REMIND model.

3.2.5. *Comparison with other studies*

Laurenti et al. (2023) used an alternative method for calculating the waste footprint of 1400 activities in ecoinvent version 3.5, which contains only a generic 'market for battery, Li-ion, rechargeable, prismatic'. The inventory of this battery most closely resembles that of the NMC 111 battery in this case study. Table 3 presents a comparison of the results from the two studies, where possible. For liquid, solid, and recycled waste, the results were closely aligned, however for hazardous waste, Laurenti et al. reported 95% of the total waste, whereas the WMF tool reported only 3%. The reason for this discrepancy is explained by the fact that in the method of Laurenti et al., a "waste flow was regarded as hazardous when the hazardousness was clearly stated in its subsequent waste treatment activity". The authors continue: "It should be noted that the high hazardousness ratios for many products might indicate a weakness in the validity of this measure". In the WMF method, the source database is exploded into a list of separate exchanges, and only those explicitly defined as hazardous are marked as such.

Table 3: Comparison of the results from the WMF 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	WMF	Laurenti et al.
Total solid waste (kg/kg)	50.9	62.5
Total liquid waste (kg/kg)	3.53	3.63
Hazardous waste (kg/kg)	1.47	62.6
Recycled waste (kg/kg)	1.59	1.98

4. Discussion

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

The WMF tool, in contrast, gives LCA practitioners a simple, flexible, and transparent way to calculate the supply chain waste and material footprints, delivering results in standard units as direct aggregations of the relevant demand inventories. Once the databases have been processed with the WMF tool, the user can then easily apply the WMF methods to calculate the supply-chain waste and material footprints for any activity in the same way that they would calculate any LCIA indicator.

The simple case study presented in this paper demonstrates both the utility and the limitations of the WMF tool. It was shown the WMF tool was able to calculate categorised aggregates and contribution analyses of both the waste generated and material demands in the present and future supply chains of the Li-ion batteries under consideration. Further, integration of the WMF methods as 'pseudo-LCIA' methods allows the user to easily make use of the WMF tool in their preferred LCA software, be it code-based like `brightway2` or graphical like `ActivityBrowser`.

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

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

Section word count: 450

5. Conclusions

Section word count: 250

We have written the WasteAndMaterialFootprint (WMF) tool, an extension to the brightway2 LCA framework that enables the user to calculate the waste and material footprints of a product or service in an LCA database. It explodes the database, identifies upstream waste and material exchanges, edits them, and writes matching custom WMF methods. These exchanges become pseudo-biosphere flows and thus, the footprint can be calculated as with the existing LCIA methods. The WMF tool can be easily customised by the user to calculate the footprints of other supply-chain flows such as water, gas, and critical raw materials.

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

Data availability

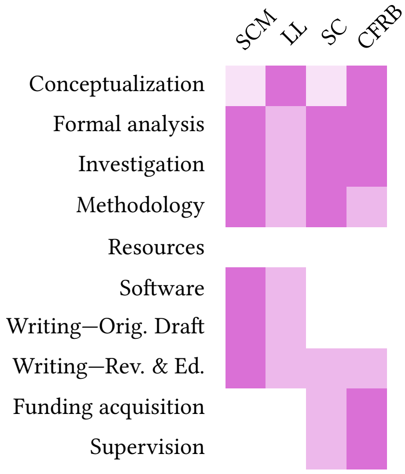
All data used in this analysis are publicly available online under the noted sources. The WasteAndMaterialFootprint tool is installable via the Python Package Index (PyPI) and is available at https://pypi.org/project/WasteAndMaterialFootprint. The full source code for the WasteAndMaterialFootprint tool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

CRediT authorship contribution statement

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

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

Alternative CRediT statement



Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary material

The supplementary material contains the following:

1. List of waste and material categories
2. Example output of the WasteAndMaterialFootprint tool
3. List of identified waste and material exchanges
4. Code (python script) used for case study
5. Inventory and methods used in the case study
6. Complete tabulated results of the case study
7. Complete visualisations of the case study

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