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A generalized schema to publish and share life cycle inventories (LCI): Exemplary case of an aviation fuel supply chain

Rahul Ramesh Nair *, Komal Mallesh Chougule, Juan Camilo Gomez, Urte Brand-Daniels

Institute of Networked Energy Systems, German Aerospace Centre, Carl-von-Ossietzky-Straße 15, Oldenburg, 26129, Germany

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ABSTRACT

Life cycle assessment (LCA) has become a crucial technique for evaluating environmental impacts across various stages of emerging clean production technologies and sustainable processes. This assessment plays a key role in guiding decision-making and policy development. Recent years have seen a substantial increase in such LCA investigations in the peer-reviewed literature. However, only a small fraction of these studies have transparently reported the foreground life cycle inventory (LCI) data of the technology under investigation. The available data are often poorly organized and lack a standard structure and metadata making them ambiguous and non-reusable. This leads to a situation where LCA outcomes must be accepted at face value due to irreplicable results. Currently, there are no standardized methods for publishing and sharing foreground LCIs with the relevant contextual information. To address this gap, this work develops a novel, minimalistic, user-centric, machine-accessible, and extensible schema based on the Brightway LCA framework to share the foreground LCI of standard (non-temporal) LCA investigations. In this schema, an inventory is made up of five components: dataset, dataset properties, metadata, dependencies, and network. A Python-based open-source tool has also been developed to convert LCIs according to the specifications of this schema. The proposed schema and the tool are demonstrated for the exemplary use case of an aviation fuel supply chain. This schema can improve the reusability and reliability of LCI datasets, a first step towards transparent, replicable, and robust LCA studies.

1. Introduction

Life cycle assessment has become one of the most widely used methods for evaluating the environmental impact of existing and emerging technologies. A simple Scopus search reveals that, between 2010 and 2023, more than 9800 original research articles and reviews were published with "life cycle assessment" in the title alone. LCA also shows a growing influence in decision- and policy-making concerning the validation of nascent technologies for industrial implementation (Pryshlakivsky and Searcy, 2021; Seidel, 2016). The precursors to this method emerged as early as the 1960s (Hauschild et al., 2018), with the past decade witnessing a growing interest in the research behind its methodology, frameworks, and applications. In LCA, the most resource-intensive and time-consuming phase is the life cycle inventory modelling, which constitutes data collection and compilation of the foreground life cycle inventory (LCI) for a defined product system.

Despite open data initiatives (Hertwich et al., 2018), only a small fraction of the studies transparently report the foreground LCI datasets used in calculations (Saavedra-Rubio et al., 2022). To address this glaring gap in the reproducibility and robustness of studies, data collection methods and a standard schema for sharing LCI datasets are needed. In terms of data collection, there are a few field-specific strategies (Hischier et al., 2014) and guidelines (Dissanayake, 2023). Still, only one study (Saavedra-Rubio et al., 2022) has proposed a common framework for LCI data collection. However, to the extent of the authors' knowledge, there have been no attempts to standardize and propose a schema to disseminate and share the LCI after the completion of an assessment. A recent investigation into the status quo of Findable, Accessible, Interoperable and Reusable (FAIR) (Wilkinson et al., 2016) data sharing in the LCA community has also concluded the necessity for LCI data sharing guidelines (Ghose, 2024).

According to DIN ISO 14040/44, an LCA consists of four iterative stages – goal and scope, inventory analysis, life cycle Impact assessment, and interpretation. The ensuing results and the goal-scope document are usually published as part of reports, environmental impact assessments, and scientific publications. The inventory data is crucial for the reproduction and validation of these results. There are no standardized methods for the compilation and sharing of inventories. Thus, many LCA

* Corresponding author.
E-mail addresses: rahul.nair@dlr.de, rahulgenesis@hotmail.com (R.R. Nair).

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investigations share the inventory ineffectively and ambiguously (Neo et al., 2021; Parsons et al., 2019; von Drachenfels et al., 2021), often with gaps in data, while other studies do not provide these inventories or only upon request (Najjar et al., 2019; Wernet et al., 2010). This makes it arduous to reconstruct the inventory to replicate and validate LCA results and/or reuse the data. In a meta-study (Ghose, 2024), only seven out of 25 LCA studies were found to supplement LCI inventories in data formats that could be directly imported to any software, albeit lacking metadata.

Numerous general-purpose proprietary (e.g., GABI, SimaPro) and open-source (e.g., OpenLCA) tools are widely used for the compilation of LCI and subsequent life cycle analysis. But, for customized, field-specific, and non-standard LCA research, custom tools are designed and employed on a per-case basis (Goglio et al., 2018; Huang et al., 2009; Paraskevas et al., 2015). Due to a lack of development, validation, and/or sufficient documentation, these tools, the subsequent inventories, and results become unadaptable, non-reusable, and, finally, abandoned. This resulted in the proliferation of expendable tools for LCA research for different non-standard use cases. This gap was filled by the open-source Python-based Brightway framework (Mutel, C., 2017). It has gained widespread traction in the LCA research community (Steubing et al., 2020). Hence, in the current investigation, Brightway is used as the framework to model the inventory schema.

Herein, this study develops and details a schema for the sharing of life cycle inventories based on existing literature standards, best practices, and conventions to promote open data. An open-source Python tool is also developed and published for the conversion of life cycle inventories in compliance with this schema. Then, this schema is demonstrated for the exemplary LCI model of an aviation fuel supply chain.

2. Terminology

While a few definitions are provided in the ISO 14040 standard, it is important to highlight that there does not currently exist any standardized glossary of LCA terminology (Ghose et al., 2021). The definitions, synonyms, and their different dialects are scattered across multiple software knowledge bases, reviews, and studies. The lack of a harmonized general glossary and the varying dialects of existing definitions lead to inconsistencies in LCI modelling and interpretation of LCA results (Gradin and Björklund, 2020). Within the context of this proposed schema, Table 1 elaborates some of the key terms and their abbreviations. It aims to delineate and clarify some important definitions that are relevant to understanding the schema's components and facilitate their unambiguous use. The terminology is based on ISO 14040:2006–07 (ISO, 2006), Life Cycle Initiative, Ecoinvent (Wernet et al., 2016), one of the most widely used life cycle databases, and the Brightway LCA framework (Mutel, C.L., 2017).

3. Methodology

This study proposes a generalized schema for the compilation and sharing of foreground LCIs as part of scientific journal publications and in digital repositories. According to this schema, a foreground inventory of the product system (hereafter also referred to as LCI or inventory) is shared as a collection of five components, namely Dataset, Dataset Properties, Metadata, Dependencies, and Network, and an environment file. This inventory decomposition is shown in Fig. 1. All these components are constructed and compiled in English (ISO 639-1, en) using the ASCII printable characters (code 32 to 127) to avoid complications arising from character encodings. The core objective of this schema is to enable the human-centric sharing of LCI datasets to make inventories more reviewable, replicable, confirmable, auditable, and reproducible (Stodden et al., 2013) with minimal technical overheads and complications stemming from complex tools, ontologies, and semantics. The schema draws inspiration from minimalistic approaches (Moresis et al.,

Table 1
Definition of key terms that are generally used in Life cycle assessment within the context of the proposed Life cycle inventory (LCI) Schema.

Schema	A structured framework for the representation of a plan about the logical interrelated components within a concept.
Template	A guide or pattern for performing "something" based on an existing and established schema. It is the format or layout for the starting point of design and customization.
Standard	An agreed way of doing something (product, service, evaluation, supply, metrics or analytics). It is usually a set of criteria and/or guidelines agreed upon by international bodies and experts and widely adopted in industrial and/or research applications (ISO, 2024).
Product system	According to ISO 14040 standard, it is a "collection of unit processes with elementary and product flows, performing one or more defined functions, and which models the life cycle of a product". It is part of the industrial (anthropogenic) systems and is characterized by a functional unit depending on the objective of the LCA.
Foreground LCI	The inventory directly contributes to and is specific to the product system under study. In other words, the foreground constitutes the data that is directly attributable to the product system. This is usually under the control of the decision-maker or LCA practitioner (hereafter referred to as practitioner).
Background LCI	The data of the background processes (usually part of the industrial economy and/or the environmental ecosystem) that indirectly influences the product system. They are delivered to the foreground systems as aggregated datasets and are not under the direct control of the practitioner. Commonly used background datasets include Ecoinvent®, Sphera® (GaBi) etc.
Dataset	The data of the foreground inventory data that has been modelled for a product system during the LCI phase consisting of the materialistic and energetic inputs and outputs that define the product system. It is usually represented in a tabular format and does not contain any metadata (contextual information) regarding the data itself.
Life cycle inventory (LCI) phase	It is the collection, quantification, and modelling of input/output (energy, materials, and emissions) data about the product system involving the collection of the data necessary for the calculation of the corresponding environmental impacts throughout the system's lifecycle.
Activity	It represents a unit process of a human activity that produces a reference product (and by-products for aggregated activities). It consumes inputs from the technosphere (e.g. energy, processed raw materials) and the environment (e.g. raw materials), and releases waste output to the environment.
Activity properties	The activities are uniquely identified based on properties such as name, location, code (unique identifier within Brightway), etc. In the schema, they are collectively referred to using the prefix "ap_". For example, the location for activities is called "ap_location".
Flows	The input and output exchanges to and from the activities. The different types of flows include elementary exchanges with the natural environment called biosphere flows; and technosphere/economic exchanges between activities, also called intermediate exchanges. A production exchange is a sub-category of intermediate exchanges and comprises the end-product that is produced or supplied by the activity (e.g. manufacturing of a product, production of electricity, etc.)
Flow properties	The characteristics of the constituent flows (Technosphere/economic and Biosphere/environmental) within a transforming or market activity. Some examples of such properties include name, location, unit, amount, comments, and formula. Within this work, flow properties are collectively invoked with the prefix "fp_". For instance, the property amount is represented as fp_amount.
Product properties	The characteristics of the reference/primary product resulting from an activity as part of its production flow. The product properties are collectively referred to with the prefix "pr_" followed by the property name. For example, the unit of a reference product will be "pr_unit".

(continued on next page)

Table 1 (*continued*)

Parameters	The custom variables that are defined for establishing mathematical relations amongst the various flow properties such as amounts. They can exist at the database, activity and/or project level.
Parameter properties	The characteristics (name, comments, amount, etc) of the parameters at the activity, database, or project level. Here, a specific parameter property will be referred to with the prefix "par_". For example, the property 'amount' of parameters is collectively called par_amount.
Data quality indicator (DQI)	The quality of the foreground LCI data that is usually estimated (as semi-quantitative numbers) based on the spatio-temporal representativeness, technological and geographical correlation, and reliability of the data that models the foreground inventory.

2024; The Turing Way Community, 2022) in other domains. The design principle of the schema tries to prioritize ease of replicability and reusability (Leipzig et al., 2021) of LCI data with low resource (time, effort) overheads. In other words, this compartmentalized schema profile aims at a univocal representation of the inventory data that is accessible by both humans and machines. Due to the rapidly evolving and malleable nature of LCA research, this schema may have to be revised in the future to accommodate new necessities to improve the sharing of inventories. Therefore, the authors refer to the current version of the schema as LCIS2024. The different parts of the schema (Fig. 1) are explained in the following sub-sections.

3.1. Dataset

The Dataset files are saved in character (comma delimited) separated value (csv, UTF-8 encoding) and Excel Open XML Spreadsheet (xlsx) formats. Brightway and other LCA software, such as SimaPro and openLCA support import/export operations with csv (albeit with their own data structure). A properly formatted xlsx dataset improves the human readability of LCI and enables quick reviews by practitioners. The csv format is one of the most widely used plain-text data formats for open sharing of tabular data and features backward compatibility with numerous tools, machine readability, and is already employed in many established repositories such as the Data portal of the European Union, Zenodo, etc.

3.2. Dataset properties

The data properties file provides high-level contextual information on the foreground dataset in csv format that constitutes the property names and their associated alpha-numeric values. It is primarily designed for machine accessibility, enabling automation for efficient import/export LCI of large product systems along with their dependencies (see sec. 3.4) while maintaining data integrity. The properties are classified into three types. The first type comprises the identifying details about the dataset, such as name, version, schema version, and the creation time (*yyyymmdd-hhmmss*, according to ISO 8601). The schema version enumerates the version of the LCI schema used for exporting the dataset and can facilitate translation layers with schema variants, revisions, and/or other types of LCI schemas in the future. The second type contains the Unique dataset identifier (UDI), software version (e.g., Brightway 2.4.1) used to model the inventory, and names of external datasets (background and/or foreground, where applicable) used to build the foreground. Finally, the third type of property also provides an overview of the total counts of activities, flows, and parameters.

3.2.1. Name and versioning of the dataset

The user-assigned name of the dataset must only contain ISO basic Latin alphabets (A-Z, a-z), Latin numerals (0–9), hyphenated words, and the underscore separator between words and digits. Special characters (such as #, %) are avoided, and the total length is limited to 250 characters to comply with the 255 bytes maximum filename length used in popular filesystems such as exFAT, ext4, APFS, NTFS, etc. The name provides a concise summary of the dataset's purpose (e.g., aviation-fuel-production) and avoids any contextual information, metadata, and/or timestamps.

There is a necessity for systematic versioning and organization of collected data to facilitate the reproducibility and extensibility of the scientific findings. This prerequisite spans all the STEM fields, and domain-specific methodologies must be developed, adopted, and agreed upon for a fundamental improvement in research dissemination. The domain of LCA includes the accounting and aggregation of data from multiple thematic areas for the construction of life cycle inventories (LCI). All newly created, revised, or bug-fixed datasets can be versioned for FAIR distribution and usage in future applications. This schema is based on the recommendations of the Research Data Alliance (RDA) for the field of engineering (Klump et al., 2021). It has to be emphasized that dataset versioning is only applicable during the release phase of the dataset at the end of the life cycle assessment. It does not pertain to the iterative revisions during the modelling of LCI. Hence, error corrections and/or rectifications during the iterative LCA phases are not classified as changes and do not warrant a separate version. Since the majority of LCI

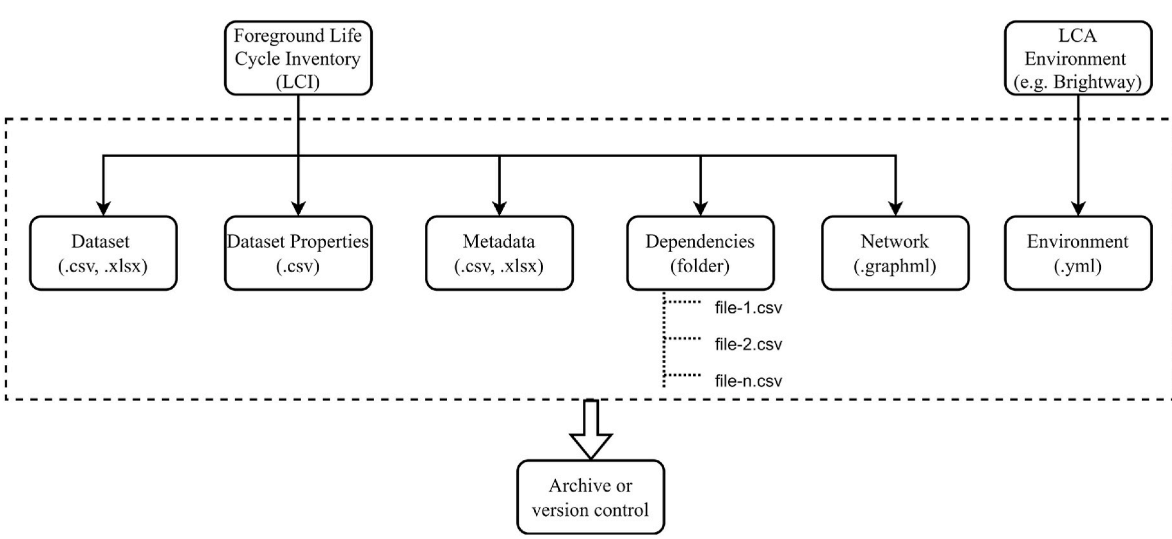

Fig. 1. The various components of a life cycle inventory according to the proposed inventory schema.

datasets primarily consists of secondary data collected from literature and/or information provided by third parties at face value, the stages of data transformations (work, expression, manifestation, item) detailed by the Functional Requirements for Bibliographic Records (FRBR) (IFLA, 1998) can be safely neglected, at least in the first version of this proposed schema. The semantic versioning (Semver) follows the convention of major. minor.patch, starting from 0.1.0 during LCI modelling, and 1.0.0 for the first public release. These three elements are updated in increments of 1 when the dataset changes, as elaborated in Table 2. A question arises as to when an LCI has undergone critical updates and changes such that it warrants a stop to versioning and the declaration of a new dataset. This is rather semi-quantifiable and depends on the subject expert. Nevertheless, it is recommended to declare a new dataset when there are changes to the goal and scope of the LCA study, and changes in system boundaries.

3.2.2. Unique dataset identifier (UDI)

The objective of a UDI is to uniquely identify and compare data and metadata to enable easier revision and reuse of inventory datasets across different projects, reports/studies, repositories, and digital resources (such as scientific publications). It especially supports those cases where inventories are shared without any globally resolvable persistent identifiers (PIDs), such as in pre-publications, supplementary files, or within on-premise/local data infrastructures, etc. The UDI is generated using version 5 of the Universally Unique Identifier (UUID) (Leach Paul and Rich, 2005). The UDIs are not directly resolvable but can also be integrated in the future with PIDs as a <UID, PID> pair for seamless integration into publication workflows using an online data storage infrastructure. For example, the UDI in an online repository that issues DOIs can enable schema-specific local consistency and global discoverability. A UDI is a 16-octet (128 bits) label generated from the text string, UDI_name, as follows.

UDI_name = ‘dataset name’-‘schema version’-‘dataset version’-‘timestamp’

Table 2
Criteria to increment the semantic version of the LCI datasets based on the type of changes to the different sections of the inventory.

Element to increment	Type of Changes	Applicable Details
Patch	Bug fixes such as spelling and grammatic corrections, and rewording without loss in contextual meaning	Changes to ap_name, ap_description, fp_name, fp_comment, pr_name, pr_comment, par_name, par_comment. The bugfixes that do not influence the final LCA scores and/or interpretation.
Minor	Updates to values, units, formulas, and regions	Changes to ap_amount, ap_unit, ap_formula, ap_location, fp_amount, fp_unit, fp_formula, fp_location, pr_amount, pr_unit, par_amount, par_formula
	Updates to data uncertainties	Uncertainties and pedigree matrices (data quality indicators) of flows and parameters.
Major	Foreground LCI Activities, flows, parameters	Addition or deletion of foreground LCI Activities, flows, parameters that influence functional units.
	Function and functional units	Changes to the function and functional units of the system, except the size of functional units.
	Changes to the system background	Using new background LCI or changes to its versions (e.g. from ecoinvent 3.8 to 3.9)

3.3. Metadata

The definition of metadata can be construed according to the context and domain of application (Guerra E, 2013), though the fundamental principle remains unambiguous. It is a structured organization of information/data about data to enable its accessibility, reliability, reproducibility, and reusability. There are numerous studies and initiatives (Weibel et al., 1998; Wolfgang zu Castell et al., 2024) to harmonize general metadata design and practices in different fields. However, metadata conventions with overcomplicated definitions, taxonomies, semantics, and tools/software result in a lower adoption rate (Ulrich et al., 2022), incompleteness, and errors (Yasser, 2011). In fact, it may be argued that a poorly implemented/utilized and convoluted metadata system can be detrimental compared to its absence due to the higher probability of errors, misinterpretations, and misappropriations. The metadata structure for the LCI dataset aims to cater to human interaction while retaining simplicity and sufficiency using a minimal set of descriptors for general LCA studies. It is structured mainly for generalized LCA and is inspired by existing schema standards (DataCite, 2024; Weibel et al., 1998), and their minimalistic adaptations in other domains of research (Brandt et al., 2024; Moresis et al., 2024)

The structure of the metadata is shown in Table 3 and further detailed in the metadata template (xlsx workbook) in the supplementary material. Briefly, it consists of 7 elements, namely dataset, authors, background, license, acknowledgments, sources of primary data, secondary data sources, and glossary. These elements and their attributes encapsulate the necessary information to facilitate a qualitative understanding (by the end-user) of the inventory, context, and the associated background details. The license element provides the necessary information to set the constraints, scope, and/or limitations in the data reuse. The sources consist of bibliographic information such as identifiers (DOIs, PIDs) of the primary/experimental data and secondary literature information used in the LCI model. Conventionally, LCA studies can usually span multiple disciplines and technology types. For example, an aviation fuel supply chain can comprise technologies ranging from Fischer-Tropsch reactors to carbon capture systems. Thus, the glossary enumerates domain-specific jargons and acronyms to promote data intelligibility. This metadata structure can lay the groundwork for FAIR data sharing of inventories while minimizing the time and resources required for compilation by end-users. However, this structure has its limitations, which are further discussed in sec. 4.

3.4. Dependencies

The dependencies folder consists of all the dependencies of the foreground LCI provided as csv files. We have previously defined dataset dependencies as other foreground inventories from which the LCI of a product system inherits activities and/or flows. For instance, in the study by Terlouw (Terlouw et al., 2021), the foreground dataset of the direct air capture (DAC) system borrows exchanges from other foreground datasets, specifically the solar collector (PV) and carbon storage (CS). Thus, CS and PV act as the dataset dependencies of DAC. There are two types of dependencies. First, a foreground LCI may have to inherit certain activities or flows from other LCIs available in the literature. This is common since LCIs are usually modelled based on secondary literature rather than primary data. Second, some product systems are large and complex, such that they must be modularly built from the inventories of their sub-components (groups of activities). For example, at the German Aerospace Center, the LCIs of next-gen aircrafts are modularly constructed from the inventories of different aircraft modules such as fuel cells, LH_2 storage tanks, fuselage, etc. This approach supports both the aggregated and disaggregated assessments of the product system (aircraft) and its modules. In such cases, the dependencies and the database properties files may be used to automatically verify, import, and integrate multiple inventories to form the desired product system while minimizing import errors and maximizing data integrity. This

Table 3
The structure of the metadata file according to the life cycle inventory schema, depicting the various elements and their attributes.

Elements	Label	Definition
Dataset	Name	Name of the dataset
	Description	Detailed description of the inventory
	Year	The year of compilation of the inventory
	Language	The language used inside the inventory
	Keywords	Keywords highlighting the key technologies included in the inventory
	Type of Data	The nature of the data present in the inventory, such as primary, secondary, mixed, etc.
	LCI Model	The type of the life cycle inventory model, such as attributional, consequential, etc.
	System boundary	The extent of the system boundary, such as cradle-to-cradle, or gate-to-gate
	Functional Units	The functional units of the product system
	Region	The geographical region in which the product system is defined in the LCA study
	Time Period	The temporal range of data used to compile the inventory
	LCI Assumptions	The technology-related assumptions used in the compilation of life cycle inventory
	LCI Schema	The name and version of the LCI schema used to export the inventory. E.g., LCIS2024
Authors	Name	The names of the authors who compiled the inventory
	Email	The primary email of the corresponding author
	Affiliation	The affiliation of the corresponding author
	Comments	Other remarks concerning the authors
Background	Name	The name of the background inventory
	Version	The semantic version of the background inventory (e.g. 0.1.1).
	Type	The type of background inventory. E.g. ecoinvent has types such as consequential, cutoff, etc.
	URL	The hyperlink to the details of this inventory
	Comments	Any other comments pertaining to the use of this background
License	Name	Name of the license for the reuse of the dataset
	SPDX Identifier	The SPDX Identifier corresponding to the license name
	Attribution	Any applicable license attributions
	Obligations	Other license obligations for data source (s) that do not have an SPDX identifier (e.g., terms of use/service) (if necessary, add text of license obligations in an additional file)
	Comments	Any other comments about the license and usage
Acknowledgements	Contributors	Name of the other contributors, if applicable, and their affiliation
	Funding	If available, the relevant funding sources and/or grant names
Primary data	Type	The nature of the primary data, if applicable, that is used in the inventory. E.g., experimental, models, simulation, mixed, etc.
	Year	Year of acquisition of experimental data and/or data analysis and validation of model/simulation
	Format	The data format of the primary data
	Language	Language of the primary data
	Availability	Indication of whether the raw data is available for download from online repositories (open-access or otherwise)
	URLs	The hyperlinks or PIDs to access the primary data.
	Comments	Other applicable details regarding the nature, availability, and type of primary data.
Secondary data	Source	The nature and type of the secondary data used in the compilation of the life cycle inventory
	Year	The range of years in which the secondary data was collected
	Language	Language in which the secondary data is available. en has precedence over other languages for multi-lingual data
	Availability	Indication of whether the secondary data used in the study is available for download from the literature or digital repositories.
	DOIs	The references for the secondary data used to compile the dataset are provided as a list of digital object identifiers of secondary data sources (such as journal articles, reports, etc.).
	ISBN	The ISBN of the source of the secondary data (such as journal articles, reports, etc.) Used only when the corresponding DOIs are not available. If both are available, DOIs take precedence.
	ISSN	The ISSN of the sources of the secondary data (such as journal articles, reports, etc.). Used only when the corresponding DOI/ISBN is not available. If both are available, DOI/ISBN takes precedence
	URLs	The hyperlinks to the secondary data (such as journal articles, reports, etc.). Used only when corresponding DOI, ISBN, and/or ISSNs are not available.
	Comments	Other relevant details regarding the nature, availability, and type of secondary data.
Glossary	List of Abbreviations	The list of key abbreviations that can help read the dataset.

modular import method will be incorporated into a future version of the Python tool (sec 3.7).

3.5. Network

The network file is a directed network graph that graphically represents all the processes and their relationships within an inventory. Many LCA studies (Chen et al., 2023; Shinde et al., 2020) employ block diagrams to delineate the boundary of the product system. However, these studies refer to these diagrams as process flow diagrams, which is a misnomer. Block diagrams can only provide a high-level overview of the major components in the inventory, and do not comprise any detailed flow (material and energy) associations as in process flow diagrams, commonly used in chemical engineering (Ansarinasab et al., 2020). The necessity for such details is increasing since, as a tool, LCA is being increasingly adopted by domain experts (chemists, engineers, etc.), and not anymore limited to technology evaluators. The concept of network in this schema is borrowed from graph theory, where a network is a coupled system made up of nodes/vertices interconnected through links/edges (Lewis, 2011). This network model of systems is used in many real-world applications in the fields of biology, chemistry, economics, etc. The integration of networks into life cycle assessments also opens opportunities for future LCI research, such as supply chain optimization (Kim and Holme, 2015; Nakatani et al., 2018; Navarrete-Gutiérrez et al., 2015). In this schema, a foreground LCI is converted into a directed network graph for a detailed visual analysis and may be extended to the study of supply chain dynamics, if necessary. The network can inherit all or any essential information contained within the parent dataset. The nodes represent the activities and reference products from production flows, which are interconnected through the edges, and carry information on amounts and units of exchanges. The network file is stored as GraphML based on the xml schema, a common format for the exchange of structural data of graphs.

3.6. Environment

The environment file is a configuration file that lists all the packages needed to recreate the virtual environment in which the inventory was compiled. It is written in YAML (.yml), a human-readable data-serialization language, and allows a platform-independent replication of the LCA environment used for creating the inventory and performing impact assessments. Scientific data can often outlive (Gamalielsson and Lundell, 2010) the software applications and specific configurations used to produce it. By appending the environment configuration along with the shared inventory data, it is possible to minimize the errors in data analysis and outcomes that stem from prospective software version changes and package compatibilities.

3.7. Python tool

An open-source tool for the conversion of foreground LCIs according to the specifications of this schema is written in Python based on the Brightway framework (Mutel, C.L., 2017). For simplicity, it mainly consists of two Jupyter notebooks supported by Python scripts. It is built on top of established libraries such as NetworkX. It must be reiterated that the proposed schema is robust and is not coupled with this tool. Rather, the algorithm behind this Python tool is just one method to implement the proposed schema. The central premise is that an end-user can write their code/tool to interface with their LCA software to share life cycle inventories according to this schema. The tool is available on GitHub (Nair, 2024) through an MIT license with detailed documentation. Future updates and improvements to this tool will focus predominantly on usability and automation (e.g., ability to install as a package from PyPI or Conda, automated imports of multiple inventories by reading their dataset properties, etc.).

4. Exemplary use case and discussion

This schema is showcased through the exemplary product system of an eco-friendly aviation fuel supply chain following the Power-to-Liquid (PtL) route. The PtL concept is a promising way to sustainably produce liquid fuels and chemicals, which utilizes renewable electricity to combine hydrogen production from electrolysis, direct air capture of CO_2, and Fischer-Tropsch synthesis. The environmental evaluations of such fuel supply chains using LCA are becoming more prevalent due to the ongoing clean energy transformation across different transport sectors, including aviation. The LCA framework is guided by the ISO 14040/44 standard and is divided into four iterative stages, namely goal and scope definition, life cycle inventory modelling, impact assessment, and interpretation. The usual goal in the LCA of such fuel chains is to evaluate the life cycle environmental impacts of the LH_2 and PtL production across the entire production chain. For this exemplary case, the results are limited to the inventory that has resulted from the iterative modelling of the product system. The discussion of impact assessment results is beyond the scope of this work. The considered activities and the system boundary of the supply chain are shown as a block diagram in Fig. 2.

The LCI of this aviation fuel supply chain is compiled using a process flow approach (Suh and Huppes, 2005) for the functional units of production of 1 kg LH_2 and 1 kg PtL fuel (e-kerosene), based on lower heating value. Transportation and distribution of fuels are outside this gate-to-gate system boundary (Fig. 2). The Brightway framework, along with its user interface, Activity Browser, is used to build the LCI. Ecoinvent™ v3.9.0 acts as the background database. Foreground processes use renewable electricity (wind-based) as their primary power source. The production steps include direct air capture of CO_2, and alkaline water electrolysis (AEL), followed by the compression of hydrogen. Then, the fuel is produced using a reverse water-gas shift process, followed by Fischer-Tropsch synthesis. A hydrogen liquefaction stage leads to the co-production of LH_2. The secondary data used to construct the foreground inventory is collected from peer-reviewed scientific publications, appropriately cited within the dataset. The literature research faced numerous hurdles concerning the nature of the currently available LCI data on PtL systems. These include bottlenecks

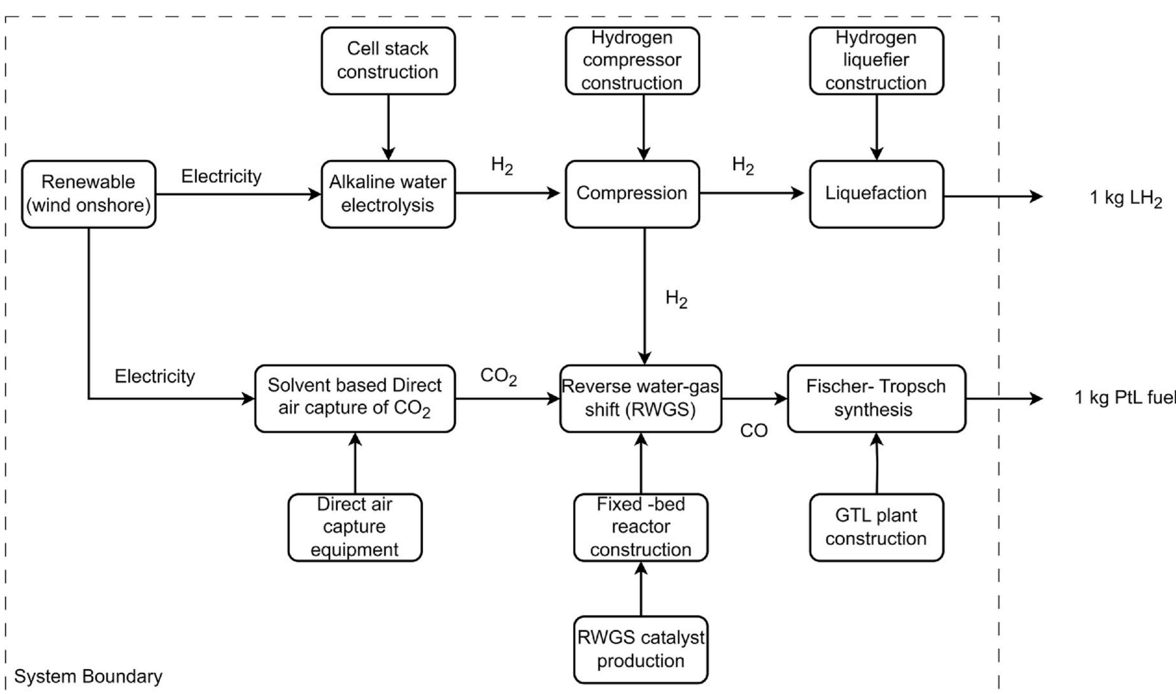

Fig. 2. Block diagram showing a high-level overview of various activities and the system boundary of the aviation fuel supply chain.

such as a) the lack of a uniform approach in sharing the inventory data, which results in data being scattered across different locations (e.g. excel files, tables, and figures, and within different paragraphs of the main document) in a peer-reviewed publication, b) missing citations, references and/or documentation regarding the data sources used in the compilation of foreground LCI, c) difficulty in linking the foreground activities to those in the background due to the missing version number and relevant details (such as geographical location) of the background database and d) lack of contextual information on the data such as technology assumptions, spatio-temporal considerations etc. During this work, the consideration and evaluation of such bottlenecks also contributed to the conceptual design and optimization of this schema's structure.

The final version of the LCI, labelled as *power-to-liquid*, is generated according to the schema as shown in Fig. 3. It is available in the supplementary information as a zip archive. The hierarchical folder structure is mainly classified into dataset, metadata, network, and dependencies. The dataset in xlsx format constitutes a well-formatted human-readable version of the dataset. The formatting of this Excel file is automated and customizable through the Python tool. The metadata expresses contextual details of the inventory in the form of descriptive, provenance, and license information. It also encapsulates the modelling assumptions, background details, and domain-specific technical glossary that are necessary for LCI comprehension with minimal reference to the parent publication.

Though the block diagram (Fig. 2) shows a high-level schematic of the product system, a detailed relationship among the various activities and exchanges cannot be easily inferred from this diagram or the tabular inventory data. Certain commercial software (e.g., Umberto™) intrinsically offers this capability since, here, the inventories are graphically assembled. In this schema, such detailed flow diagrams can be created from the network file. A graphical rendering of the network file is not included within this schema as these renders are subjective and depend on the use case, objective, and the rendering tool. However, for demonstration purposes, the network file in this use-case was rendered in Cytoscape v3.10.0 to produce the flow diagram as shown in Fig. 4. Furthermore, it can be seen that the block diagram, in Fig. 2, is essentially a subset of the network diagram, and the network file can, in theory, be used to generate consistent schematic block diagrams in LCA investigations at the desired granularity. This PtL LCI is not disaggregated into any component inventories. Hence, the dependencies folder is empty. The environment file preserves a snapshot of the production environment used in the compilation of the inventory. The provenance metadata of libraries in this file can be reviewed and executed in most operating systems (Win/Lin/Mac) through Conda or even other package managers after translation. Thus, the environment in which this LCI was created and exported can be replicated to verify, reuse, and/or modify the foreground LCI.

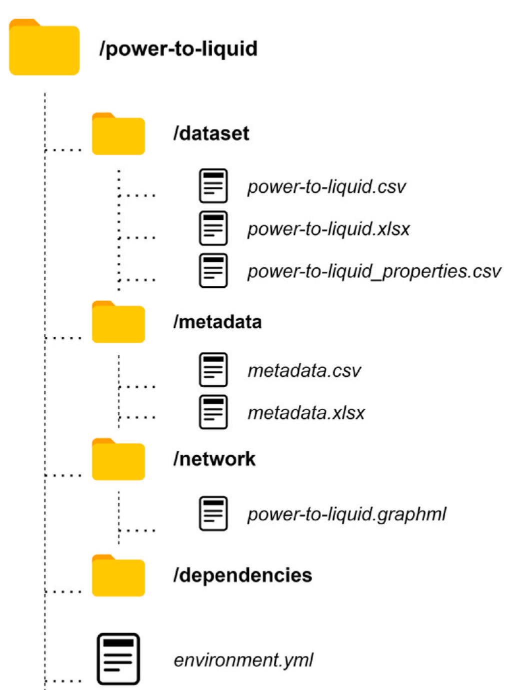

Fig. 3. The structure of the life cycle inventory, titled power-to-liquid, files that are shared according to the proposed LCIS2024 schema.

Similar to this use case, the schema can be readily applied to other product systems since the structure of its components – such as the folder structure, and metadata template – are modular and largely sector-independent, except for the foreground dataset. Once the dataset has been compiled for a generalized LCA, end-users can utilize the Python tool and the metadata template to convert the LCI according to this schema. The responsibility of data collection and quality assurance lies entirely with the LCA practitioner compiling the inventory. The metrics for data quality assessment are beyond the scope of this schema and constitute a vast research domain in their own regard (Moutik et al., 2024). The schema functions only as a medium to share and effectively communicate the foreground LCI. However, the authors recommend at least employing pedigree matrices (Weidema and Wesnæs, 1996) and assigning data uncertainties, where possible. For large product systems such as aircrafts, it is advisable to construct the inventory modularly, with each critical sub-system compiled as a disaggregated dataset. This approach can support iterative revisions during the LCA and data review post-publication. The terms "large" and "critical" are subjective and rely solely on the expert judgment of the LCA practitioner for a given analysis. Regarding metadata, the authors strongly recommend a) fully utilizing the metadata template, which demands only the most essential information; b) logging the provenance (e.g., ISBNs and DOIs) of primary and/or secondary data sources; and c) demark any forms of non-disclosable data sources in the provenance section i.e., comment fields for primary and secondary data. This is crucial to ensure the transparency of the shared dataset. A future version of the Python tool will feature a simple graphical user interface to streamline this process of metadata entry further, perform basic checks such as the resolvability of PIDs for the linked literature, and enhance overall usability. Finally, during data review by other stakeholders after the publication of LCI, the network graph can be used as a starting point to verify and crosscheck the dataset since they have a one-to-one relation as opposed to the commonly used system boundary diagram, which only provides a high-level overview.

The application of this schema has a few boundary conditions. It mainly caters to LCA research using Python (Brightway). Considering the growing relevance of LCA and the large number of available software with differing semantics for the same underlying concepts, it is practically impossible to design and maintain a functional schema compatible with all the tools and their data structure. The schema closely follows the naming conventions used within ISO 14040/44 and Ecoinvent, one of the most widely used background databases in the community (Viere et al., 2024). Due to the availability of open-access data translation layers, this schema can be theoretically extended to other LCA software. At present, such translation layers for data exchange between Brightway and other popular tools, such as openLCA are being actively developed by the open-access community, which will also be implemented as part of a future iteration of the Python tool. The schema does not address specialized analysis approaches such as prospective LCA with background scenarios. For FAIR data sharing, the authors recommend future revisions and extensions to this schema to meticulously tailor it to the exigencies of such esoteric LCA methods. The metadata structure does not tackle datasets and/or dependencies that fall under the category of restricted/redacted data that is protected by non-disclosure agreements. In such cases, even though the metadata

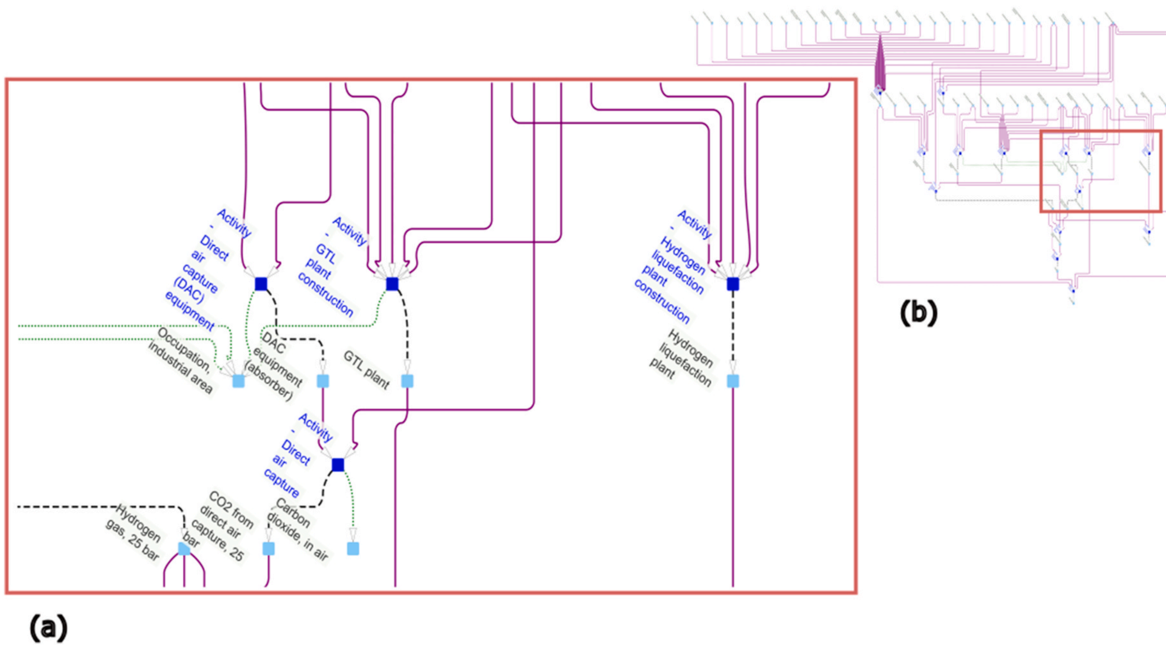

Fig. 4. A magnified section (a) of the network diagram (b) plotted from the life cycle inventory for the production of aviation fuel. *Legend: purple (solid), black (dashed), and green (dotted) lines indicate technosphere, production, and biosphere flows, respectively. Activities are indicated as blue nodes. The magnified section zooms in on the red-colored rectangular area in the network (b).*

could identify such restrictions, reconstruction of the foreground LCI would become impossible due to the lack of data. Nonetheless, this challenge of data restriction transcends LCA research and extends to all scientific domains striving to adopt the FAIR data principles. Finally, the metadata is currently generated in the csv and xlsx formats mainly for the purpose of simplicity. For specialized LCA approaches, the metadata structure may need to be extended to include more elements and attributes such as scenario details, assumptions behind parametrization, etc. In such cases of nested information structure, JSON-LD (JavaScript object notation for linked data) is more efficient than csv for machine accessibility. This is because, in such situations, features of JSON-LD, such as representation of relationships and interoperability with other linked data sources may supersede the simplicity and ease of use offered by csv files, making JSON-LD an optimal choice.

5. Conclusion

Life cycle assessment is an exponentially growing research field with large amounts of heterogeneous data from different technical domains being published as part of LCA datasets. It is difficult to design a singular and panoptic schema that can support all types of foreground LCIs without a considerable increase in complexity and usability. Unlike the standards and templates that exist in quantitative analysis and experimental data collection (e.g. PXRD, NMR databanks), it may not be feasible to harmonize an inventory schema for all domains of LCA research due to the intrinsic subjectivity in LCA (Seidel, 2016), variants, platform dependence (Lopes Silva et al., 2019), backgrounds, various modelling approaches, and requirements. However, as a method, LCA is witnessing an increasing research interest in the literature, and studies of technologies that claim novel findings about the life cycle environmental footprints of emerging technologies are becoming ubiquitous. Despite this, there is a lack of emphasis on sharing LCI data that is used to generate these LCA outcomes, leading to irrefutable results and conclusions. Hence, this generalized schema aims to *set the wheels in motion* to address the reproducibility crisis (Baker, 2016) that is creeping into the LCA research community due to the lack and/or incomplete sharing of the foreground LCI datasets associated with investigated product systems.

The adoption of this schema in future LCA studies can improve the data accessibility and transparency of the inventories in peer-reviewed published literature. This can improve the reuse of LCI datasets and support the transparent comparisons of the life cycle impacts of product systems across studies and regions. Furthermore, this can also indirectly aid the quality and reliability of LCA background databases, which often source data from such published literature. Future research is recommended in the direction of extending this schema to specialized LCA approaches such as prospective and social life cycle assessments.

CRediT authorship contribution statement

Rahul Ramesh Nair: Writing – original draft, Validation, Methodology, Conceptualization, Visualization, Software, Formal analysis, Writing – review & editing, Investigation. **Komal Mallesh Chougule:** Writing – review & editing, Data curation. **Juan Camilo Gomez:** Writing – review & editing, Data curation. **Urte Brand-Daniels:** Supervision, Funding acquisition, Writing – review & editing, Resources, Project administration.

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 Information

- Life cycle inventory dataset of the exemplary use case of aviation fuel production that is structured according to this proposed schema.
- The metadata template file (.xlsx) for life cycle inventories that is recommended by this schema.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jclepro.2025.146120.

Data availability

Data is shared in the supplementary material. Code is available at DOI: 10.5281/zenodo.12200856

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