

Technical Guidance

Supplementary document to the PAS
2090:2025, Pharmaceutical products – Product
category rules for environmental life cycle
assessments – Specification

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Document Information

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Supplementary document to the PAS 2090:2025, Pharmaceutical products – Product category rules for environmental life cycle assessments – Specification

Leading organization [Pharmaceutical LCA Consortium](#)

Liability statement

This Technical Guidance has been developed to support companies in conducting Life Cycle Assessments (LCAs) for pharmaceutical products in alignment with the principles and requirements of PAS 2090. It is intended as a practical aid to facilitate understanding and implementation of LCA best practices within this context.

While every effort has been made to ensure the accuracy, relevance, and completeness of the information provided, this document does not constitute a formal interpretation of PAS 2090, nor does its use guarantee compliance with the standard. Users of this guidance are solely responsible for ensuring that their own LCA methodologies, data, and reporting meet all applicable requirements of PAS 2090 and any other relevant standards, regulations, or contractual obligations.

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Sustainable Markets Initiative

Version 1.1 change log

Page	Section	Figure/ Table/ Note	Change
11	Introduction	NA	Change Life-Cycle for Life Cycle
20	4.4 geographical scope	NA	change Section 5.1.2 for Section 4.4
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74	5.6 Packaging manufacturing modelling rules	table 41	<p>Move the introductory text "Tertiary packaging can be modelled using the datasets provided in Table 41." and table 41 to 5.6</p> <p>Change the numbering and linked references of all tables 39 and 40</p>
77	5.8.1 Key parameters		Change the words "table 12" to "table 13"
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81	5.8.2 Transport scenarios	Table 43	Review the words as per the PDF
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89	5.11.2	NA	<p>Change the whole paragraph to the attached</p> <p>The PAS 2090 prescribes the recovered content cut-off approach for recycled content and end-of-life impact, as defined in clause 3.1.35. The product generating the waste is cut off at the point of collection: it bears no recycling or recovery process burdens and receives no end-of-life credits. Recovered materials or energy enter the next product system burden-free, and any burdens associated with the recovery process (e.g. material recycling, incineration for energy recovery) are accounted for in that next life cycle.</p> <p>In some cases, alternative allocation approaches may offer additional insights, though their results must always be reported separately to remain compliant with PAS 2090. Such methods can be useful for sensitivity or comparative analyses, but the recovered content cut-off approach remains the required method for PAS 2090-compliant LCAs.</p>
89	5.11.3	NA	Change the words "table 21" to "table 22"

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Page	Section	Figure/ Table/ Note	Change
94	5.11.4.1	NA	Change the words "table 22" to "table 23"
96	6.2	NA	Change the words "Annex B, Table B.1" to "Annex A, Table A.1"
98	Appendix I	NA	Change the words "Table B.1" to "Table A.1"
101	Appendix II	NA	Change Life-Cycle for Life Cycle

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Acronyms and abbreviations

ABS	Acrylonitrile Butadiene Styrene
API	Active pharmaceutical ingredients
BSI	British Standards Institution
CHP	Cogeneration of heat and power
CMO	Contract manufacturing organisation
CO ₂	Carbon dioxide
COD	Chemical oxygen demand
DC	Distribution centre
DOC	Dissolved organic carbon
DP	Drug product
DS	Drug substance
EF	Environmental Footprint
EoL	End-of-life
EPS	Expandable polystyrene
ETBE	Ethyl tert-butyl ether
FU	Functional unit
g	Gram
HDPE	High density polyethylene
HMDS	Bis(trimethylsilyl)amine
HVAC	Heating, Ventilation, and Air Conditioning
IEA	International Energy Agency
kg	Kilogram
km	Kilometre
kWh	Kilowatt-hour
l	Litre
LCA	Life Cycle Assessment
LCS	Life Cycle Stage
LDPE	Low density polyethylene
LHV	Lower heating value
LUC	Land use change

m ³	Cubic meter
mAb	Monoclonal antibodies
mg	Milligram
MJ	Megajoule
NaHMDS	Sodium bis(trimethylsilyl)amide
P	Phosphorus
PA	Polyamide
PC	Polycarbonate
PCR	Product Category Rules
PE	Polyethylene
PEF	Product Environmental Footprint
PET	Polyethylene terephthalate
PiE	Product-in-Environment
pkm	Person kilometre
PLA	Polylactic acid
PP	Polypropylene
PS	Polystyrene
PU	Polyurethane
PVC	Polyvinyl chloride
PVDC	Polyvinylidene chloride
PTFE	Polytetrafluoroethylene
RP	Representative product
SAN	Styrene-acrylonitrile
SDS	Safety data sheets
SKU	Stock keeping unit
t	Tonne (metric tonne=1000kg)
THF	Tetrahydrofuran
TOC	Total organic carbon
TMSCI	Trimethylsilyl chloride
tkm	Tonne kilometre
WW	Wastewater
WWTP	Wastewater treatment plant

Introduction

The [Pharmaceutical Life Cycle Assessment Consortium](https://www.pharmalcaconsortium.com/) (“Pharma LCA Consortium”) is made up of eleven members: AstraZeneca; GSK; Johnson & Johnson Innovative Medicine; Merck KGaA, Darmstadt, Germany; MSD; Novartis; Novo Nordisk; Pfizer; Roche; Sanofi; Takeda Pharmaceuticals; and SLR Consulting as project management entity. The creation of the consortium was led by the Pharmaceutical Environment Group (PEG) and the Sustainable Markets Initiative (SMI) Health Systems Task Force. The consortium has sponsored the development of a standard through the British Standards Institution (BSI), Quantis is the Technical Author of the Standard. The PAS 2090:2025 <https://knowledge.bsigroup.com/products/pharmaceutical-products-product-category-rules-for-life-cycle-assessments-specification>, Pharmaceutical products – Product category rules (PCR) for environmental life cycle assessments – Specification, was published 30 November 2025. In the present document, the standard will be referred to as PAS 2090.

The aim of this technical guidance is to support the practical application of the PAS 2090. It also uses the key findings from Representative Product (RP) studies conducted by Quantis, as well as from pilot projects led by Pharma LCA consortium members. These studies were based on the initial PCR draft and contribute to refined recommendations for Life Cycle Stages (LCS) modelling, including guidance on data requirements, calculation approaches, and background dataset selection.

This technical guidance is divided in two parts. Part I provides general recommendations and findings from the development of the PCR and testing of its early versions. Then, Part II mirrors Sections 4, 5 and 6 of the structure of PAS 2090, providing complementary guidance to the equivalent section, such as suggestions on dataset selection from third-party data providers, calculation examples and illustrations of approaches. This document is targeted at LCA practitioners that seek to conduct an LCA in alignment with PAS 2090, to support conformity with PAS 2090 in offering practical interpretation of its requirements and facilitate adoption of the standard following its publication.

→ *The aim of this technical guidance is to support the practical application of the PAS 2090.*



I. General recommendations

To support the development of a successful and credible LCA aligned with PAS 2090, practitioners are encouraged to follow these overarching recommendations across planning, stakeholder engagement, methodological choices, and execution.

Lay the groundwork

- **Understand the product and process**
Develop a supply chain map of all manufacturing processes life cycle stages of the product, including upstream and downstream flows and the manufacturing network (locations, roles, and responsibilities).
- **Define a “single source of truth”**
Establish a centralised, agreed-upon data collection sources for relevant data points and storage location to ensure consistency across studies and teams.
- **Plan for iteration and time**
Conducting LCAs is an iterative process. Allocate enough time for refinement, feedback, and stakeholder engagement throughout the process.



→ *These recommendations are complemented by the results of the representative product (RP) studies and pilot studies, which offer practical insights into the environmental profiles of pharmaceutical products.*

Engaging the right stakeholders

- **Start with people, not data**
Identify the key internal stakeholders and process owners early, such as finance, planning, sustainability, product lead, drug substance and drug product experts, packaging, operations, and involve them from the beginning.
- **Clarify roles and responsibilities**
Establish a clear governance model, outlining who is responsible for data ownership, review, decisions, and the audiences of the LCA study results.
- **Engage suppliers early**
Where possible, collaborate with suppliers and contract manufacturing organisations (CMO) with support from internal stakeholders to improve data quality.

Choosing methods

- **Select an appropriate modelling approach**
Selected modelling approach (e.g., system boundaries, allocation procedures, data granularity, systematic inclusion or exclusion of non-attributable activities) and assessments should reflect the intended use of the results and remain consistent with PAS 2090 requirements. Where applicable, alignment with organisational objectives and sector-specific guidance can support coherence across assessments.
- **Plan for results aggregation**
Determine how results will be aggregated (e.g., by market geography, product lines, or sales volume) to support meaningful reporting and decision-making.

Ensuring transparency

- **Document assumptions and decisions**
Keeping thorough and accessible documentation of modelling choices, data sources, system boundaries, and assumptions provides the basis for traceability, verification, and future updates.

These recommendations are complemented by the results of the representative product (RP) studies and pilot studies, which offer practical insights into the environmental profiles of pharmaceutical products. Together, they provide a general orientation on typical impact distributions and can help identify environmental hotspots early in the assessment process, supporting more targeted data collection and modelling efforts.

1.0 Representative products and pilot studies

After completing the first draft of the PCR, various pharmaceutical products were selected for LCA to test and refine its rules. These LCAs were conducted in two sets of studies: the RPs, for which the analysis was led by Quantis, and the pilot studies, which were modelled and analysed by the consortium members.

For reference, the system boundaries for the LCA of pharmaceutical products evaluated in the RPs and pilots are found in “**Figure 1 – System boundary for pharmaceutical products**” of PAS 2090 (see the PAS 2090 for further details of inclusions and exclusions).

The products chosen for the RP and pilot studies covered the following aspects:

- | | |
|--|--|
| <ul style="list-style-type: none"> • Therapeutic purposes: <ul style="list-style-type: none"> • Curative treatments. • Preventive vaccines. • Disease management. • Administration methods: <ul style="list-style-type: none"> • Infusion. • Injection. • Nasal. • Inhalation. • Oral. • Drug substance production methods: <ul style="list-style-type: none"> • Recombinant proteins. • Monoclonal antibodies (mAb). • Live attenuated virus. • Cell therapies. • Peptides. • Small molecules. | <ul style="list-style-type: none"> • Products sold with or without device. • Storage and transport: <ul style="list-style-type: none"> • Refrigerated or frozen conditions (particularly biologics and vaccines). • Ambient temperatures. • Transportation with or without air transport. • Use stage location: <ul style="list-style-type: none"> • Administration by healthcare professional in or outside of hospital settings. • Home administration. • No specific scenarios for end-of-life. |
|--|--|

The following sections (1.1 to 1.4) focus on the material aspects of LCA for pharmaceutical products, based on insights gained from said RP and pilot studies. The PEF method was applied (Zampori & Pant, 2019) to determine the most relevant impact categories, LCS and processes. Note that these analyses are indicative and refer to the outcomes of a limited sample of products, hence, findings cannot be generalized for all individual pharmaceutical products. Product design choices and environmental improvement initiatives can significantly shift environmental hotspots over time. This highlights the need for iterative and flexible LCAs to reassess hotspots as improvements are implemented.

Nota Bene: the trends presented emerge from a limited number of studies, performed using a previous version of the PCR, developed as a draft for the PAS 2090, and shall be considered as general information. They must not overrule any findings from future studies performed using PAS 2090.

1.1 Overall trends

Across the LCAs performed for both the RPs and pilot studies, some common trends were observed regarding the main contributors to the environmental footprint of pharmaceutical products.

In terms of impact categories, climate change, fossil resource use, mineral and metal resource use, and particulate matter consistently emerged as the most significant contributors to total environmental impact.

Regarding most relevant LCS, DS manufacturing was identified as the dominant contributor across nearly all relevant impact categories. This stage typically drives impacts through energy consumption, use of raw materials and waste treatment. The distribution and use stages also showed notable contributions in certain cases, primarily through transportation and consumables. Though their relative importance may vary depending on the product's formulation, storage conditions, and administration route.

Conversely, the DP manufacturing and end-of-life (EoL) stages generally exhibited the lowest contributions across all studied impact categories. However, these findings should be interpreted as indicative trends based on a limited sample of products rather than generalised conclusions for the entire pharmaceutical sector.

Overall, the results underscored the importance of detailed modelling within DS manufacturing, as well as the potential influence of packaging, device manufacturing, and distribution stages depending on product characteristics.

1.2 Most relevant impact categories

The set of impact categories corresponds to the [Environmental Footprint \(EF\) reference package 3.1](#) released by the European Commission. The most relevant impact categories are those cumulatively contributing to at least 80% of the PEF single score, starting from the largest to the smallest contribution. Note that weighting factors are based on value judgements on the respective importance of the life cycle impact categories considered (Zampori & Pant, 2019).

The most relevant impact categories of RPs and pilots included:

- Climate change
- Fossil resource use
- Mineral and metal resource use
- Particulate matter

Additional impact categories identified as relevant across the RPs and pilot studies were:

- Water use
- Human toxicity (non-cancer)
- Human toxicity (cancer)
- Acidification
- Freshwater ecotoxicity¹
- Photochemical ozone formation
- Freshwater eutrophication
- Terrestrial eutrophication
- Ozone depletion

¹ Results for toxicity-related impact categories may be underestimated, due to the limited availability of the respective characterisation factors for certain substances.

The following categories were not identified as most relevant for either the RPs or the pilots:

- Ionising radiation
- Marine eutrophication

The main drivers of the average relevant impact categories are further discussed in sections 1.3 and 1.4. While other impact categories were not consistently among the most relevant across all RPs and pilots, they may be significant for other products and should be considered on a case-by-case basis.

1.3 Most relevant life cycle stages

In alignment with the PEF method, the most relevant LCS are those cumulatively contributing at least 80% to any of the most relevant impact categories that are identified, starting from the largest to the smallest contribution within that impact category.

From the RP studies and pilots:

- Drug substance manufacturing was the most relevant LCS for all relevant impact categories.
- Distribution stage occasionally resulted in significant impacts for some products for all relevant impact categories.
- Overall, packaging had a low contribution to the total score, with higher relevance for mineral resource uses, relative to other impact categories.
- For products including a device, said device represented one of the most relevant LCS in some cases, but not consistently across all products. This indicated that the presence of a device did not always drive the overall environmental impact.
- Use stage was relevant for a subset of products requiring certain medical devices like needles, consumables or direct emissions of aerosol products, which can drive significant environmental impacts.
- Drug product and EoL stages had low relevance across all impact categories of the studied products, as Product-in-Environment (PiE) considerations were not included in this assessment.

Table 1 shows a summary of the above findings, with most relevant LCS for all products marked with an X, whereas most relevant LCS for some products are marked with (X).

Table 1. Relevant contribution of LCS per most relevant impact category from RPs and pilots.

Most relevant impact category	LCS						
	Drug substance	Drug product	Packaging	Device	Distribution and storage	Use	End of life
Climate change	X			(X)	(X)	(X)	
Resource use, fossil	X				(X)	(X)	
Resource use, mineral	X		(X)	(X)	(X)	(X)	
Particulate matter	X				(X)	(X)	

Most relevant LCS for all products are marked with X, whereas most relevant LCS for some products are marked with (X).

1.4 Most relevant processes

The most relevant processes are those that cumulatively contribute at least 80% (aligned with the PEF threshold) to any of the most relevant impact categories identified across all LCS, starting from the largest to the smallest contribution within each category.

Table 2 presents the most relevant processes identified from the RPs for each impact category. Only these processes are listed in the table. Due to confidentiality constraints, an analysis of the most relevant processes for pilot studies was not conducted.

Table 2. Most relevant processes per impact category from the RPs. Relevance of process for impact category is marked with an “X”.

LCS	Process	Most relevant impact category (relevance of process for impact category is marked with an “X”)			
		Climate change	Resource use, fossils	Resource use, minerals and metals	Particulate matter
Drug substance manufacturing	Energy	X	X	X	X
	Reagents / precursors	X	X	X	X
	Solvents	X	X	X	X
	Growth medium (biologicals)	X	X	X	X
	Catalysts (synthetics)			X	
	Non-attributable chemicals & other materials (sterilisation, cleaning)	X	X	X	X
	Consumables (biologicals)			X	X
	Direct emissions				X
	Other (solid and liquid) waste*	X	X	X	X
	Drug product manufacturing	Energy	X	X	
Materials for formulation (e.g. excipients, consumables)		X			X
Packaging & device manufacturing	Energy (forming, assembly, filling...)	X	X	X	
	Raw materials (packaging / device composition)	X	X	X	X
Distribution	Product transport	X	X	X	X
	Product collection	X	X	X	X
Use stage	Consumables (production and disposal)	X	X	X	X
End-of-Life	Packaging disposal	X	X	X	X
	Device disposal	X	X	X	X

* Waste impact comprises impact of solvent waste treatment and hazardous solid waste treatment.

There is a set of processes that drive the environmental footprint of pharmaceutical products. The drug substance manufacturing LCS, often the most impactful LCS, includes most of the processes influencing all most relevant impact categories:

- Energy
- Reagents/precursors
- Solvents
- Growth media
- Non-attributable chemicals
- Solid and liquid waste treatment.

For other LCS, the following processes were consistently found as key drivers for all the relevant impact categories:

- Raw materials in the packaging and device manufacturing LCS
- Transportation steps in the distribution LCS
- Consumables in use stage
- EoL of packaging and device materials (especially aluminium and plastic) in EoL stage.

Compared to other LCS, the processes within the drug product manufacturing stage of the evaluated products were contributing to a maximum of two of the most relevant impact categories. Energy in this stage contributes to climate change and fossil resource use, and materials for formulation (e.g., excipients, consumables, etc.) show relevance to climate change and particulate matter impacts.

Any other processes not listed in [Table 2](#) were not identified as significant for the relevant impact categories of the RPs but may be relevant for other impact categories.

The results of the pilots generally confirm the observed trend for RPs, except for one study with significant impact arising from water supply in the DS stage. Sporadically, results included other relevant processes:

- air freight needed for transportation within the DS manufacturing stage,
- propellant emissions during use stage,
- the catalysts having more relative contribution in other relevant impact categories.



Overall, the results highlight common patterns observed across the assessed cases, offering insight into the main drivers of environmental impacts within pharmaceutical life cycle stages based on a sample of products. The findings presented in this chapter are intended for informational purposes and should be interpreted accordingly.

II. Technical guidance of PAS 2090

This section is drafted to mirror the structure of the PAS 2090. Sections 1, 2 and 3 of PAS 2090 are not discussed in this document. The technical guidance starts at chapter 4: Life Cycle Assessment. *Where a section does not apply, it has been intentionally left blank.*

4.0 Life Cycle Assessment

4.1 Goal of the life cycle assessment

In accordance with PAS 2090 and ISO 14044, the goal of the life cycle assessment (LCA) must be clearly defined by addressing the following four elements:

- a. the intended application;
- b. the reasons for performing the study;
- c. the intended audience for the communication of results; and
- d. whether comparative assertions resulting from the study are intended to be publicly disclosed.

These elements form the foundation of the LCA study and directly influence key methodological decisions. Such as the functional or declared unit, system boundaries, geographical scope, and review requirements. For example, if the LCA is intended to generate cradle-to-gate LCA results for internal company use, a simplified scope and internal review may suffice. In contrast, a comparative public claim would require harmonised boundaries and an independent critical review.

The goal of the study will shape the scope of the LCA, notably (but not limited to): declared and/or functional unit, system boundaries and geographical representativity. Sections 4.2 to 4.4 contain some tips intended to support the definition of said aspects.



→ *These elements form the foundation of the LCA study and directly influence key methodological decisions.*

4.2 Declared unit

The declared unit is the reference quantity that must be used following PAS 2090, irrespective of the chosen system boundaries. It should be physically measurable, unambiguous, and relevant to the recipient. If the system boundaries include any packaging (primary, secondary, tertiary), the specification shall be included in the declared unit as per PAS 2090. It is recommended to specify the point of delivery or boundary in the declared unit.

Some examples of use cases could include:

- Customer-facing LCA of drug substance for pharmaceutical customer: 1 kg of packaged bulk drug substance at production warehouse exit gate.
- Reporting a product footprint to a regulator or procurement body: 1 pack of 32 x 500 mg paracetamol ready for distribution from producer's final packaging site.

A functional unit should be defined as indicated in PAS 2090 where relevant for the goal of the study, but also for product comparisons in accordance with ISO 14044.

4.3 System boundaries

The system boundaries shall be defined in accordance with the study's goal and scope, specifying whether the assessment is cradle-to-grave or cradle-to-gate, clearly stating the selected gate.

Note that all attributable activities, inputs, and outputs within the defined perimeter shall be included. Non-attributable processes, capital goods and infrastructure (e.g., employee travel, R&D) are included only when relevant to the study's objective. Clearly document any such inclusions in the inventory.

Document all assumptions, inclusions, and exclusions, particularly regarding non-attributable activities and boundary cut-offs, to maintain transparency, reproducibility, and alignment with the standard's requirements.

4.4 Geographical scope

It is recommended to refer to Section 4.4 of PAS 2090, which provides detailed requirements on reporting and modelling the geographical scope of life cycle stages, as well as to the informative Annex B, where illustrative examples (Cases A, B and C) are provided to support consistent application of these rules.

4.5 Allocation rules

Guidance on the application of allocation rules can be found in [5.3.2](#), [5.4](#) and [5.5](#), where the allocation burdens for modelling chemical products and co-products are shown.

When applying system expansion or substitution, it is recommended to use production-mix datasets rather than market-mix datasets (e.g. in ecoinvent), as the latter includes transport to the entry gate. Using datasets that include transportation impacts in substitution may lead to an overestimation of the credit assigned to the substituted material.

4.6 Cut-off criteria

It is important to note that, as per PAS 2090, no cut-off is allowed for the bill of materials (BOM) of drug substance and drug product LCS, with further specification in the respective LCS sections.

4.7 Impact categories

Refer to PAS 2090 for specific requirements of the impact categories.

5.0 Life cycle inventory modelling

This chapter includes information to support modelling calculations and recommendations of background datasets to be used for modelling in each life cycle stage.

When preparing the life cycle inventory for pharmaceutical products, the following general recommendations should be considered to ensure consistency, transparency, and completeness:

- Perform mass balance checks to confirm that all relevant flows are accounted for and that material inputs reflect net quantities, including yields, losses, and internal recycling, rather than gross or theoretical amounts.

$$\text{Input} = \text{Output} + \text{Loss} + \text{Waste}$$

- A specific mass balance to be conducted is also the water balance. Account for all water inflows and outflows, including process water, cleaning water, and wastewater.
- Check unit consistency across data points (e.g., mass, energy, and volume units) and apply appropriate conversion factors when combining data from multiple sources and when applying LCI datasets.
- Document all data sources, assumptions, and exclusions clearly to enable transparency and reproducibility.
- Prioritize data quality in accordance with the defined data quality requirements.
- Ensure alignment with system boundaries and functional unit definitions established in the goal and scope phase.

The datasets in this document are based on the [ecoinvent database v3.11 cut-off \(2024\)](#), as it is one of the most used databases for LCA. While this document references ecoinvent due to its widespread use, practitioners are reminded that other relevant datasets and databases may also be available and should be considered where appropriate. Some relevant databases include:

- [ecoinvent database](#): wide range of sectors and global scope.
- [Sphera's Managed LCA Database](#): covers various industries, including energy, transportation, materials, chemicals, packaging, electronics, etc. with global scope
- [US LCI by NREL \(National Renewable Energy Laboratory\)](#): predominantly for environmental impact of material, products and processes in US.
- [Agri-footprint by Mérieux NutriSciences | Blonk](#) and [World Food LCA Database \(WFLDB\) by Quantis](#), with focus on agricultural goods.

Note that dataset names may have different English spelling than this document.

Geographical references are removed from the dataset name, as this is the choice of the practitioner, except where some guidance or specification has been given in the standard. PAS 2090 specifies where the use of primary data is mandatory.

In cases where primary data is not available and the use of secondary data is allowed; users may follow the recommended datasets provided here. However, if primary data or more representative datasets are available, for example, from other databases offering greater technological or geographical accuracy, these should take precedence to increase data quality of the study.

5.1 Overall requirements

5.1.1 General

Note the PAS 2090 requirements for use of supplier-specific data.

5.1.2 Data quality requirements

Under PAS 2090, practitioners are required to ensure that data quality is consistent with the goal and scope of the study and to document the quality and source of data used for each key impact driver. This includes specifying whether the data applied in the life cycle inventory (LCI) are primary, secondary, or proxy. The objective is to increase transparency and reproducibility of the assessment by linking each major contributor to its data source type and quality.

To apply this requirement in practice:

- Identify the most impactful process (also called the primary impact driver) for each environmental impact category.
 - Example: For the climate change category, electricity use is found as the main contributor.
- Report the activity data for that process.
 - Example: Document the total electricity consumption (e.g., kWh per functional unit or per process).
- Indicate the data source type used to model this process:
 - Primary data measured or directly collected from operations.
 - Secondary data obtained from LCI databases.
 - Proxy data estimated or substituted when no representative dataset is available.
- Repeat this procedure for each life cycle stage and for all impact categories assessed, ensuring that the data source and quality are clearly reported for every major input or output contributing significantly to the results.

Some examples (non-exhaustive) on setting data quality requirements based on the goal and scope are shown in Table 3.

Table 3. Examples of data quality requirements definition according to LCA goal and scope.

Goal and Scope	Example of data quality requirements
Internal, early-stage assessment to obtain an overview of environmental hotspots and main contributors across life cycle stages.	<ul style="list-style-type: none"> • Primary data on the minimum required inputs and outputs for the LCS under focus. • Use default secondary data for all other stages. • Accept broader technological and geographical representativeness.
Internal decision-making or supplier engagement, focusing on improving data accuracy for key hotspots.	<ul style="list-style-type: none"> • Measured primary data on energy, water, and main materials used in DS & DP manufacturing. • Representative secondary data for upstream suppliers and downstream activities.
Internal and external communication, tracking progress toward climate or sustainability targets.	<ul style="list-style-type: none"> • Primary data for all manufacturing sites and critical suppliers contributing >20% of impacts. • Secondary datasets are region- and technology-specific. • Evaluation and reporting of data completeness, representativeness, and uncertainty per life cycle stage.
External disclosure, verification, or comparative assertions (e.g., public reports, certifications).	<ul style="list-style-type: none"> • Auditable primary data for all direct operations and critical suppliers. • Perform a data quality assessment as per PAS 2090 requirements.

5.1.3 Secondary data

Apart from dataset suggestions for specific materials or processes, some examples of application of secondary data choice as per PAS 2090 are developed in other sections of this document (5.2.2 Energy consumption modelling, 5.3.2 Chemical products, 5.4 Drug substance manufacturing modelling rules, 5.5 Drug product manufacturing modelling rules). Pay attention to the database requirements listed in section 5.1.3 PAS 2090.

5.2 Energy modelling

5.2.1 Allocation at product level

According to PAS 2090, the inventory on energy demand for the assessed product(s) in manufacturing stages can be developed using three data sources: data at product level, data at building level, and data at site level.

In practice, the quality and granularity of available energy data vary significantly between organisations and facilities. Therefore, a structured approach is required to ensure that the allocation of energy demand across processes and products is transparent and consistent. Where product data or process is not available, building-level or site-level data can be used, with allocation keys applied to distribute the energy consumption. The choice of allocation key should be based on a physical or causal relationship with the assessed product as per PAS 2090.

Each organisation has its own configuration for manufacturing operations; therefore, there may be different ways to allocate energy demand per process or product. Supporting buildings, such as wastewater treatment (WWT) facilities, should be carefully reviewed. If primary data on the energy demand of WWT is available for use in the assessment and secondary datasets for WWT are also applied, the energy demand included in the secondary dataset should be removed to avoid double counting and to ensure that primary data is prioritised.



Figure 1 provides a stepwise approach for determining how to allocate energy data depending on the level of data availability (site, building, or process level). The figure should be read in combination with the recommended allocation guidance Table 4 (allocation approaches by data availability), Table 5 (examples of allocation keys for different product categories and manufacturing stages), and Table 6 (allocation methods for multi-stage and multimodality sites).

Figure 1. Decision tree for allocating energy demand data based on data availability.

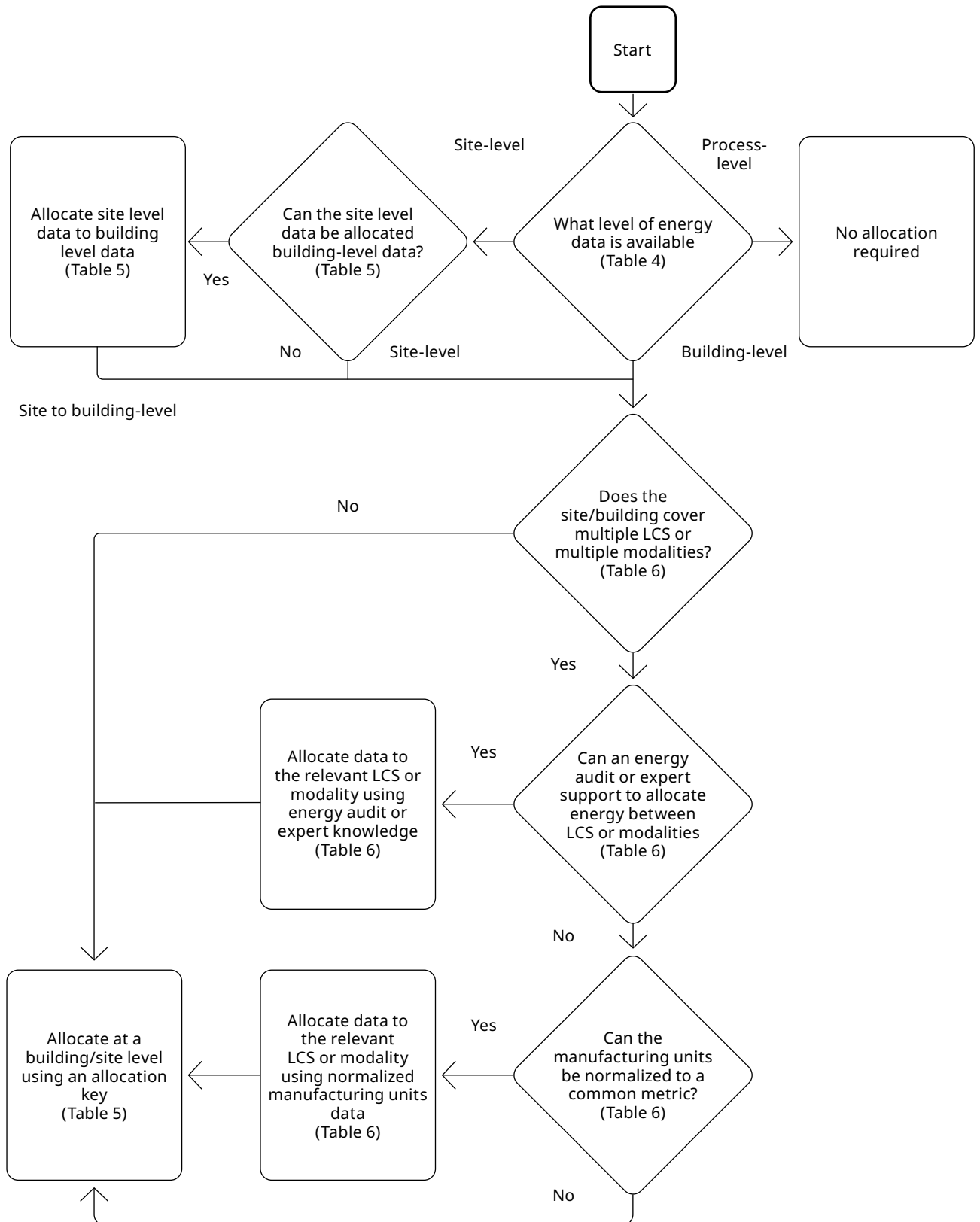


Table 4. Recommended approaches for allocating energy demand according to data availability.

Availability of data	Recommended approach
Site level data	<p>Option 1 Use allocation key to allocate site to building level.</p> <p>Classify buildings of the site into a) production building b) in scope supporting building (e.g. WWT) c) out of scope building (to be excluded from the analysis). Remove any in scope supporting buildings if the activity is already covered by secondary datasets (e.g. WWT).</p> <p>Option 2 Use allocation key to allocate site to product level.</p>
Building level data	<p>Option 1 Use allocation key(s) to allocate energy to product level for each building in scope.</p> <p>Option 2 Use an allocation key to allocate the energy of supporting buildings to production buildings (e.g. by area). Then use further allocation key to allocate energy to product level.</p>
Building level data, separated between activities (such as manufacturing and overheads)	Use best available allocation key(s) to allocate energy across products for each activity in scope.
Process specific data	<p>Identify which steps include process level data and which steps do not.</p> <p>Sum process level data for each product per process step, considering the yield output (see Equation 1, page 27).</p> <p>Where process level data is not available: utilize site level or building level data to estimate process level data.</p>

Table 5. Examples of allocation keys for different pharmaceutical product categories and manufacturing stage.

Allocation key	Recommended approach for...				
	Small molecule drug substance	Biologic drug substance	Drug product	Pack	Device
Number of units/ production volumes	N/A	N/A	Tablet, capsule, vial, etc.	Stock keeping unit (SKU), box, piece of packaging etc.	Inhaler, syringe, device unit etc.
Mass	kg of API	kg of bulk DS	kg of formulated product (for liquids, a volume unit may be more appropriate)	kg of packs	kg of filled devices
Floor area			m ²		
Room volume			m ³		
Time in plant/ Machine hours			hours/days		
Number of batches			count of batches		
Cost to manufacture			Relevant currency (EUR, USD, etc.)		

Table 6. Recommended energy allocation methods for multi-stage and multimodality sites of site/building-level energy data.

Context	Recommended approach A (energy based)	Recommended approach B (floor area based)	Recommended approach C (normalization based)	Default
<p>Multiple lifecycle stages</p> <p>The site/building is involved in more than one LCS of the product manufacturing process.</p>	<p>Use expert knowledge or energy audit data to allocate energy to specific modality.</p> <p>Example: biologics DP floor uses more HVAC so should consume more energy than biologic packaging floor. Between the two buildings, biologics DP should be attributed more than 50% of the energy consumption.</p>	<p>Allocate the energy to a specific LCS using floor area.</p> <p>Example: Packaging takes place in floor 1, devices in floor 2. Between the two floors, each floor gets 50% of the energy consumption.</p>	<p>Normalize the allocation keys prior to performing allocation.</p> <p>Example: convert each SKU into kg of API, or convert each kg of API into number of tablets etc.</p>	<p>Use equal shares, see Table 4.</p>
<p>Multimodality</p> <p>The site/building manufactures products from vastly different modalities with very different energy needs.</p>	<p>Use expert knowledge or energy audit data to allocate energy to specific modality.</p> <p>Example: biologics DS building has a higher energy consumption through HVAC compared to the synthetic DS building. Between the two buildings, biologics DS should be attributed more than 50% of the energy consumption.</p>	<p>Allocate the energy to a specific modality using floor area.</p> <p>Example: building 1 for synthetic DS production has an area of 50,000m², building 2 for biologic DS production has an area of 100,000m². 33:66 allocation to each.</p>	<p>N/A</p>	<p>Use equal shares, see Table 4.</p>

Note: Recommended approach A (energy-based) is preferred over approach B (floor area-based), which is preferred over approach C (normalization-based). All three are more robust than the default equal-share allocation.

Once process level data is available or obtained, the concatenation of processing steps should account for the output yield of each step.

Equation 1

$$\text{Energy}_i = e_{i,1} \frac{1}{Y_{i,2}Y_{i,3}\dots Y_{i,N}} + e_{i,2} \frac{1}{Y_{i,3}\dots Y_{i,N}} + e_{i,3} \frac{1}{Y_{i,4}\dots Y_{i,N}} \dots + e_{i,N}$$

Where:

i= product index (e.g. Product 1, Product 2)

s= step index (e.g., process step 1, process step 2, ...)

e_{i,s}= energy of step *s*, reported per unit of output (e.g. kg) of that step.

Y_{i,s}= yield of step *s* for product *i* (fraction output/input)

Energy_i = total energy per product, in energy unit (e.g. kWh) per product output (e.g. kg).

Each earlier step is divided by all downstream yields, since more intermediate material is needed to end up with 1 unit of final product.

Building on this framework, the following section provides three worked examples that reflect real manufacturing configurations, see overview in Table 7.

Table 7. Overview of energy allocation modelling examples.

Example	LCS	Allocation key	Short description
A	Synthetic drug substance	Mass	This example demonstrates an allocation method for a synthetic drug substance facility, using batch size and number of synthesis steps to distribute energy consumption
B	Packaging	Floor area	This example covers a packaging case, where building-level utility consumption is allocated based on floor area, due to the dominance of HVAC (Heating, Ventilation, and Air Conditioning) and lack of suitable production-based allocation keys.
C	Biological drug substance	Time	This example introduces a time-based allocation approach across multiple buildings representing distinct process steps (fermentation, recovery, and purification), with further adjustments for product-specific yields (applying Equation 1).

Together, these examples provide some solutions for translating facility-level energy data into product-level environmental impacts, in alignment with PAS 2090.

Example A for energy allocation

Data at building level for synthetic drug substance

In this example, yearly energy consumption data is available at the building level, but not per product or process step (Table 8).

Table 8. Example A energy allocation - Data on energy consumption per year.

Energy carrier	Consumption [kWh/year]
Steam	6 200 000
Electricity	2 200 000

The building is dedicated to batch production of synthetic drug substances, with each product requiring a different number of synthesis steps yielding different batch sizes. In this example, data on the number of synthesis steps and final mass of product are available, however the intermediate output quantities per steps are not known.

In accordance with PAS 2090 section 5.2.1(b), energy use is allocated to all product outputs from the building using mass as a common physical parameter, with the number of synthesis steps used to approximate the process intensity. This allocation method is based on the assumption that both the final mass of product and the number of synthesis steps are directly related to energy use. Mass captures the production volume, while the number of synthesis steps serves as a proxy for process complexity and operational intensity. This combined metric is applied to allocate more complex and energy intensive processes with proportionally greater share of the building-level energy consumption.

$$\text{final mass product [kg]} \times \text{number of synthesis steps}$$



Table 9 summarises the manufacturing data of this building: synthesis steps, batch size, number of batches per year, and the resulting weighted production (kg × number of synthesis steps).

Table 9. Example A energy allocation - Data on production volumes and synthesis steps per product.

Product ID number (#)	Number of synthesis steps (A)	Amount produced per batch [kg/batch] (B)	Batches produced per year [batch/year] (C)	Annual amount and NSS (D = A × B × C)
1	1	8.0	1	8
2	9	1.3	14	168
3	9	36.5	6	1 971
4	8	37.0	21	6 216
5	2	11.0	4	88
6	7	9.7	2	136
7	11	37.0	6	2 442
8	3	44.7	34	4 559
9	8	28.0	26	5 824
10	5	28.0	8	1 120
11	2	6.5	9	117
12	7	16.3	9	1 027
13	2	7.7	86	1 324
Total	-	-	-	25 000

Using the total burden (25 000 kg•number of synthesis steps/year), the building level energy is allocated as follows:

$$\text{Steam} = \frac{6\,200\,000 \text{ kWh/year}}{25\,000 \text{ kg} \bullet \text{ number of synthesis steps/year}} = 248 \frac{\text{kWh}}{\text{kg} \bullet \text{NSS}}$$

$$\text{Electricity} = \frac{2\,200\,000 \text{ kWh/year}}{25\,000 \text{ kg} \bullet \text{ number of synthesis steps/year}} = 88 \frac{\text{kWh}}{\text{kg} \bullet \text{NSS}}$$

These energy consumption rates can now be used to estimate energy consumption for any product made in this building. For instance, hypothetically, an LCI shows that product #7 of this building is utilized at 3 g or 0.003 kg (30 tablets of 100 mg) for a given functional unit. Based on the data from Table 9, this product would require 11 synthesis steps, then the energy requirements are estimated as shown in Table 10.

Table 10. Example A energy allocation - Data for energy consumption rate applied to product #7.

Energy carrier	Energy consumption [kWh/kg ×NSS]	Product #7		Energy consumption per FU [kWh/FU] (D = A × B × C)
		Quantity per functional unit [kg/FU]	Number of synthesis steps	
		(A)	(B)	
Steam	248	0.003	11	8.2
Electricity	88			2.9

It should be acknowledged that this method provides an estimation per product, however it has limitations, as some intermediate manufacturing stages may not have been active during the reporting year, or that processes can be operated at different scales across different time periods. If more granular data were available, such as information on when specific synthesis steps took place, corresponding yields, etc., the accuracy of the estimations could be improved, albeit with additional effort.

Example B for energy allocation

Data at site and building level for packaging

Similar to example A, in this example the yearly energy and other utilities consumption data is available at the building level, but not per product or process. The goal is to allocate the data at the process level, for an intermediate process step of the packaging LCS.

This building handles a wide variability of product types and outputs, for which an allocation based on mass, batch, or unit count is impractical. Floor area was therefore selected as the most suitable allocation key, as it is practical and consistently available across processes. This choice is also supported by the fact that HVAC systems, which scale with spatial volume, represent the primary energy demand in the facility.



This approach assumes that HVAC demand scales proportionally with floor area, which may not hold true for all process types or unevenly loaded facility areas. Alternative allocation keys, such as machine hours or process duration, could provide a more precise representation of energy use for directly attributable processes; however, such data are often unavailable or inconsistent across production areas.

In this example, the area where the relevant process takes place represents 2% of the total building area; this factor is applied equally to all utilities. Table 11 summarises the building-level data and the corresponding attributable share allocated to the process.

Table 11. Example B energy allocation - Data on energy, water, steam and electricity consumption per year allocated to process based on area.

Energy carrier/flow	Consumption of building	Unit	Allocation factor %*	Attributable share to process	Unit
Cooling water	600 000	kWh/year	2%	12 000	kWh/process
Steam	900 000	kWh/year		18 000	kWh/process
Purified water	700	m ³ /year		14	m ³ /process
Electricity	700 000	kWh/ year		14 000	kWh/process

* Calculated based on the floor area where the process takes place and total building area.

The resulting attributable shares can be further scaled per product by dividing by the total output in units, mass or volume produced. When assessing the impacts of these flows, it is important to verify whether the energy for water purification, steam production or other utility generation is already included in the reported consumption data. It should also be noted that building-level data may not capture site-wide energy uses, such as shared utilities, warehousing or distribution losses. Where relevant for the goal and scope of the LCA, these should be included within the system boundaries and allocated appropriately (see also [Table 4](#)).

Example C for energy allocation

Data at building level for process

In this example, a company has yearly energy consumption data available at the building level within a site and per year, but not per product or process. The drug substance manufacture follows a sequential process consisting of fermentation, recovering and purification. The site comprises three buildings, each hosting one or more of these process stages for each product.

The company has data on yearly output quantities per product and process step.

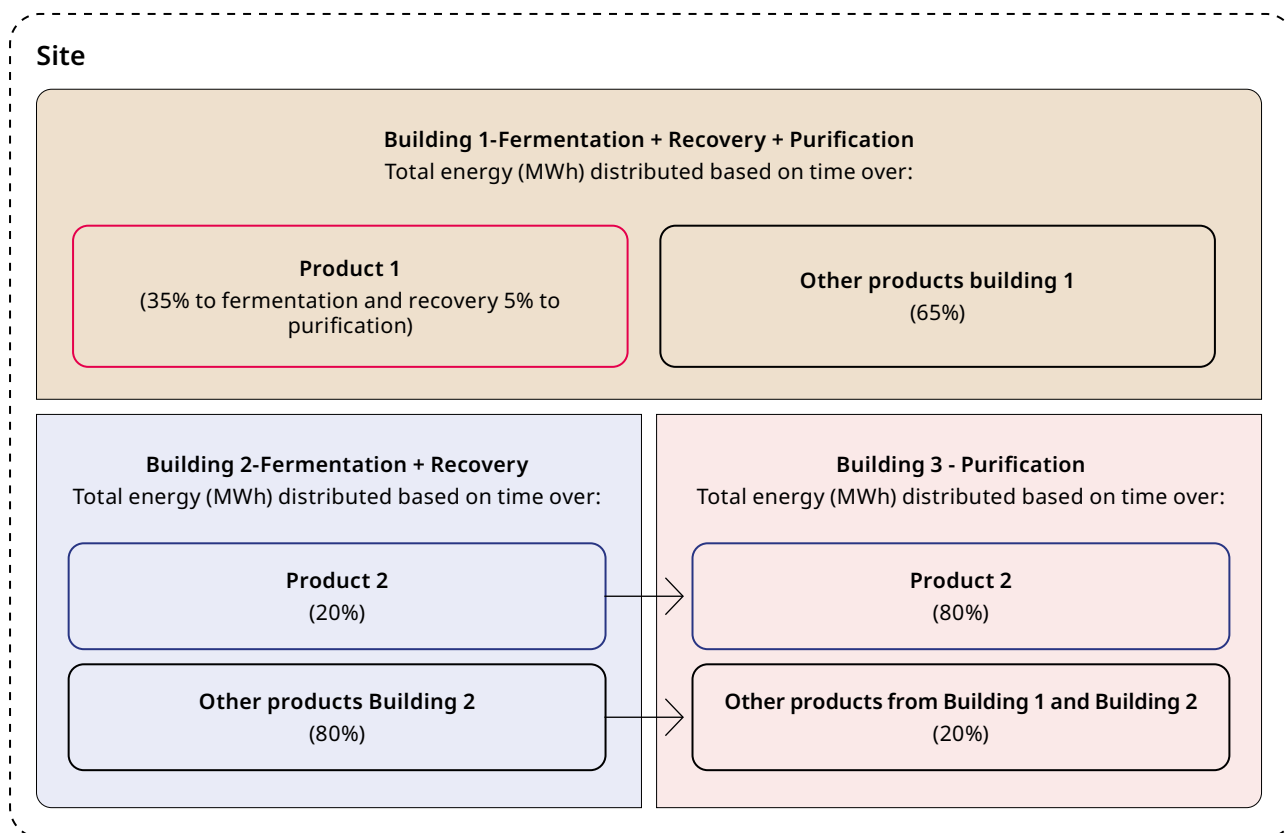
Figure 2 shows a simplified flow mapping of products manufactured at each building.

Several products are manufactured here, but the goal is to estimate the energy consumption for Product 1 and Product 2, per kg of product.

Because direct metering at the process or product level is not available, a first allocation based on time spent is applied. Each product’s share of energy is calculated based on the proportion of time it was produced in a given building over the course of a year. This is determined based on the number of batches for each product and each production step in each building and the time used per batch (including downtimes), all these data points are tracked by the company. The product flows of Product 1 and Product 2 and their time shares across the three buildings can be summarised as follows:

- Building 1 hosts the full production of Product 1, including fermentation, recovery, and purification. Based on its production time share, 35% of the building’s energy consumption is allocated to Product 1, while the remaining 65% is attributed to other products made in the same building.
- Building 2 is used for fermentation and recovery of Product 2, as well as other products. Product 2 accounts for 20% of the building’s operational time, and receives 20% of its energy; the rest (80%) is assigned to other products.
- Building 3 handles purification. Here, Product 2 accounts for 80% of the operational time, and receives a corresponding share of energy use. The remaining 20% is allocated to other products, which may originate from Building 1 or Building 2, and are purified in Building 3.

Figure 2. Example C energy allocation - Illustration of product flows between buildings and time allocation of product per building.



The energy per building, distributed based on time, is presented in Table 12, along with relevant information on process breakdown and yield. Although Product 1 and Product 2 undergo the same processes, they differ in function, properties, and specifications. Additionally, the reported produced amounts associated with each product and process vary significantly. Therefore, an additional allocation step is required to account for the process intensity per unit of output, as shown in Table 12.

Table 12. Example C energy allocation - Building-level energy distribution by product and process step (based on time and yield of process).

Building	Total energy consumption of building (electricity) [kWh/year]	Product	Process	Time allocation share [%]	Energy allocated to product and process based on time [kWh product*-year]	Amount produced [kg of active kg of product/year]	Energy allocated to product and process per unit of output [kWh/kg process output*year]
	(A)			(B)	(C = A × B)	(D)	(E = C ÷ D)
1	33 000	Product 1	Fermentation and recovery	35	11 550	12 600	0.92
			Purification	5	1 650	4 600	0.36
2	42 000	Product 2	Fermentation and recovery	20	8 400	3 200	2.63
3	3 600	Product 2	Purification	80	2 880	1 600	1.8

Now that process- and product-specific energy consumption has been calculated, it is possible to estimate the combined energy demand for the fermentation, recovery, and purification steps of Product 1 and Product 2. To determine the impact per kilogram of product (after purification), the yield of the purification process must be taken into account. This yield is required to calculate the necessary input quantities from the preceding fermentation and recovery stages. The yield of the purification step is known and is specific to each product.

The energy consumption per product is calculated using the Equation 1, which specifically for this example would be:

$$\text{Energy}_i = e_{i,p} + \frac{e_{i,f}}{Y_{i,p}}$$

Where:

i = product index (Product 1 or Product 2).

$e_{i,p}$ = energy of purification of product i , obtained from Table 12 (E column), in kWh per kg product.

$e_{i,f}$ = energy of fermentation and recovery of product i , obtained from Table 12 (E column), in kWh per kg product.

$Y_{i,p}$ = yield of purification of product i , available at the company and available in Table 13 below (C column), in % output per input.

A summary of the data and calculated results for energy consumption per product is presented in Table 13 below. Although the process steps are the same, the differences between Product 1 and Product 2 and respective yields are captured in this allocation procedure, leading to the estimation of specific energy consumption per unit of product mass.

Table 13. Example C energy allocation - Calculation of total energy consumption per product.

Building	Product	Energy consumption of fermentation and recovery ($e_{i,f}$) [kWh/kg process output*year] (see Table 12, column E) (A)	Energy consumption of purification ($e_{i,p}$) [kWh/kg process output*year] (see Table 12, column E) (B)	Yield of purification process ($Y_{i,p}$) [%] (C)	Energy allocated to product [kWh/kg product] (see applied Equation 1 for this example) (D = B + (A ÷ C))
1	Product 1	0.92	0.36	55%	2.0
2	Product 2	2.6	1.8	60%	6.1

Note: some calculations may not match on second digit due to rounding.

Although both products follow the same process steps, their yields and process intensities differ. The allocation approach described above captures these differences, allowing estimation of specific energy consumption per unit of product mass.

The time-based allocation method was selected as a practical and transparent approach to allocate building-level energy consumption data. Production time per product and process step is routinely tracked by the company, allowing for a verifiable and data-driven allocation of energy. Alternative allocation keys, such as floor area, are considered less suitable because physical space does not necessarily correlate with energy demand due to differences in process intensity.

However, this method has some limitations. It assumes that energy consumption per unit of time is constant within each building, without differentiating between operating modes such as active production, cleaning, or downtime. Consequently, potential variations in process intensity or equipment efficiency are not captured. The method also does not consider product-specific characteristics that may influence energy use, such as differing temperature or pressure requirements.

5.2.2 Energy consumption modelling

5.2.2.1 Overall requirements

Modelling of fuel and heat supply

This section recommends a list of datasets to be used for i) upstream impact of the energy supplied to manufacturing facilities (Table 14) and for ii) supply and combustion of the fuel (heat) that can be used for manufacturing and use stages (Table 15). If a dataset for the required energy carrier is unavailable, an approximation can be done by using a dataset of a similar fuel of the same source (i.e. biogenic or fossil).

Information of the technology consuming the fuel in the facility should be obtained, as the environmental impacts could be significantly different:

- Cogeneration of heat and power (CHP) plant: produces electricity and steam or hot water
- Heat dedicated units (non-CHP): furnace or boiler technologies to produce direct heat gas, steam or hot water for processes

If the technology is unknown, a conservative assumption should be made and the dataset with higher impact per functional unit should be chosen.



For the distribution stage, default energy carrier for storage steps is electricity and default transport datasets for transportation scenarios (see section 5.8.2, [Table 41](#)) already account for fuel supply and combustion.

Note that the datasets recommended in [Table 14](#) can be used to model the upstream impact of the fuel at the entry point to the facility (prior to combustion), whereas [Table 15](#) datasets refer to the output heat of the combustion.

The choice to use [Table 14](#) or [Table 15](#) depends mostly on data availability:

- If the output heat is known and primary data on measured combustion emissions are available, use the datasets listed in [Table 14](#) to represent the upstream impacts of the fuel, and apply the primary data for the on-site combustion process. As specified in PAS 2090, where heat is supplied by a CHP (combined heat and power) system, allocate impacts in accordance with the PAS 2050 method (BSI, 2011).
- If the output heat is known but measured combustion emissions are not available, or if the heat is purchased externally, use the datasets listed in [Table 15](#). These datasets already include the upstream impacts of the fuel; therefore, the datasets from [Table 14](#) must not be added.
- If heat/steam outputs are unknown but fuel input quantities are known, use the datasets listed in [Table 15](#) to estimate combustion emissions per unit of fuel input. In this case, the dataset should be adjusted to express impacts per unit of fuel consumed:
 - Identify the amount of fuel input represented in the dataset.
 - Change the reference flow from 1 MJ or 1 kWh to the corresponding amount of fuel (kg, m³, etc.).
 - Check that the fuel unit in the dataset corresponds to the unit of the primary data, based on the energy content reported or a defined specific energy value.
 - Verify that all inputs and emissions are correctly scaled, and that the dataset now calculates impacts per unit of fuel consumed rather than per MJ of heat output.

If the energy carrier for industrial or district heat is unknown, use site-specific data where available, regional statistics, or refer to [IEA statistics](#) for representative heat sources in the relevant region.

Table 14. Recommended datasets for energy supply*.

Energy carrier	Recommended datasets	
Natural gas	Market for 'Natural gas, low pressure'.	
Coal	Anthracite or hard coal	Market for 'Hard coal'.
	Lignite	Market for 'Lignite'
	Other coal or unknown	Use anthracite or hard coal dataset as proxy, this is a conservative assumption.
Diesel	Market for 'Diesel'.	
Fuel oil	Heavy fuel oil	Market for 'Heavy fuel oil'.
	Light fuel oil	Market for 'Light fuel oil'.
Petrol or gasoline	Market for 'Petrol'.	
Wood	Market for 'Wood chips, wet, measured as dry mass'	
Biomethane	Market for 'Biomethane, low pressure'.	

*The datasets only include upstream impact.

Table 15. Recommended datasets for heat, including combustion and impact of energy carrier supply.

Source type	Energy carrier	Technology type*	Dataset selection
Industrial or district heat*	Natural gas	CHP	'Heat, district or industrial, natural gas heat and power co-generation, natural gas, conventional power plant, 100MW electrical'.
	Non-CHP	<p>'Heat, district or industrial, natural gas heat production, natural gas, at industrial furnace >100kW'.</p> <p>'Heat, district or industrial, natural gas heat production, natural gas, at boiler modulating >100kW'.</p>	
Coal	Hard coal	CHP	Heat, district or industrial, other than natural gas {TW} heat and power co-generation, hard coal
		Non-CHP	Market for 'Heat, district or industrial, other than natural gas heat production, at hard coal industrial furnace 1-10MW'.
	Lignite	CHP	'Heat, district or industrial, other than natural gas heat and power co-generation, lignite'.
		Non-CHP	'Heat, central or small-scale, other than natural gas heat production, lignite briquette, at stove 5-15kW'.
Other or unknown	CHP or Non-CHP	Use anthracite or hard coal heat dataset as proxy, this is a conservative assumption.	
Wood Non-CHP		CHP	'Heat, district or industrial, other than natural gas heat and power co-generation, wood chips, 6667 kW'.
			'Heat, district or industrial, other than natural gas heat production, wood chips from industry, at furnace 5000kW'.
Biomethane		Non-CHP	Market for 'Heat, central or small-scale, biomethane'.
Oil		CHP	'Heat, district or industrial, other than natural gas heat and power co-generation, oil'.
Fuel oil	Heavy fuel oil	Non-CHP	'Heat, district or industrial, other than natural gas heat production, heavy fuel oil, at industrial furnace 1MW'.
	Light fuel oil	Non-CHP	'Heat, district or industrial, other than natural gas heat production, light fuel oil, at industrial furnace 1MW'.
Unknown		CHP and non-CHP	Market for 'Heat, from steam, in chemical industry'.

Source type	Energy carrier	Technology type*	Dataset selection	
Local heating units**	Natural gas	Non-CHP	Market for 'Heat, central or small-scale, natural gas'.	
	Coal	Hard coal	Non-CHP	Market for 'Heat, central or small-scale, other than natural gas heat production, anthracite, at stove 5-15kW'.
		Lignite	Non-CHP	'Heat, central or small-scale, other than natural gas heat production, lignite briquette, at stove 5-15kW'.
		Other or unknown	Non-CHP	Use anthracite or hard coal heat dataset as proxy, this is a conservative assumption.
	Wood	Non-CHP	Market for 'Heat, central or small-scale, other than natural gas heat production, wood pellet, at furnace 9kW'.	
	Biomethane	Non-CHP	'Heat, central or small-scale, biomethane'.	
	Fuel oil	Heavy fuel oil	Non-CHP	'Heat, district or industrial, other than natural gas heat production, heavy fuel oil, at industrial furnace 1MW'.
Light fuel oil		Non-CHP	'Heat, district or industrial, other than natural gas heat production, light fuel oil, at industrial furnace 1MW'.	

* Technology type is subdivided into CHP and non-CHP. For some fuels, no specific CHP or non-CHP datasets were available in ecoinvent, and thus CHP and non-CHP are not consistently available for all fuels in this table.

** Oil is not used for local heating units. It is assumed that average local heating units are mostly non-CHP, based on the information of Market for 'Heat, central or small-scale' datasets in ecoinvent.

According to PAS 2090, the allocation of impacts to the CHP energy outputs can be conducted using the PAS 2050 method (BSI, 2011) or the exergy allocation method, where exergy refers to the maximum useful work obtainable from a form of energy as it moves toward thermodynamic equilibrium with its environment.

In principle, the PAS 2050 method is based on exergy as well but provides default ratios of exergy depending on the technology and type of fuel, whereas the exergy allocation method (also known as Carnot method) is more precise and requires specific temperatures of the heat output.

Allocation using PAS 2050 method

The allocation of impacts to heat and electricity relies on the process-specific ratio of heat to electricity from each CHP system.

Below is the formula to allocate the impacts to heat output:

Equation 2

$$AF_Q = \frac{Q}{Q+n \cdot E}$$

Where:

AF_Q : allocation factor of impacts for heat,

Q : heat output,

E : electricity output,

n : intensity coefficient based on useful energy.

Q and E must be expressed in the same energy unit (e.g. MJ, kWh, etc.).

The allocation factor for impacts to electricity (AF_E) is calculated as shown below:

Equation 3

$$AF_E = 1 - AF_Q$$

For boiler-based CHP systems (coal, wood, solid fuel), the coefficient n is **2.5**, while for turbine-based CHP systems (natural gas, landfill gas) $n = 2.0$. For other forms of CHP, PAS 2050 requires the calculation of the process-specific ratio.

Below (Table 16) is a typical example of heat and electricity outputs for a turbine-based natural gas CHP system, based on a fuel input of 100 MWh:

Table 16. Example of allocation of energy outputs for turbine-based natural gas CHP system, parameters for calculation according to PAS 2050.

Parameter	Value	Unit	Source
Q	55	MWh	Assuming heat efficiency of 55%
E	30	MWh	Assuming electrical efficiency of 30%
n	2.0	-	PAS 2050 intensity coefficient for turbine-based natural gas CHP system

First, the AF_Q is calculated using Equation 2:

$$AF_Q = \frac{55 \text{ MWh}}{55 \text{ MWh} + (2.0 \cdot 30 \text{ MWh})} = 0.48$$

Then, AF_E is calculated using Equation 3:

$$AF_E = 1 - 0.48 = 0.52$$

With the PAS 2050 method, the allocation factors reflect an almost equal split of environmental impacts between the electricity and heat.

Allocation using the exergy method

The allocation of impacts to heat and electricity relies on their exergy content, i.e. the maximum useful work that can be performed by the energy product. The ratio between the energy and exergy content is referred to as the quality factor.

From the thermodynamic point of view, electricity produced during cogeneration has an exergy factor of 1, so the exergy of electricity is equal to its energy ($Ex_e = E$). This means that 100% of electricity can be converted to any form of energy. In contrast, heat can be converted to power or any other form of energy only to some extent, so the heat exergy can be calculated as:

Equation 4

$$Ex_Q = \left(1 - \frac{T_0}{T}\right) \cdot Q$$

Where:

T_0 : is the average ambient temperature during the heating period in K,

T : is heat transfer media thermodynamic logarithmic mean temperature in K, calculated with equation below

Equation 5

$$T = \frac{(T_S - T_R)}{\ln\left(\frac{T_S}{T_R}\right)}$$

Where:

T_S : supply or delivery temperature in K

T_R : return temperature in K

Then, impacts are allocated to heat output through this equation:

Equation 6

$$AF_Q = \frac{Ex_Q}{Ex_Q + Ex_E}$$

Ex_Q and Ex_E must be expressed in the same energy unit (e.g. MJ, kWh, etc.).

The allocation of impacts to electricity is calculated as shown below:

Equation 7

$$AF_E = 1 - AF_Q$$

To demonstrate the application of the allocation based on exergy method, we use the example of a turbine-based natural gas CHP system, similar to the one applied under PAS 2050 (Table 17).

Table 17. Example of allocation of energy outputs for turbine-based natural gas CHP system, parameters for calculation through exergy allocation.

Parameter	Value	Unit	Source
Q	55	MWh	Assuming heat efficiency of 55%
E	30	MWh	Assuming electrical efficiency of 30%
T ₀	298	K	25 °C converted to K
T _s	393	K	120 °C converted to K Typical value for low-pressure steam for heating
T _R	333	K	60 °C converted to K

First, T (heat transfer media mean temperature) is calculated applying Equation 5, in order to obtain the efficiency factor needed to calculate the exergy of heat.

$$T = \frac{(393 \text{ K} - 333 \text{ K})}{\ln\left(\frac{393 \text{ K}}{333 \text{ K}}\right)} = \frac{60 \text{ K}}{\ln(1.18)} = \frac{60}{0.17} = 362 \text{ K}$$

Then, Ex_Q is calculated applying Equation 4.

$$Ex_{Q=} \left(1 - \frac{298}{362}\right) \cdot 55 \text{ MWh} = (1 - 0.82) \cdot 55 \text{ MWh} = 0.18 \cdot 55 \text{ MWh} = 9.8 \text{ MWh}$$

Finally, impacts to heat and electricity are calculated with the allocation factors by applying Equation 6 and Equation 7.

$$AF_Q = \frac{9.8 \text{ MWh}}{9.8 \text{ MWh} + 30 \text{ MWh}} = 0.25$$

$$AF_E = 1 - 0.25 = 0.75$$

With this method, the allocation factors show that a greater share of environmental impacts is attributed to electricity, due to its higher exergy content compared to heat.

The calculations above can be applied to other fuels, provided that the relevant parameters are collected. Temperature and heat values can be obtained from the following sources:

- Process or plant instrumentation and monitoring data.
- Thermodynamic property tables to determine enthalpy or heat content for specific streams.
- System operating data, such as flow rates and heater temperatures.

5.2.2.2 Electricity

Datasets are recommended for the electricity mix modelling at country level (Table 18), as well as datasets to be used to model renewable energy impacts (Table 19).

Following the PAS 2090 requirements, medium voltage datasets are suggested for manufacturing stages, which are associated with large industrial facilities, whereas low voltage is suggested for distribution (unknown voltage) and use stage (households). For the datasets listed in Table 19, two separate adjustment factors can be applied:

- A factor of 1.05 to account for conversion losses when converting from high to medium or low to medium voltage; and
- A factor to account for average transmission losses, which can be obtained from publicly available sources such as [World Bank - Electric power transmission and distribution losses \(% of output\)](#).

Table 18. Recommended datasets for electricity mix.

LCS	Reporting approach	Electricity mixes	Recommended dataset
Manufacturing	Market-based	Residual mix	Market for 'Electricity, medium voltage, residual mix'.
	Location-based	Consumption mix	Market for 'Electricity, medium voltage'.
Distribution	Location-based	Consumption mix	Market for 'Electricity, low voltage'.
Use stage	Location-based	Consumption mix	Market for 'Electricity, low voltage'.

Table 19. Recommended datasets for renewable energy.

Electricity sources for contractual instruments	Recommended dataset
Hydropower	Electricity, high voltage electricity production, hydro, run-of-river.
Solar power, photovoltaic	Electricity, low voltage electricity production, photovoltaic, 570kWp open ground installation, multi-Si.
Windpower	Electricity, high voltage electricity production, wind, >3MW turbine, onshore.
Geothermal	Electricity, high voltage electricity production, deep geothermal.
Nuclear	Electricity, high voltage electricity production, nuclear, boiling water reactor.

Where the country or region-specific residual grid mix is unavailable, the user can follow the PEF method section 4.4.2.3 to model this data.

5.2.3 Energy recovery modelling

All requirements and guidance for energy recovery modelling are provided in PAS 2090, including the treatment of internally recovered energy, the application of co-product rules where energy is sold externally, and the use of appropriate regional or country-specific energy mixes. Practitioners shall refer directly to section 5.2.3 and “**Figure 4 – Decision tree for modelling on-site electricity generation when electricity produced equals the consumption**” of PAS 2090 for the methodology and allocation rules.

5.3 Raw materials supply modelling rules

5.3.1 Production and packaging

In line with PAS 2090 requirements, raw materials shall be modelled as 100% virgin production when the recycled content is unknown. Where recycled content is known, it can be modelled by replacing the corresponding share of virgin material inputs with recycled-material datasets, according to the actual percentage of recycled content.

Since the cut-off approach must be applied according to PAS 2090 requirements in section 5.11.2:

- only the impacts of recycling processes (e.g., collection, sorting, reprocessing) are included within the system boundary for recycled content,
- recycled material enters the system with no upstream burden from its previous life/virgin production.



→ *In line with PAS 2090 requirements, raw materials shall be modelled as 100% virgin production when the recycled content is unknown.*

5.3.2 Chemical products

According to PAS 2090, when a chemical raw material is relevant² for the pharma LCA and the specific dataset is not directly available (e.g., from suppliers or databases), a chemical proxy model shall be modelled. This section outlines the information required and the applied procedure to create such proxies following the PAS 2090.

As indicated in “**Table 2 – Modelling chemical proxies**” of PAS 2090, in the lack of primary data, the following information is required to model a chemical proxy:

- Stoichiometric equation of the chemical reaction used to produce the compound.
- Yield.
- Energy consumption.
- Solvent use.
- Catalyst (if relevant).
- Water consumption.
- Waste.

When modelling a chemical proxy, it is also necessary to identify whether the compound is a base, specialty, or advanced chemical, as this influences the selection of default energy and input data from PAS 2090:

- “Base chemicals” are high-volume building blocks used to produce other chemical products.
- “Specialty chemicals” are value-added or function-specific compounds tailored to meet the requirements of a particular application, customer, or industry, for example, intermediates used in drug development or performance additives.
- “Advanced” chemicals (Note B in Table 2 of PAS 2090) result from complex, multi-step syntheses involving several chemical transformations, purification stages, and the use of specialised reagents or technologies.

To identify the appropriate category in practice, users may:

- Consult process or synthetic chemists familiar with the compound’s synthesis and industrial context.
- Review literature sources, patents, or safety data sheets (SDS) to understand production steps, scale, and use.
- Use retrosynthesis or chemical process modelling tools (see [Table 20](#)) to estimate reaction complexity, number of steps, and reagents required.
- Refer to chemical production statistics or supplier information (e.g. large-scale commodity vs. limited-use compound) to assess whether the compound fits the characteristics of a base, specialty, or advanced chemical.

Several retrosynthesis and chemistry modelling tools can provide relevant information for chemical product modelling, by estimating the quantities of input chemicals required to produce a given target compound. [Table 20](#) provides an overview of these retrosynthesis and chemistry modelling tools, comparing their functionalities and accessibility. The columns capture whether each tool supports retrosynthesis, forward synthesis, or both, and whether they provide postulated conditions (i.e., named reagents and solvents that underpin calculations), stoichiometry, or other relevant outputs. The table also indicates whether tools can link back to simple chemicals inecoinvent and whether they are open source or require a paid license. Empty cells represented with dashes (-) reflect cases where a definitive yes/no conclusion of the feature could be reached for the specific tool.

² According to the PAS 2090, a chemical raw material is deemed relevant if the weight % in the bill of materials is $\geq 1\%$ (it does not apply to catalysts).

Table 20. Overview of available retrosynthesis modelling tools and their features.

Tool Name	Provider	Does it give you solvent & reagent amounts and yields?	Does it give you a forward synthesis?	Does it give you other outputs?	Does the tool provide stoichiometry (quantities) of reactants?	Is this tool able to go back to the simple chemicals in ecoinvent?	Is this open source or requires a paid licence?	Does it give you a paid licence?	
AiZynthFinder	AZ	✓	✓	✗	✗	✗	-	✗	Open Source
ASKCOS	MLPDS consortium with MIT	✓	✓	✓	✗	✗	-	-	Open Source
AZsynth /Info-Chem	ICSynth	✓	✓	✓	✗	✗	✗	✗	Paid licence
ChemAIRS	Chemical AI Inc.	✓	✓	✓	✓	✗	-	✓	Paid licence
Chemprop	GitHub	✗	✗	✗	✗	✗	-	-	Open Source
EPI Suite	EPA	✗	✗	✗	✗	-	-	-	
FineChem	ETH Zurich	✗	✗	-	✗	✓	-	-	Open Source
FineChem2	ETH Zurich	✗	✗	✗	✗	✓	✗	✗	Open Source
Muir AI	Muir AI	✓	✗	✓	✓	✓	✓	✓	Paid licence
QSAR toolbox	OECD & ECHA	✗	✗	✗	✗	✗	✗	✗	Open Source
Reaxys	Elsevier	✓	✓	✓	✓	✗	✓	-	Paid licence
RXN for Chemistry	IBM	✓	✓	✓	✓	✗	✗	✓	Paid licence
SciFinder	CAS	✓	✓	✓	✓	✗	✓	✓	Paid licence
SYNTHIA® Retrosynthesis Software	Merck KGaA	✓	✓	✓	✓	✓	✓	✓	Paid licence
VEGA	Istituto di Ricerche Farmacologiche Mario Negri IRCCS	✗	✗	✗	✗	✗	✗	✗	Open Source

For a general chemical reaction:

Equation 8



Where:

A, B, C = reagents.

X, Y = products.

$\gamma, \delta, \varepsilon, \alpha, \beta$ = stoichiometric coefficients.

To calculate the mass of a given reagent (e.g., reagent A) required to produce 1 kg of product X:

Equation 9

$$m_{\text{tot}}(A) = \frac{\alpha \cdot M(X)}{\gamma \cdot M(A)} \cdot \frac{1}{\text{yield}}$$

Where:

$M(X), M(A)$ = molar masses of X and A (in g/mol).

$m_{\text{tot}}(A)$ = total mass of A required (kg).

Yield = reaction yield (expressed as a decimal).

To calculate the amount of waste from unreacted A:

Equation 10

$$m_{\text{waste}}(A) = m_{\text{tot}}(A) - \frac{\alpha \cdot M(X)}{\gamma \cdot M(A)}$$

These equations can be used to estimate material inputs and waste in LCI datasets.

In addition, to apply some of the default data (solvent and catalyst quantities), a limiting reagent should be selected. The limiting reagent is the reagent that is completely consumed first in a chemical reaction, which is determined through the chemical reaction and actual available quantities. As the actual quantities are often unknown in the context of chemical product modelling, the following recommendations can be applied:

- Limiting reagents are always the main building block, the structural foundation of the targeted molecule.
- Reagents cost can serve as an indication, in practice, the limiting reagent is usually the most expensive input in the reaction.

The necessary inputs can be modelled in combination with the datasets shown in Table 21, in the lack of primary data. Note that these datasets are generic for production of chemicals and using technology mixes. The data quality of the study can be improved with technological representativeness of the datasets.

Table 21. Recommended datasets for water supply to manufacturing.

Process or input	Recommended dataset
Catalysts (when applicable)	Metallic catalysts: Market for 'Palladium' as a common catalyst. If the catalyst is a compound, for example Palladium acetate, the content of Palladium should be modelled with the suggested dataset, along with a dataset for the respective ligand. Enzymatic catalysts: Market for 'Enzymes'
Solvents (when applicable)	If solvent is unknown: Market for 'Solvent, organic'
Water consumption	Market for 'Water, completely softened', see also Table 22
Waste treatment	Market for 'Hazardous waste, for incineration'
Wastewater	'Treatment of wastewater, average, wastewater treatment'.

Water is used for different processes in chemical product production and drug substance manufacturing, with various types of water depending on the specific requirements for purity and sterility. [Table 22](#) provides an overview of water specifications and corresponding datasets that can be utilized to model the water supply for manufacturing processes. The datasets recommendations within this section are applicable to chemical products modelling, DS and drug product DP manufacturing. It is important to note that energy inputs for purification, distillation, and other treatment processes are included in the proposed datasets. This may lead to double counting if site or building-level energy data of DS and DP manufacturing allocated to processes and products are also used. If site or building-level energy data includes energy for water supply treatment, these inputs should be removed from the proposed datasets.

Some chemical inputs may be provided as aqueous solutions, and their water content should be reflected in the model. This can be done either by selecting a dataset representing the appropriate solution concentration or by manually adding the corresponding water input. The related water output should also be included to maintain a consistent mass balance. If the exact water content of a chemical input is unknown, the practitioner may assume the use of an anhydrous dataset, for which no water balance adjustment is required.

Table 22. Recommended datasets for water supply to manufacturing.

Water specification	Description*	Recommended dataset
Tap water	Water supplied through municipal or other potable water systems.	Market for 'Tap water'
Purified water	Water processed via distillation, ion exchange, reverse osmosis, or other purification techniques to remove organic, inorganic, microbial, and particulate impurities. It must meet pharmacopeial purity requirements but is not sterile. Purified water in pharmaceuticals is mainly used for non-parenteral product formulation (oral, topical), synthesis, manufacturing processes, cleaning production equipment and vessels, and as feed water for producing higher-grade waters like Water for Injection (WFI).	Market for 'Water, deionised'
Demineralized water	Demineralized water is primarily utilized for removing dissolved minerals and ions, important in industrial applications such as boiler feed water, cooling systems, and steam generation. Distilled water can be assumed as demineralized water.	Market for 'Water, deionised'
Water for injection (WFI)	Water of the highest purity used in the preparation of parenteral solutions. WFI is produced to be free of pyrogens, microorganisms, and endotoxins, meeting stringent chemical and microbial quality standards. Sterile water can be assumed as water for injection.	Market for 'Water, ultrapure'
Other water (e.g. utilization in energy equipment, etc.)	Water primarily utilized for removing dissolved minerals and ions, important in industrial applications such as boiler feed water, cooling systems, and steam generation.	Market for 'Water, completely softened'

* Description of water specifications as per (EMA, 2020) and (WHO, 2011).

This guidance also includes some illustrative examples on how to model chemical products when datasets are not available in common commercial databases, which are summarised in Table 23. The classification of these chemicals as base, specialty, or advanced was primarily based on the technical knowledge and experience of the consortium members. Where possible, this was complemented with information from literature, supplier data, and general chemical industry knowledge.

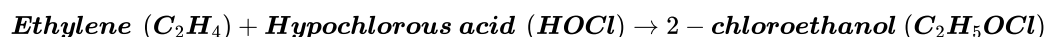
Table 23. Overview of chemical product modelling examples.

Example	Chemical product	Type	Application	Solvent or catalyst use
A	2-chloroethanol	Basic chemical	Drug substance manufacturing and other industrial uses	None
B	Boc-D-alanine	Specialty chemical	Building block in peptide synthesis and drug development	Solvent only
C	API precursor and related starting material [3-(hydroxymethyl)phenyl] boronic acid	Advanced chemical	Intermediate used MET tyrosine kinase inhibitor synthesis.	Solvent and catalyst
D	Sodium bis(trimethylsilyl) amide (NaHMD) in tetrahydrofuran (THF)	Specialty chemical	Non-nucleophilic base for deprotonation and enolate formation in organic and pharmaceutical synthesis	Solvent only

Example A

For chemical product 2-chloroethanol

The chemical reaction for production of 1 mol of 2-chloroethanol requires 1 mol of ethylene and 1 mol of hypochlorous acid (see balanced chemical equation below).



As a base chemical, the yield is assumed as 95% and the energy requirements are assumed for simple organics. The quantities of inputs are calculated by applying Equation 9, as shown in Table 24.

To select the appropriate datasets for modelling the upstream impacts of ethylene and hypochlorous acid, the hierarchy for chemical products outlined in “Figure 5 – Decision tree for selecting datasets of chemicals” is applied. Ethylene is modelled with an available direct match of dataset, whereas no dataset is available for hypochlorous acid.

Hypochlorous acid can be modelled based on publicly available information, hence it is modelled based on the chemical reaction to produce it: 1 mol of chlorine gas (produced via electrolysis of brine) and 1 mol of demineralized water. Furthermore, in this case, two products are obtained: HOCl and HCl. According to the allocation decision tree for multi-output processes illustrated in Figure 2 of PAS 2090, allocation can be avoided by applying system expansion for HCl, provided that it is known, measured and documented that substitution occurs, in line with Note 2 of Figure 2 in PAS 2090.



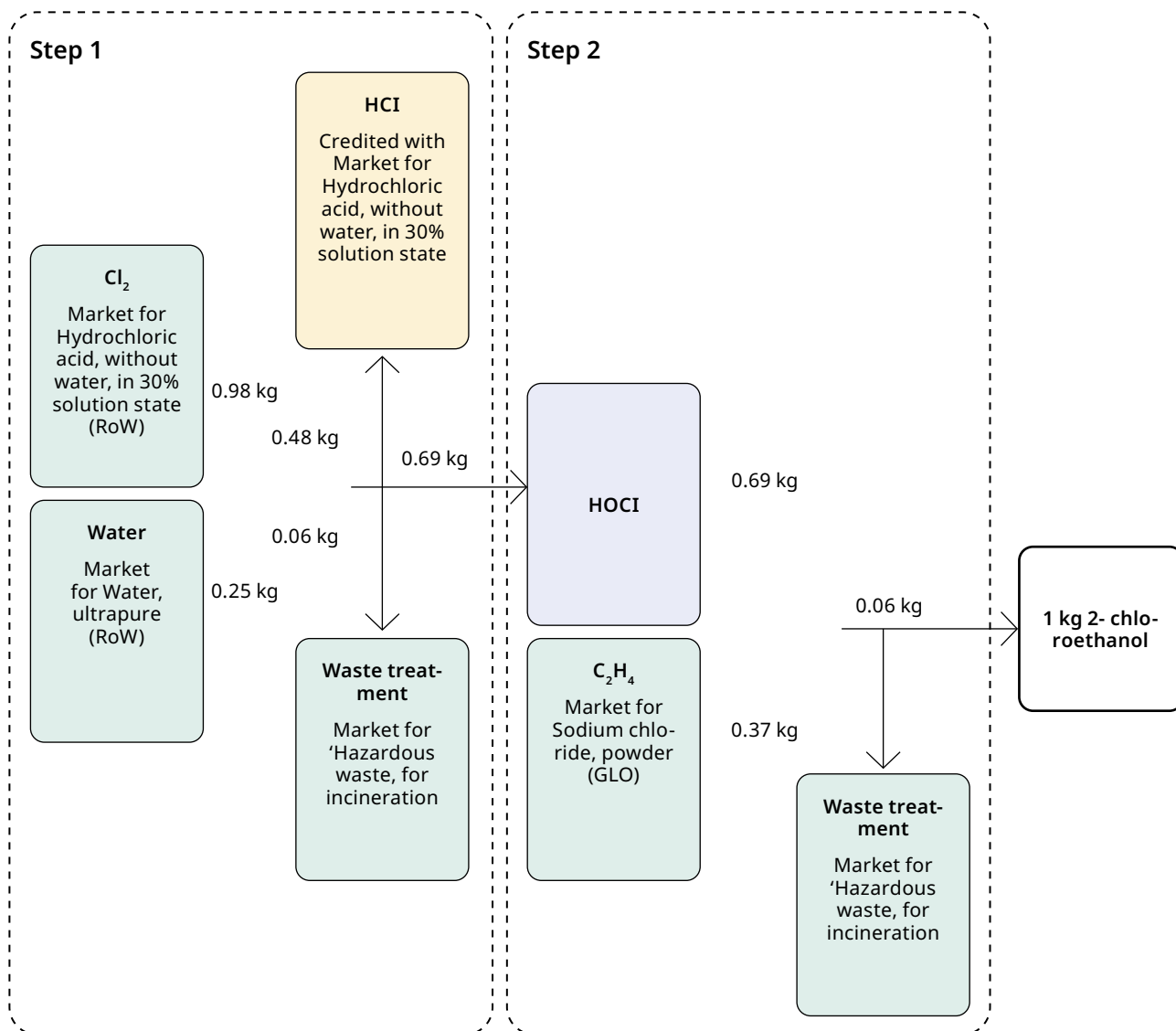
Table 24. Stoichiometry and reagent requirements for 2-chloroethanol production, including dataset recommendation.

Role	Compound	Molar mass [g/mol]	Required inputs, calculated using Equation 9	Unit of required inputs	Recommended dataset
Reagent	Ethylene (C ₂ H ₄)	28.06	0.37	kg/kg of 2-chloroethanol	Market for ‘Ethylene’.
Reagent	Hypochlorous acid (HOCl)	52.46	0.69	kg/kg of 2-chloroethanol	Modelled with chlorine gas from brine electrolysis and water.
Reagent	Chlorine gas (Cl ₂)	70.90	1.42	kg/kg of hypochlorous acid	Chlorine, gaseous sodium production, sodium chloride electrolysis, molten salt cell.
Reagent	Water (H ₂ O)	18.02	0.36	kg/kg of hypochlorous acid	Market for ‘Water, completely softened’ (see also Table 22).
Product	Hydrochloric acid (HCl)	36.46	0.73	kg/kg of hypochlorous acid	Substitution of hydrochloric acid market for ‘Hydrochloric acid, without water, in 30% solution state’.*
Product	2-chloroethanol	80.52	-	-	-

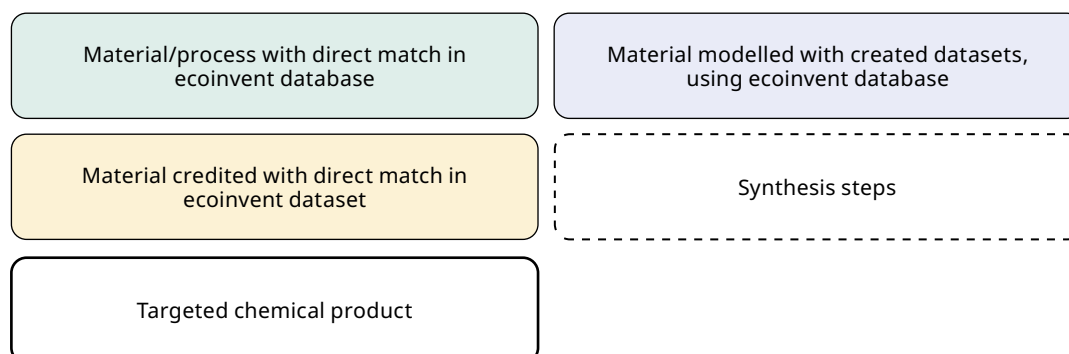
* Note that ‘Market for’ datasets include transportation impacts to entry gate, hence the credited environmental impacts may be overestimated. In this example, the ‘market’ dataset was chosen as it represents the market of hydrochloric acid production technologies.

Figure 3 summarises the production steps, mass flows and datasets of 2-chloroethanol, which combines the utilization of modelling chemical proxies (HOCl) together with dataset matching and allocation procedure, applying the PAS 2090 rules to overcome data gaps. For this chemical product, production routes are available from public sources, though it is acknowledged that a market of production technologies may not be represented.

Figure 3. Example A chemical product - Visualization of modelling of 2-chloroethanol (materials only, solvents excluded).



Legend



Additional inputs and outputs to be modelled based on PAS 2090 “**Table 2 – Modelling chemical proxies**” are listed in Table 25, scaled to the 2-chloroethanol output. Note that the same inputs and outputs apply to the production of HOCL, which are included in Table 25. These were derived by multiplying the amount of HOCL input for 2-chloroethanol production times the default data from Table 2 of PAS 2090.

Table 25. Other inputs and outputs required for modelling of 2-chloroethanol production.

Input/output	Synthesis step	Amount*	Unit [-/kg of 2-chloroethanol]	Recommended dataset
Electricity	1	0.43	kWh	Market for ‘Electricity, medium voltage’, see also Table 18.
	2	0.62		
Heat	1	1.91	MJ	Market for ‘Heat, central or small-scale, natural gas’, see also Table 15.
	2	2.77		
Steam	1	0.25	MJ	Market for ‘Heat, from steam, in chemical industry’, see also Table 15.
	2	0.36		
Water	1	15.9	L	Market for ‘Water, completely softened’
	2	23		
Catalyst	1 and 2	0 (not considered)	kg	N/A
Solvent	1	0.98	kg	Market for ‘Solvent, organic’
	2	0.69 (basic reaction)		
Waste (incl. solvent)	1	0.06 (95% molar yield) + 0.98 (solvent) = 1.04	kg	Market for ‘Hazardous waste, for incineration’
	2	0.06 (95% molar yield) + 0.69 (solvent) = 0.75		
Wastewater	1	15.9	L	‘Treatment of wastewater, average, wastewater treatment’.
	2	23		

* Amounts for synthesis step 1 are normalized to obtain the 0.69kg of HOCL needed for the production of 1kg of 2 chloroethanol through step 2 (according to the default data of PAS 2090 Table 2).

Example B

For specialty chemical Boc-D-alanine

The chemical reaction for production of 1 mol of Boc-D-alanine requires 1 mol D-alanine, 1 mol of Boc anhydride and 1 mol of sodium hydroxide.

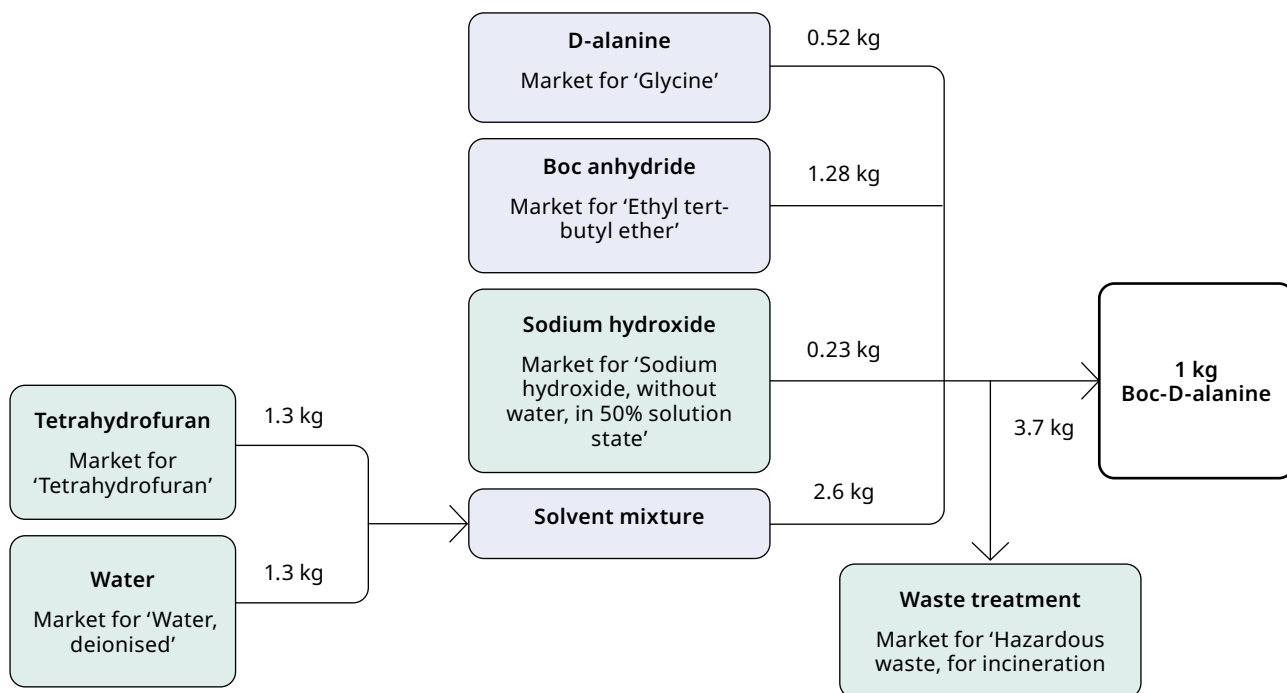
Following the PAS 2090, as a specialty chemical, the yield is assumed as 90% and the energy requirements are assumed for any other chemicals (i.e. not simple organic). The quantities of inputs are calculated by applying Equation 9, as shown in Table 26 (see also Figure 4 for visualization of the process steps). Sodium hydroxide can be modelled with a direct dataset match. However, the reagents are matched with datasets of similar materials³, following consultations with inhouse process chemists.

Table 26. Stoichiometry and reagent requirements for Boc-D-alanine production.

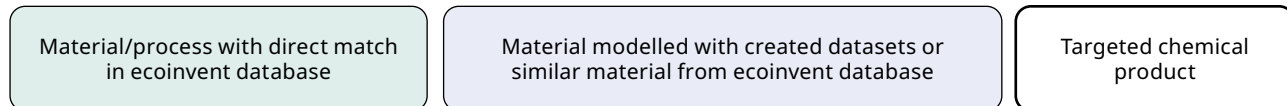
Material type	Compound	Molar mass [g/mol]	Required inputs, calculated using Equation 9 [kg/kg of Boc-D-alanine]	Recommended dataset
Reagent	D-alanine	89.09	0.52	Market 'Glycine'
Reagent	Boc anhydride	218.3	1.28	Market for 'Ethyl tert-butyl ether'
Reagent	Sodium hydroxide	40	0.23	Market for 'Sodium hydroxide, without water, in 50% solution state'
Product	Boc-D-alanine	189.2	-	-

³ **D-alanine and glycine** are both simple, single-carbon-side-chain α -amino-acids. They share similar synthesis via Strecker, enzymatic or fermentation routes that share the same nitrogen-carbon building blocks and both derive from ammonia, formaldehyde or other aldehydes and hydrogen. **Boc anhydride and ethyl tert-butyl ether (ETBE)** molecules are dominated by the tert-butyl group attached through an oxygen. ETBE: t-Bu-O-CH₂CH₃; Boc 2O: (t-Bu-O)₂C=O. From the synthesis route perspective, both compounds originate from isobutylene or tert-butyl alcohol chemistry under mild, acid-catalyzed conditions and share isobutylene/iso-butane chains as raw materials

Figure 4. Example B chemical product - Visualization of modelling of Boc-D-alanine (materials only).



Legend



Similar to example A, Table 27 shows the modelling of other required inputs and outputs for Boc-D-alanine. Following the default data from “**Table 2 – Modelling chemical proxies**” of PAS 2090, Boc-D-alanine is classified as a specialty chemical. As such, its energy requirements per unit of product are higher than those of simple organics. Additionally, the use of solvents must be considered, in this case, THF in water. THF was selected as a representative solvent because it is commonly used in pharmaceutical synthesis, following consultation with inhouse process chemist.

Table 27. Other inputs and outputs required for modelling of Boc-D-alanine production.

Input/output	Amount	Unit [-/kg of Boc-D-alanine l]	Recommended dataset
Electricity	65	kWh	Market for ‘Electricity, medium voltage’, see also Table 18.
Heat	212	MJ	Market for ‘Heat, central or small-scale, natural gas’, see also Table 15.
Steam	13	MJ	Market for ‘Heat, from steam, in chemical industry’, see also Table 15.
Water	23*	L	Market for ‘Water, completely softened’**.
Catalyst	0 (not considered)	% of limiting reagent amount	N/A
Solvent	2.6 kg of solvent mix= 1.3 kg THF + 1.3 kg water (specialty chemical step, 5 kg/kg of D-alanine)	kg	Market for ‘Tetrahydrofuran’. Market for ‘Water, deionised’, see also Table 22**.
Waste	3.7 kg + 1.3 (90% molar yield and solvent waste)	kg	Market for ‘Hazardous waste, for incineration’.
Wastewater	23 + 1.3	kg	‘Treatment of wastewater, average, wastewater treatment’.

* Default data from PAS 2090

** Water completely softened is used for utilities, water deionised is used for the solvent solution.

Example C

For chemical product API precursor and starting material

This example illustrates how to model a multi-step route (retrosynthesis of a pharmaceutical API precursor, see Figure 5) and how to apply PAS 2090 default data consistently at each step. This example is based on a publication of the synthesis of a precursor for MET kinase inhibitors (Dorsch, 2015), for which the solvents and catalysts in each step are known.

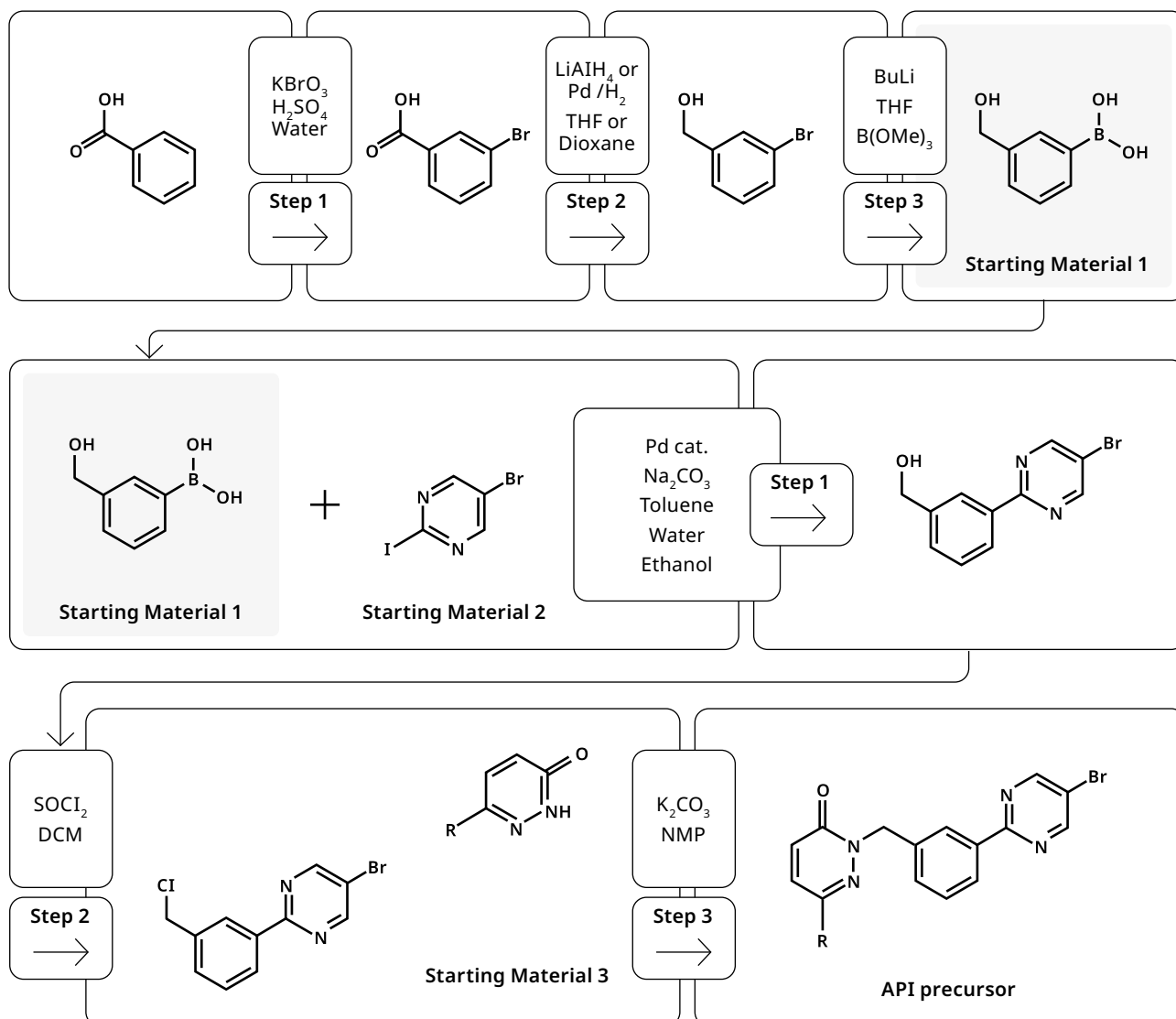
The PAS 2090 default data is applied to:

- molar yield,
- solvent quantities,
- catalyst quantity,
- energy requirements, and
- water and wastewater quantities.

The molecular weights and nature of all starting materials are available in the original publication.

The API precursor produced via three upstream synthesis steps yielding Starting Material 1, followed by three subsequent transformation steps to form the precursor (Figure 5). These reactions do not generate any co-products, and it is assumed for simplification that all reagents are equimolar.

Figure 5. Example C chemical product – Synthesis steps to produce API precursor.



As a first step, to apply the default data, each reaction step should be classified according to its complexity: as a base, specialty, or advanced chemical. None of the reactions in scope correspond to bulk commodity processes; however, the first reaction involves commodity reagents (e.g., benzoic acid) to produce a specialty chemical (3-bromobenzoic acid). All subsequent steps are classified as advanced chemical processes, as they involve multiple transformations and specialised reagents or catalysts.

Then, the limiting reagent must be identified. In this example, the selection for each reaction is based on which reagent serves as the building block for the subsequent product. These limiting reagents will then be the basis to estimate the solvent and catalyst use per reaction.

Table 28 shows an overview of the default data applied per synthesis step for molar yield, solvent quantity and catalyst. It is recommended to consult and validate assumptions of such complex reactions with process chemists.

Table 28. Example C chemical product - Default data applied to complexity of step.

Output	Synthesis step	Complexity	Limiting reagent	Molar yield (% mol limiting reagent)	Solvent quantity per kg limiting reagent	Catalyst use (Dorsch, 2015)
Starting material 1	1	Advanced chemicals	Benzoic acid	90%	5 (PAS 2090)	No
	2	Advanced chemicals	3-Bromobenzoic acid	80%	15 (PAS 2090)	No
	3	Advanced chemicals	3-(Bromophenyl) methanol	80%	15 (PAS 2090)	No
API precursor	3	Advanced chemicals	Starting material 1	80%	15 (PAS 2090)	No
	2	Advanced chemicals	Intermediate 1	80%	15 (PAS 2090)	No
	1	Advanced chemicals	Intermediate 2	80%	15 (PAS 2090)	Yes

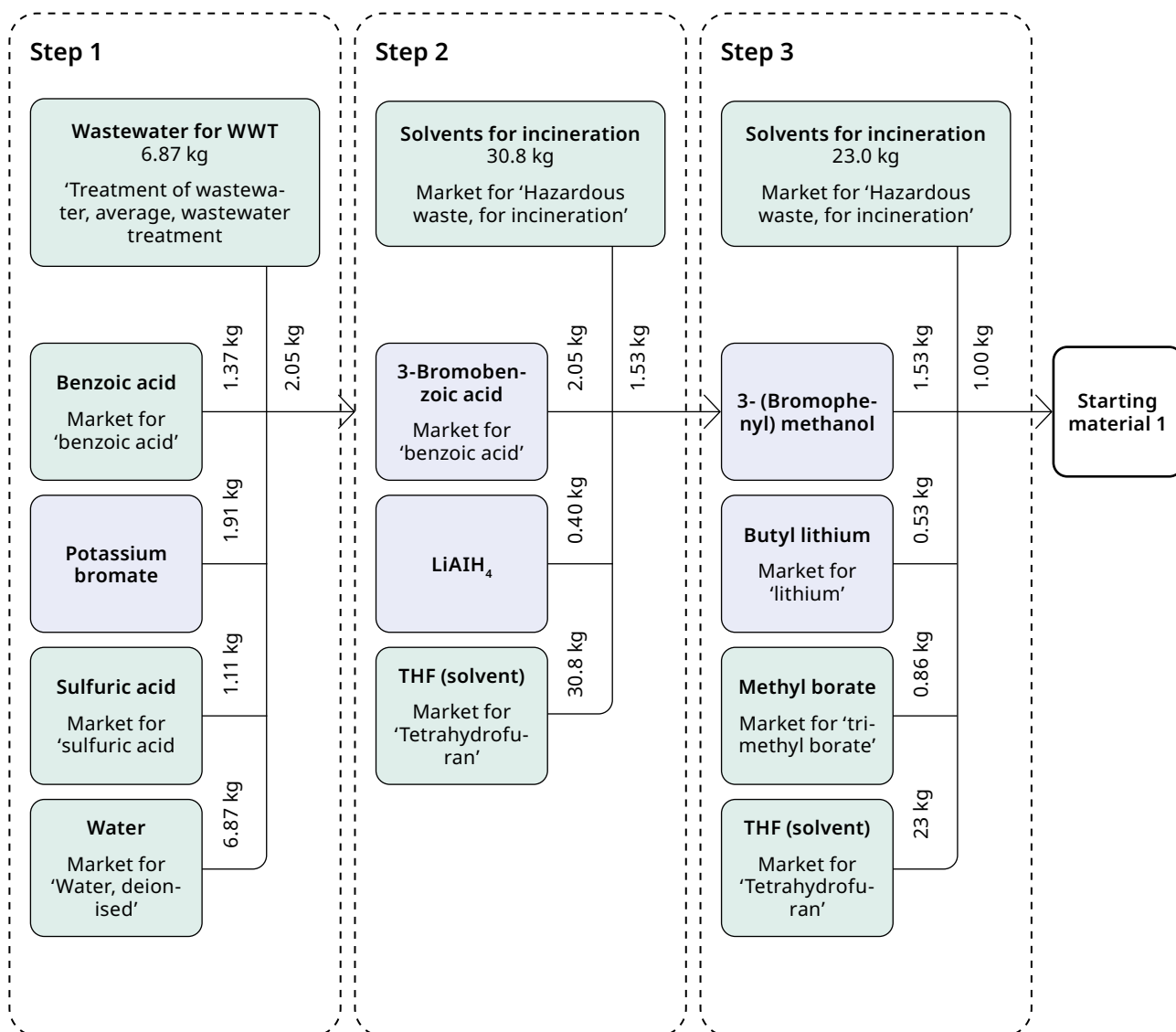
Similar to previous examples A and B:

- the inventory to produce 1 kg of the API precursor is based on the molar weights of reagents and products, factoring the molar yields in each step of the reaction,
- solvent waste and wastewater amounts are calculated performing a mass balance,
- datasets are matched for materials⁴,
- energy and utilities consumption are estimated based on default data for 'any other chemicals', as per the table 2 of PAS 2090.

A visual overview of the synthesis steps for starting material 1 and the API precursor are found in Figure 6 and Figure 7, respectively, for main materials only (excluding waste, water and energy flows) and including the recommended datasets. Through this example, the approach highlights how consistent application of PAS 2090 default data supports modelling of advanced chemical processes.

⁴ Potassium bromide is not available in the ecoinvent database. To represent it, it should be model through an additional synthesis step: Bromine + potassium hydroxide → potassium bromate + potassium bromide + water.

Figure 6. Example C chemical product – Visualization of modelling of Starting material 1 (materials only).



Legend

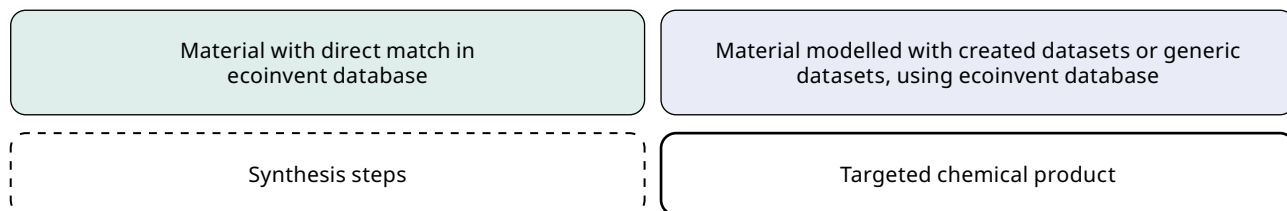
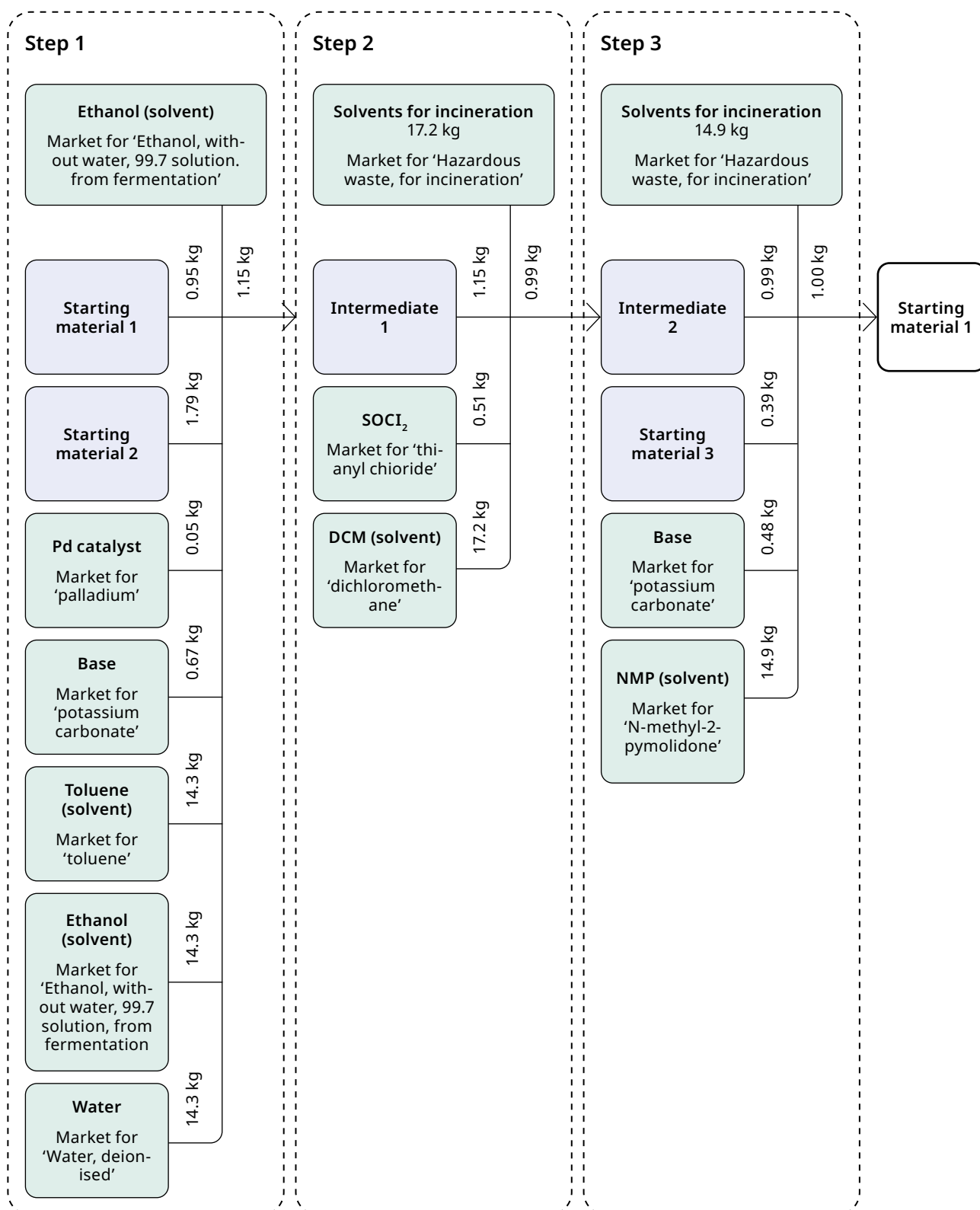
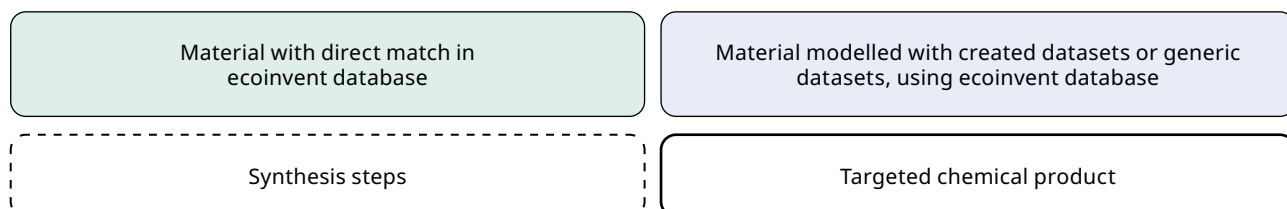


Figure 7. Example C chemical product – Visualization of modelling of API precursor (materials only).



Legend



Example D

For chemical product NaHMDS in THF

This example focuses on NaHMDS in THF, a specialty non-nucleophilic base commonly used for deprotonation and enolate formation in organic and pharmaceutical synthesis. Similar to example C, it provides a case on how to apply multiple proxy modelling criteria to a complex, multi-step synthesis involving co-products. Information of this reaction was retrieved from [PrepChem](#).

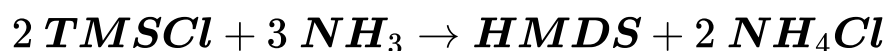
The synthesis route for NaHMDS in THF consists of four main steps, progressing from base to specialty chemical processes. In Step 1, methyl chloride reacts with elemental silicon to form TMSCl and methyltrichlorosilane as a co-product. Both are commercially relevant methylchlorosilanes produced via the Rochow process, and their outputs are managed through mass allocation, as a direct substituting dataset is unavailable and the economic values of each product are not readily available. In Step 2, TMSCl reacts with ammonia to form a nitrogen-silicon intermediate and ammonium chloride as a stoichiometric co-product; the latter is credited in the model with an available production dataset. Step 3 involves reaction of the nitrogen-silicon intermediate with sodium amide to produce NaHMDS, with ammonia, as a co-product which is also credited, only this time with a market dataset that represents the technology mix for ammonia, but also includes transportation impacts to entry gate. This could result in an overestimation of the credit, however it simplifies the choice of production route. Step 4 represents solvation of the product in THF rather than a chemical transformation; therefore, no default solvent quantities were applied, as THF is part of the final product formulation. The allocation methods applied across these reactions are in line with “**Figure 2 – Decision tree for allocation in multi-output processes**” of PAS 2090. With the exception of the intermediates modelled across the synthesis steps, it is possible to match all reagents withecoinvent datasets.

Below are the balanced chemical reactions for the above-mentioned steps. For simplification, the chemical formulas of Trimethylsilyl chloride (TMSCl), Hexamethyldisilazane (HMDS), Sodium hexamethyldisilazane (NaHMDS) and THF are not shown in this example. These can be consulted at the source website. Figure 8 summarises the synthesis steps, mass flows and datasets, following the PAS 2090 rules.

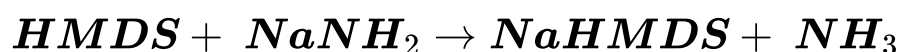
Step 1



Step 2



Step 3



Step 4

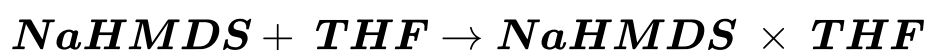
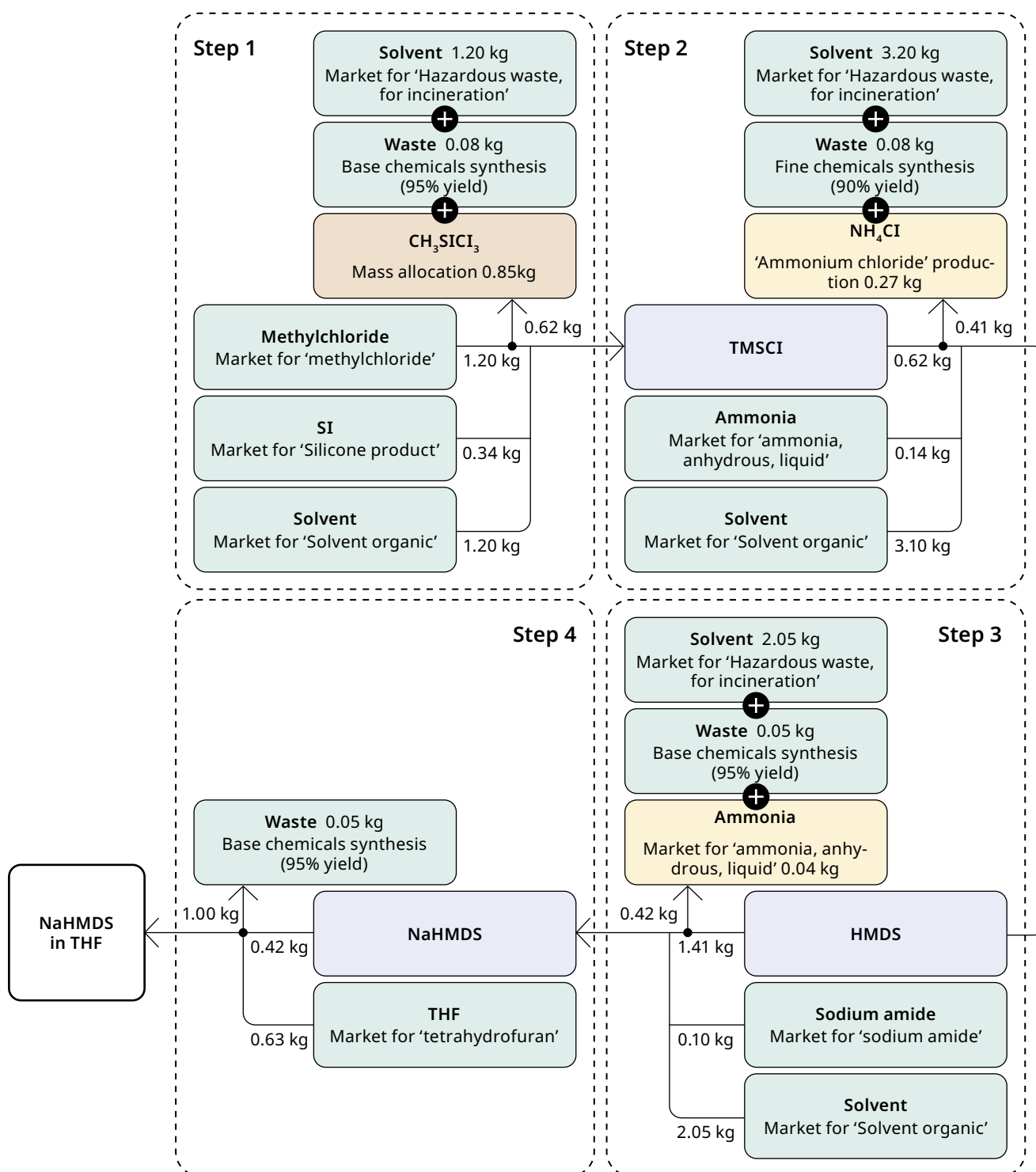
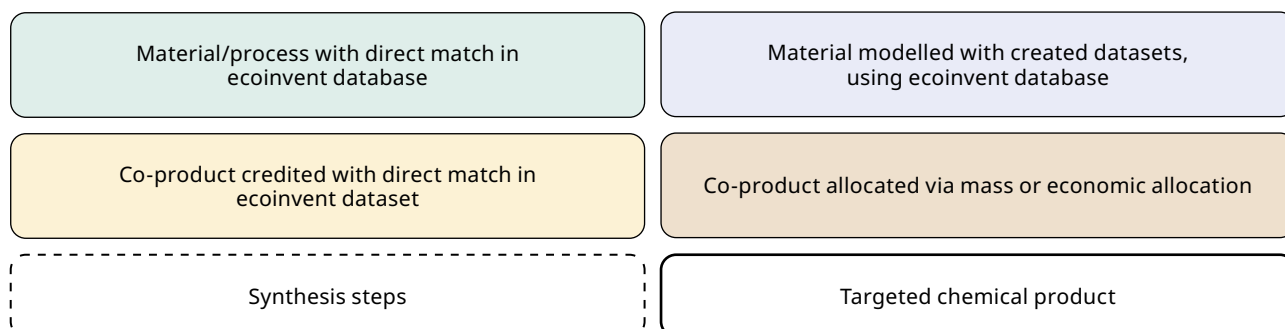


Figure 8. Example D chemical product – Visualization of modelling of NaHMDS (materials only).



Legend



Similar to example C, to apply the default data, each reaction step should be classified according to its complexity. The synthesis route includes both base and specialty chemical reactions. Step 1 involves the production of trimethylsilyl chloride (TMSCl), a widely used chemical building block classified as a base chemical. Steps 2 and 3 describe the formation of nitrogen-silicon intermediates that are produced in small quantities for specific applications; both are therefore considered specialty chemical processes. Step 4 represents a solvation step and is approximated to a base chemical reaction, and no default solvent quantities should be applied, as THF is already the reaction medium and molar quantities should be used.

As for the limiting reagents, in order to estimate solvent use, the reagents are selected based on the building blocks for the subsequent product. These reactions do not require catalyst use.

Table 29 shows an overview of the default data applied per synthesis step for molar yield, solvent quantity and catalyst.

Table 29. Example D chemical product - Default data applied to complexity of step.

Synthesis step	Complexity	Limiting reagent	Molar yield (% mol limiting reagent)	Solvent quantity per kg limiting reagent
1	Base chemicals	Methyl chloride	95%	1 (PAS 2090)
2	Specialty chemicals	TMSCl	90%	5 (PAS 2090)
3	Specialty chemicals	HDMS	90%	5 (PAS 2090)
4	Base chemicals	NaHMDS	95%	Quantity determined through balanced chemical reaction

Finally, similar to previous examples A, B and C:

- the inventory to produce 1 kg of NaHMDS is based on the molar weights of reagents and products, factoring the molar yields in each step of the reaction,
- solvent waste and wastewater amounts should be calculated performing a mass balance,
- datasets are matched for materials and co-products,
- energy and utilities consumption should be estimated based on default data from table 2 of PAS 2090, both for base chemicals (synthesis step 1 and 4) and 'any other chemical' (synthesis steps 2 and 3).

Overall, example D illustrates how PAS 2090 default data and allocation guidance can be systematically applied to represent complex, multi-step syntheses with multiple co-products.

5.3.3 Upstream transport

It refers to the upstream transport of raw materials used for pharmaceutical product and packaging or device manufacturing, i.e. from a supplier to the manufacturing plant.

When the supplier location is known, the adequate road distance can be determined using [Google Maps](#) or equivalent road distance calculators. Distances for ships and aircrafts may be determined using [SeaRates](#) and [Myclimate](#) calculators, respectively.

Datasets for transportation modes are available in section 5.8.2 Transport scenarios (steps, modes and distances), [Table 39](#). Recommended datasets for transport per refrigeration scenario.

5.4 Drug substance manufacturing modelling rules

This chapter of PAS 2090 lists the requirements to model drug substance manufacturing.

For this LCS, careful attention to process-specific elements can significantly enhance data quality and representativeness. Some broad recommendations in modelling this stage to improve precision and ensure completeness are provided below, these are based on practical experience that reflect common challenges and best practices, supported by general trends of relevant environmental impacts of pharmaceutical products highlighted in section I.1.4:

- Early data collection can often begin with basic inputs like BOMs, then be refined iteratively as more detailed or validated information becomes available.
- Where direct process data are unavailable, secondary sources, such as patents, safety data sheets, and regulatory dossiers, can offer valuable insights into process steps and material compositions. However, representative primary data can improve the quality of the LCA study.
- Consultation with technical experts, such as chemists, process engineers, or quality personnel, is important to validate assumptions, ensure process realism, and align with actual operating practices.
- In terms of specific input types, additional diligence is warranted. Growth media formulations should be reviewed for the presence of animal-derived ingredients to ensure these are properly captured in the model and their environmental impacts assessed.
- Where solvent mixtures are used, specifying the exact composition improves precision, as each solvent has a distinct environmental footprint.
- Similarly, HVAC energy consumption, especially in biologics and cleanroom environments, can represent a major portion of site-level energy use and should be accounted for using site-specific or best-available data.
- For consumables, a practical modelling approach is provided in [Appendix II – Modelling single use items](#), offering a more precise yet simplified method for handling large numbers of items used in drug substance manufacturing. The approach supports consistent and representative modelling without requiring detailed data for every individual item.
- Waste management practices, including the treatment, recovery, or disposal of general and solvent waste, should be clearly described, as they can carry significant environmental impacts. For biological drug substances, waste from consumables may also be a major contributor and should be addressed with specific attention to how it is handled.



While these recommendations focus on improving data accuracy and completeness at the process level, it is equally important to recognize the broader variability in environmental impacts across drug types and production technologies. Practitioners seeking to explore additional life cycle assessments (LCAs) and case studies in the pharmaceutical sector may consult the [HealthcareLCA database](#) and other sources.

When modelling this LCS, secondary data sources listed in Table 30 can be used if no primary data is available on the listed treatment processes.

Table 30. Recommended datasets for waste treatment processes from DS manufacturing.

Waste treatment process	Recommended dataset
Waste transport to treatment facility	In Europe 'Transport, freight, lorry >32 metric ton, EURO6 {RER}' Elsewhere 'Transport, freight, lorry >32 metric ton, EURO5 {RoW}'
Spent solvent treatment – unknown treatment market for	Market for 'Spent solvent mixture'.
Spent solvent treatment – incineration with energy recovery	'Treatment of spent solvent mixture, hazardous waste incineration, with energy recovery'.
Hazardous waste treatment	Market for 'Hazardous waste, for incineration'.
Catalyst recovery (different from 'regeneration')	For metal catalyst containing Rhodium, Palladium or Platinum: 'Rhodium Treatment of automobile catalyst'. 'Palladium Treatment of automobile catalyst'. 'Platinum Treatment of automobile catalyst'. For other catalysts (neither based on precious metals, nor metallic): No recovery performed.
Consumables – municipal waste incineration	Market for 'Municipal waste incineration' (with energy recovery).
Consumables – hazardous waste incineration	Market for 'Hazardous waste incineration' (without energy recovery).

Solvent recovery

In the specific case of solvent recovery, the PAS 2090 recommends modelling the recycling according to (Azapagic, D., R., & H., 2013). The datasets proposed for modelling this process are listed in Table 31.

Table 31. Recommended datasets for solvent recycling process.

Process/input/output	Recommended dataset
Cooling water	'Water, completely softened'
Chemicals (50:50 mix of H ₂ SO ₄ :NaOH)	Market for 'Sulfuric acid'. Market for 'Sodium hydroxide'.
Electricity	See Table 18
Steam	See Table 15
Waste (unrecovered) solvent	See Table 30, hazardous waste treatment.
Wastewater	'Treatment of wastewater, average, wastewater treatment'.
Residues (hazardous)	See Table 30, hazardous waste treatment.

For solvent incineration via regenerative thermal oxidizers, “**Table 3 – Secondary data and assumptions on waste treatment processes from manufacturing steps**” of PAS 2050 states that “*direct CO₂ emissions from incineration should be adjusted based on the carbon content of the solvent*”. To apply this, the mass fraction, molecular weight, and number of carbon atoms for each solvent in the mixture must be known. CO₂ emissions can be estimated based on the carbon content of the solvent, using 44 g/mol (the molecular weight of CO₂) as the conversion factor.

Emissions of solvent mixtures can be calculated as per Equation 11 below.

Equation 11

$$EF_{\text{mixture}} = \sum_i EF_i = \sum_i \left(\frac{n_{C,i} \times MW_{CO_2}}{MW_i} \times f_i \right)$$

Where:

EF_{mixture} = CO₂ emission factor of solvent mixture, in kg CO₂-eq per kg of solvent mixture.

EF_i = CO₂ emission factor of solvent i in the mixture, in kg CO₂-eq per kg of solvent.

$n_{C,i}$ = Number of carbon atoms in solvent i (mol⁻¹).

MW_{CO_2} = Molecular weight of CO₂ in g/mol.

MW_i = Molecular weight of solvent i , in g/mol.

f_i = Mass fraction of solvent i in the mixture (unitless).

The total emissions from the mixture are the sum of the individual solvent contributions, weighted by their respective fractions.

To guide on the application of rules for this LCS, two examples are shown in this section (excluding utilities):

- Example A: Modelling bill of materials and solvent use of synthetic drug substance, based on the average realized BOM over one year (PAS 2090 5.4a case).
- Example B: Modelling bill of materials of biological drug substance, based on the realized BOM for one batch (PAS 2090 5.4b case).

Example A

Modelling the bill of materials for yearly production of synthetic drug substance

This example shows an extract of a bill of materials, focusing on the necessary calculations to estimate quantities and suggested datasets (utilities excluded).

Table 32 shows a BOM with the inventory data for the yearly production of a drug substance, including input material and drug substance output quantities. In this example, the BOM data was originally available on a per-batch basis, along with the number of batches produced annually. Annual quantities were therefore calculated by scaling the per-batch BOM data to yearly production volumes. Similarly, solvent use for decontamination is reported on a per-campaign basis and was multiplied by the number of campaigns per year to obtain the corresponding annual quantities.

In this example, there is a direct match for all materials, except for the drug intermediate⁵. This material should be known by the manufacturing company and can be modelled with primary data or as per the chemical product modelling from **section 5.3.2 of PAS 2090**. The manufacturing locations of these materials are countries within Asia⁵. As no specific regional datasets are available for these countries, the datasets were selected for “Rest of the World” in accordance with section 5.1.3(c) of PAS 2090. If the countries of origin are known, the suggested datasets can be adapted to more accurately represent the geographical scope by substituting the underlying data with country-specific information on raw materials, energy inputs, water use, wastewater generation, and waste treatment; provided that such datasets are available. This approach can improve overall data quality. Since the manufacturing company knows the location of its suppliers, it models the transportation impact from the supplier to the manufacturing facility separately. Therefore, the selected datasets are “production datasets,” which do not include transportation impacts up to the manufacturer’s gate.

Table 32. Example A of drug substance manufacturing material inventory for synthetic drug substance, including dataset recommendation.

Main category	Material	Quantity [kg/year]	Recommended dataset
Attributable reagents/ precursors/ building blocks for drug substance manufacturing	Acetonitrile	17 000	Acetonitrile {RoW} acrylonitrile production, Sohio process Cut-off, U
	Isopropyl alcohol	30 000	Isopropanol {RoW} isopropanol production Cut-off, U
	Acetic acid	9 000	Acetic acid, without water, in 98% solution state {RoW} acetic acid production, methanol carboxylation (Monsanto), product in 98% solution state Cut-off, U
	Triethylamine	4 000	Triethyl amine {RoW} triethyl amine production Cut-off, U
	Drug intermediate	8 000	Modelled with primary data or via chemical product modelling.
	Methane sulfonic acid 160		Methylsulfonic acid {RoW} methylsulfonic acid production Cut-off, U
Total (reagents/ precursors/ building blocks)		68 160	
Non-attributable chemicals and other materials (solvents for decontamination)	Acetonitrile	12 000	Acetonitrile {RoW} acrylonitrile production, Sohio process Cut-off, U
	Methanol	320	Methanol {RoW} methanol production, natural gas reforming Cut-off, U
	Acetone	320	Acetone, liquid {RoW} phenol production Cut-off, U
	Isopropyl alcohol	4 000	Isopropanol {RoW} isopropanol production Cut-off, U
	Acetic acid	315	Acetic acid, without water, in 98% solution state {RoW} acetic acid production, methanol carboxylation (Monsanto), product in 98% solution state Cut-off, U
Total materials (solvents)		16 955	
Total drug substance output		7 250	

5 The identity of drug intermediate and country location of suppliers are not disclosed in this document.

In order to estimate the waste destined for incineration, a mass balance is performed:

$$\text{Waste} = \text{Input} - \text{Output}$$
$$\text{Waste} = 68\,160 \frac{\text{kg}}{\text{year}} + 16\,955 \frac{\text{kg}}{\text{year}} - 7\,250 \frac{\text{kg}}{\text{year}} = 77\,865 \frac{\text{kg}}{\text{year}}$$

By default, this amount is modelled as hazardous waste incineration without energy recovery, if not modelled with primary data, see [Table 30](#) for recommended datasets.

Example B
Modelling the bill of materials for one batch of biological drug substance

This example provides guidance on modelling buffers, media, and consumables used in the manufacturing of a biological drug substance. It focuses on the necessary calculations to estimate material quantities, the impacts of manufacturing and sterilisation of consumables, and the selection of relevant datasets (excluding utilities and waste treatment) for one batch of biological drug substance.

Table 33 shows an extract of the bill of materials (BOM), which lists the inventory data (materials only) to be used for modelling the drug substance. These quantities are then converted to mass (kg) for subsequent modelling with ecoinvent datasets. The mass conversion for hydrochloric acid (HCl) is based on the density of the solution, equal to 1.19 g/mL (1.19 kg/L), while the consumable mass data are based on supplier information. In biological drug-substance manufacturing, consumables are not always single-use items. In this example, the resin is reused for 100 cycles, with one cycle corresponding to one batch. Consequently, the resin quantity is scaled down to one batch.

Table 33. Example B of drug substance manufacturing material inventory for biological drug substance, categorisation and conversion of quantities.

Main category	Material	Quantity per batch	Unit	Quantity in kg per batch	Additional information
Attributable reagents/precursors/building blocks for drug substance manufacturing	Cell bank	Cut-off	-	Cut-off	Cell bank is cut-off. This is possible as per Note 2, Table 5 of PAS 2090.
	Hydrochloric acid (HCl) 37%	1	L	1.19	Buffer. Conversion based on density of solution.
	Sodium chloride (NaCl)	0.75	kg	0.75	Media component.
	Tris(hydroxymethyl)aminomethane hydrochloride (Tris-HCl)	29	kg	29	Buffer.
	Simethicone 3%	1.2	kg	1.2	Anti foam.
	Resin	400	kg per 100 cycles, 1 cycle per batch	4	Consumable.
	Storage bag, PE*	2	pieces	6	Based on unitary weight of 3 kg.
	Filter, 75% PP and 25% PA	1	piece	PP: 1.5* PA: 0.5*	Based on composition of filter and unitary weight of 2 kg.

* Composed of PE and EVA films, with PE as main material (over 80% of composition in weight).

To select the relevant datasets for modelling the upstream impacts of materials, PAS 2090 specifies a hierarchy for secondary data.

In this example, two materials in the BOM have direct dataset matches (or equivalent factors when processing impacts are included):

- Sodium chloride, and
- Storage bag (polyethylene granulate).

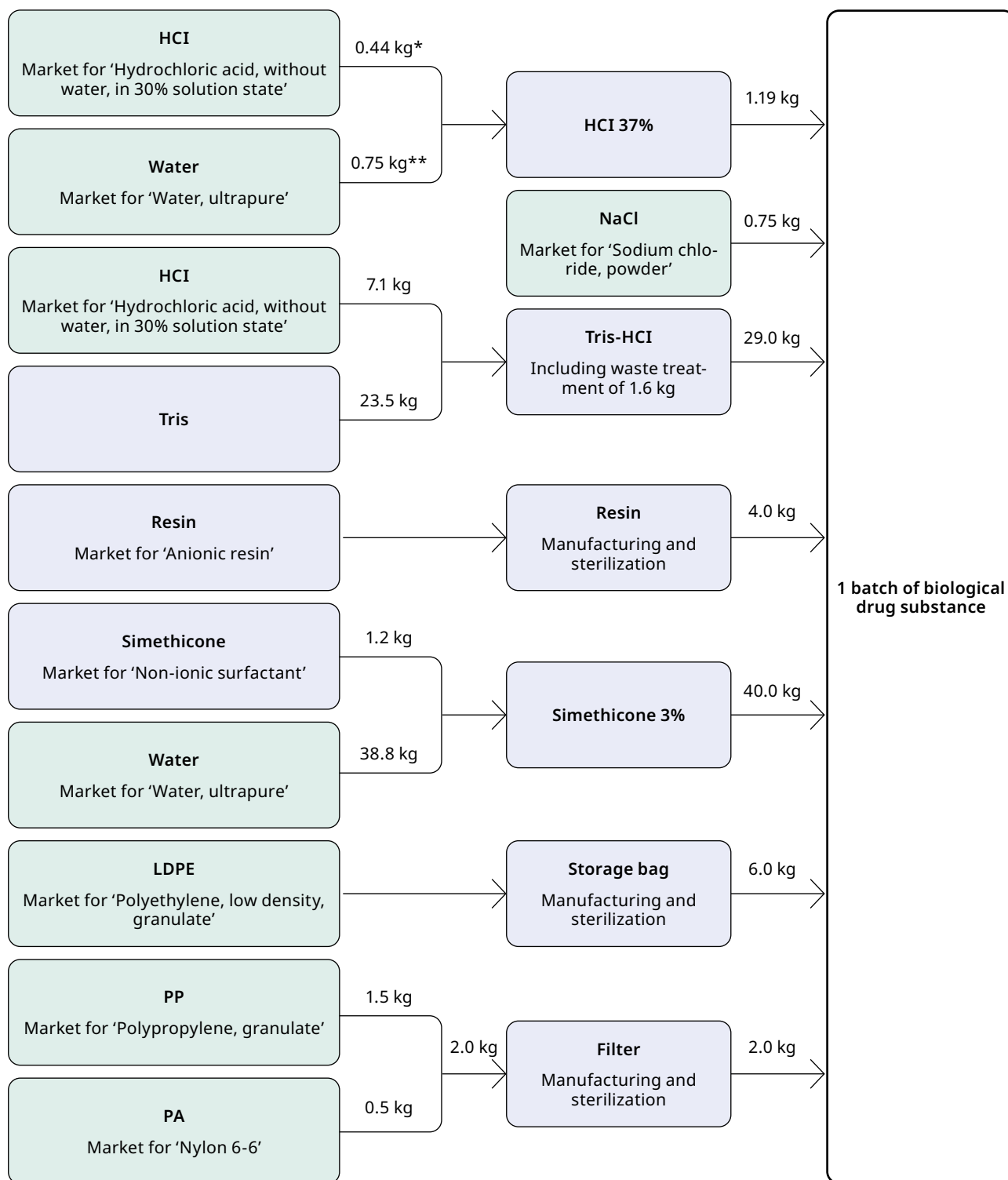
Figure 9 illustrates the upstream material flows and dataset mapping used to model the LCI for producing one batch of a biological drug substance.

For HCl 37%, the dataset is composed of HCl and water, with quantities determined according to the concentration of the solution.

For Tris-HCl, the required quantities of Tris and HCl are calculated using reaction stoichiometry and a molar yield of 95%, as commonly applied for basic chemicals. Tris can be modelled through the chemical product modelling approach.



Figure 9. Example B drug substance manufacturing - Mapping of material flows and dataset sources.

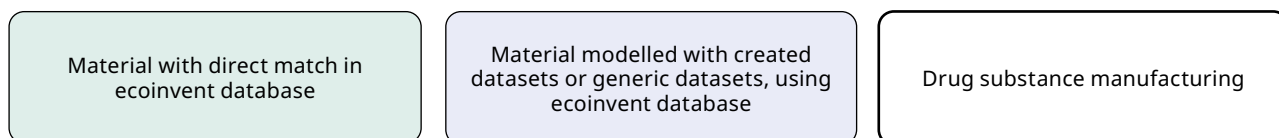


* Calculated as the mass of the solution and the concentration w/w = 1.19 kg x 37% = 0.44 kg

** Calculated applying mass balance between HCl 37% and HCl amounts = 1.19 kg - 0.44 kg = 0.75 kg

*** Calculated as the mass of the solution and the concentration w/w = 40 kg x 3% = 1.2 kg

Legend



After mapping the datasets for material production (including consumables), the next step is to account for electricity and water consumption required for consumable manufacturing and sterilisation, as required by PAS 2090.

In this example, default data from the *source A framework to support environmentally-based decision-making in the biopharmaceutical industry*, RAMASAMY, SVP is used since we know the quantity and the material used.

PAS 2090 provides **Table 6 – “Default energy and water use for consumable manufacturing and conditioning, per main consumable type, according to their size”** as a general source of default data where information of Raw material and weight of raw material is not known.

The consumables considered comprise two storage bags, one filter, and 4 kg of resin. Ramasamy (20218) and Table 6 of PAS provides data for consumables with defined specifications, listing energy and water consumption by size. The default data must be scaled to the size or quantity of the consumables used in the study, as indicated in the note to Table 6 of PAS 2090:

- This storage bag weighs 3 kg, and based on its weight, it can be assumed to have a capacity of approximately 500 L. No scaling is necessary in this case and data from Table 34 can be directly used.
- The filter weighs 2 kg, while the default data are provided for a 1 kg filter; default values are multiplied by two.
- For the resin, the batch weight is 4 kg. Table 6 provides data for both Protein A and ion-exchange resins. Given the application in biological drug-substance manufacturing, the Protein A resin is selected. Assuming a density of 1 kg/L, the resulting resin volume is 4 L, and the default data (originally provided for 26 L) are scaled accordingly.

Table 34 summarises the corresponding energy and water use per batch of biological drug substance, together with the recommended datasets.

Table 34. Electricity required for modelling the manufacturing and sterilisation of consumables required for 1 batch of biological drug substance.

Consumable	Consumable type	Input / output	Amount and unit per item	Amount and unit per batch biological product*	Recommended dataset
Storage bag	Bag 500 L	Electricity	10.1 MJ/kg 30.3 MJ	60.6 MJ (2 bags)	Market for ‘Electricity, medium voltage’.
Filter	Filter 1 kg	Electricity	10.1 MJ	20.2 MJ (1 filter, unitary weight 2 kg)	Market for ‘Electricity, medium voltage’

* Note that quantities may need unit conversion to match the unit of the dataset.

5.5 Drug product manufacturing modelling rules

Similar to drug substance manufacturing, this chapter of PAS 2090 lists the requirements to model drug product formulation. For biological products, the drug product sometimes also consists of the filling stage.

Drug product manufacturing introduces several modelling considerations that differ from the drug substance stage and may have a substantial influence on the overall environmental profile. Key aspects to consider include:

- A clear distinction between declared filling volume and the actual volume dispensed, including any deliberate overfill, is often required, since product losses at this stage translate directly into additional material demand and associated impacts.
- Where multi-component presentation formats are involved (for example, a kit that contains the finished dosage form, diluent, and device), accounting of the ancillary kit materials is needed.
- For biologic products, concentration of the API requires special attention, verify whether API mass is expressed on a “wet” basis versus a dry-solid equivalent, and process yields or potencies can shift the apparent burden per therapeutic dose.
- Using simple averages, whether for concentration, fill weight, or batch yield, without verifying their representativeness can introduce bias, especially in campaigns where variability is high.
- Other materials beyond the primary formulation such as stabilizing sugars or buffers may be recycled within the facility; however, consumable items such as stoppers, filters, or single-use bags are rarely reused and may dominate waste streams.
- Version changes to high-volume excipients (for instance, a shift from standard-grade to low-endotoxin grade) should be reflected in time-series or comparative assessments.
- Map for energy-intensive unit operations, such as lyophilization, which demands substantial refrigeration, vacuum, and heater loads.
- Similar to drug substance (DS) modelling, it is equally important in drug product (DP) assessments to consult technical experts and perform mass balance checks to ensure that assumptions are realistic, data are complete, and material flows reflect net quantities rather than theoretical inputs.

To complement the guidance provided in this section, the following example illustrates the application of PAS 2090 requirements to an extract of non-attributable materials and consumables used for filling and cleaning of biological drug product (energy excluded), focusing on the conversions to estimate quantities and suggested datasets. Further practical guidance on modelling consumables is available in [Appendix II – Modelling single use items](#).



→ *Similar to drug substance manufacturing, this chapter of PAS 2090 lists the requirements to model drug product formulation.*

Example A

Modelling materials and utilities for filling one batch of biological drug product

Table 35 shows the inventory data to be used as inputs to model the drug product filling per piece of drug product (simplified declared unit), further converted to mass in kg for its subsequent modelling with ecoinvent datasets, as well as the yearly output of drug product and batch sizes. The quantities reflect the realized consumption of attributable chemicals and other materials for one batch (PAS 2090 5.5b case), which is then divided by the batch output of drug product, and yearly consumptions for non-attributable chemicals and other materials divided by the yearly output of drug product, in order to obtain the quantities per piece of drug product. The mass data for the consumables is based on supplier data. While the relative quantity of consumables to product output is low, a cut-off cannot be applied as per the PAS 2090 requirements, “Table 8 – Minimum inventory data required for drug product manufacturing modelling”.

Table 35. Example A of drug product manufacturing material inventory for biological drug product, categorization and conversion of quantities.

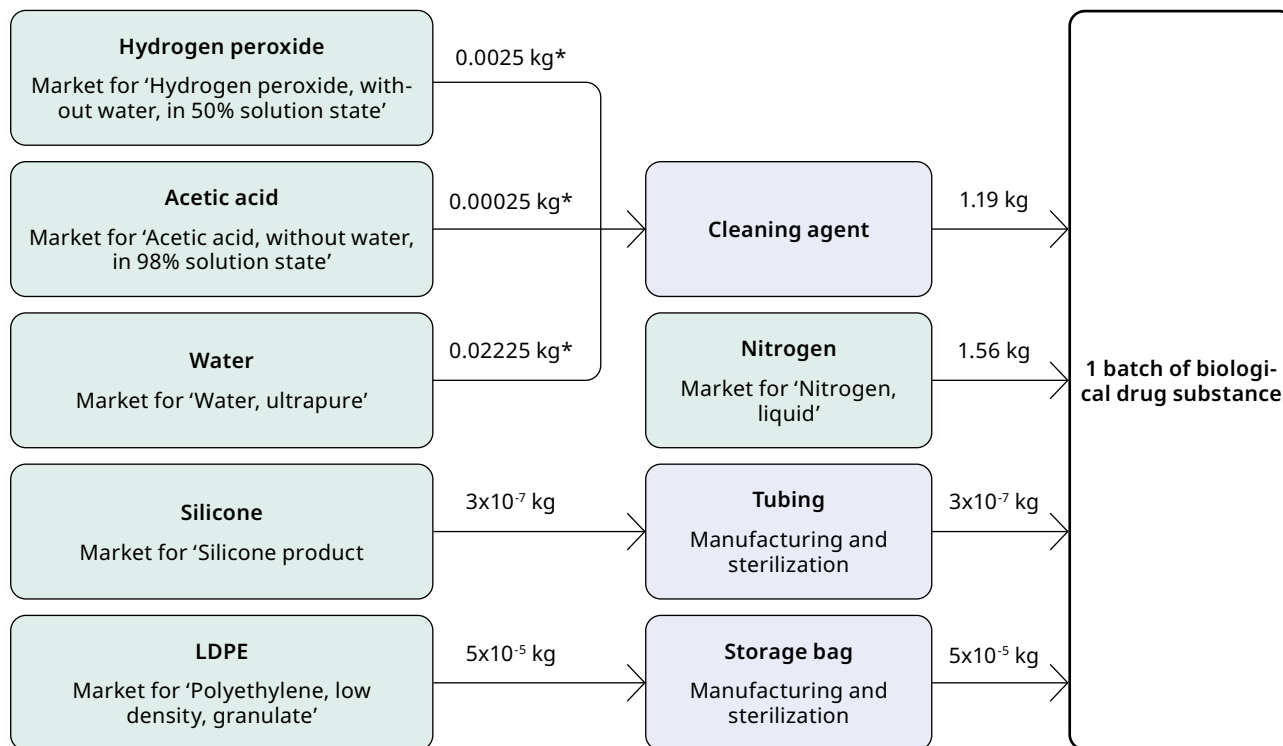
Main category	Material	Quantity	Unit	Quantity in kg per unit of product	Additional information
Non-attributable chemicals and other materials	Nitrogen	5 000	Nm ³ /year	1.56	Creating an inert atmosphere within the vial. Conversion to kg is easily obtained from online search for normal cubic meters, in this case 1.25 kg/Nm ³ . Divided by total drug output per year.
	Cleaning agent 10% hydrogen peroxide and 1% acetic acid	10 000	L/year	0.025	Cleaning. Since water makes up over 80% of the composition, density is assumed as equivalent to density of water (1 kg/L). Divided by total drug output per year.
Attributable chemicals and other materials	Tubing	1	piece/batch	3·10 ⁻⁷	Consumable. Based on unitary weight of 0.12 kg. Divided by batch size.
	Storage bag*	1	piece/batch	5·10 ⁻⁵	Consumable. Based on unitary weight of 1 kg, 200 L capacity. Divided by batch size.
Total drug product output		400 000	vials/year		
Batch size		20 000	vials/batch		

* Composed of LDPE, PBT and nylon, with LDPE as main material (over 80% of composition in weight).

In this example, there is a direct match for all materials.

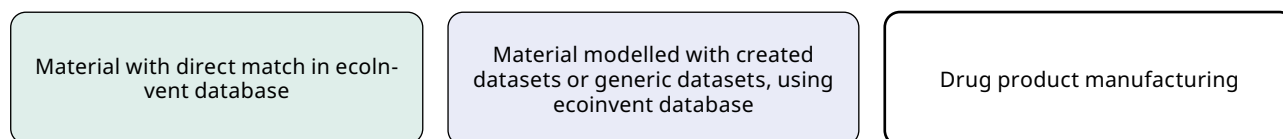
Figure 10 illustrates the upstream material flows and dataset mapping used to model the LCI for the production of one batch of a biological drug product. The quantities of hydrogen peroxide, acetic acid and water were calculated based on the composition as stated in Table 35 and the respective quantity per unit.

Figure 10. Example A drug product manufacturing - Mapping of material flows and dataset sources.



* Calculated as the mass of the solution per unit of product and the concentration w/w

Legend



Similar to Example B of drug substance manufacturing modelling rules, the next step is to account for the electricity (at a minimum) required for transformation and sterilisation of the consumable materials, in line with PAS 2090 requirements. In this example, the default data are scaled to one unit of biological product. The storage bag has a capacity of 200 L.

Table 36. Electricity required for modelling 1 unit of biological drug product.

Consumable	Consumable type (Table 6 of PAS 2090)	Input / output	Amount and unit per item (Table 6 of PAS 2090)	Amount and unit per unit of biological product (divided by batch size)*	Recommended dataset
Storage bag	Bag 200 L	Electricity	10.1 MJ/kg 60.6 MJ	5.05×10^{-4} MJ	Market for 'Electricity, medium voltage'
Tubing	Other	Electricity	10.1 MJ/kg	3.03×10^{-6} MJ	Market for 'Electricity, medium voltage'

* Note that quantities may need unit conversion to match the unit of the dataset.

5.6 Packaging manufacturing modelling rules

Tertiary packaging can be modelled using the datasets provided in Table 37.

Table 37. Recommended datasets for tertiary packaging.

Packaging material	Recommended dataset
LDPE wrap	Market for 'Packaging film, low density polyethylene'
Carton boxes	Market for 'Corrugated board box'
Corrugated board (separators)	Market for 'Corrugated board box'
Wood pallet*	Market for 'EUR-flat pallet'
Passive cold chain – Dry ice	Market for 'Carbon dioxide, liquid' for production Direct CO ₂ emission from sublimation and evaporation
Passive cold chain – Cold packs	'Polyethylene, high density, granulate' 'Injection moulding' Market for 'Tap water'
Passive cold chain – Insulated box	Market for 'Polystyrene, extruded'.

* PAS 2090 requires modelling of single use tertiary packaging. Pallets are reused and may be modelled.

Table 38 shows the datasets that can be used to model packaging manufacturing for the material production and subsequent forming or conversion, unless primary or more accurate data is available. The average market or production dataset may be used.

If the packaging is sterilised by the supplier prior delivery to the pharmaceutical manufacturing site, default data from “**Table 6 – Default energy and water use for consumable manufacturing and conditioning, per main consumable type, according to their size**” of PAS 2090 may be applied.

Table 38. Recommended datasets for packaging manufacturing.

Material production	Recommended dataset
Carton	'Carton board box production, with offset printing'
Corrugated board box	'Corrugated board box'
Folding box board	'Folding boxboard carton'
Paper (wood containing)	'Paper, wood containing, lightweight coated'
Paper (woodfree)	'Paper, woodfree, coated'
Aluminium	'Aluminium, primary, ingot'
Glass	'Glass tube, borosilicate'
HDPE	'Polyethylene, high density, granulate'
LDPE	'Polyethylene, low density, granulate'
Nylon (6 or 6-6)	'Nylon 6 / 6-6'

Material production	Recommended dataset
ABS	'Acrylonitrile-butadiene-styrene copolymer'
PA (polyamide)	'Nylon 6 / 6-6'
PC	'Polycarbonate'
PET (amorphous or bottle grade)	'Polyethylene terephthalate, granulate, amorphous / bottle grade'
PLA	'Polylactide acid, granulate'
PP	'Polypropylene, granulate'
PS (general or extruded)	'Polystyrene, general purpose/extruded'
EPS	'Polystyrene, expandable'
PTFE (polytetrafluoroethylene)	'Tetrafluoroethylene'
PU (flexible or rigid)	'Polyurethane, flexible/rigid foam'
PVC (bulk or emulsion polymerized)	'Polyvinylchloride, bulk/emulsion polymerised'
PVDC	'Polyvinylidenechloride, granulate'
SAN	'Styrene-acrylonitrile copolymer'
Steel	'Steel, low-alloyed'
Stainless steel	'Steel, chromium steel 18/8'
Synthetic rubber	'Synthetic rubber'
Material forming or conversion	Recommended dataset
Plastic thermoforming	'Thermoforming of plastic sheets'
Plastic extrusion	'Extrusion, co-extrusion'
Plastic film extrusion	'Extrusion, plastic film'
Plastic blow moulding	'Blow moulding'
Plastic injection moulding	'Injection moulding'
Polymer foaming	'Polymer foaming'
Metal sheet rolling	'Sheet rolling, aluminium/(chromium) steel'
Wire drawing*	'Wire drawing, steel'

* It has been noted that the wire drawing process dataset as a proxy to model production of needles may be underestimated, as per Consortium expertise. Further developments to improve the background modelling need to be undertaken.

The practitioner should gather information about the materials and conversion processes used for packaging and device manufacturing or investigate the relevant production processes for the intended application. Table 38 provides non-exhaustive suggestions for common combinations of materials and conversion processes for pharmaceutical packaging applications.

Table 39. Common material and conversion processes for packaging manufacturing.

Processing step	Materials	Pharmaceutical packaging applications
Extrusion and blow moulding	HDPE, LDPE, PP, PET, PVC, PVDC, Nylon, PA, PTFE, EPS, PU	Bottles (HDPE, PET), pouches (LDPE), blister packs (PVC, PVDC), films.
Thermoforming	PET, PS, PVC, PLA, Nylon	Blister packs, trays for tablets, syringes, ampoules, and thermoformed films.
Injection moulding	HDPE, PP, ABS, PC, SAN	Closures, caps, inhaler parts, syringe bodies, rigid medical components.
Moulding and foaming	EPS, PU	Insulation for vaccines, protective inserts, shock-absorbing components.
Rolling	Aluminium, steel, stainless steel	Blister foils (aluminium), containers, medical-grade equipment (steel).
Wire drawing	Steel, stainless steel	Needle making.

To model the impacts of operational packaging waste, the datasets listed in [Table 50](#) can be used for the packaging materials. According to Note 2 in “[Table 10 – Minimum inventory data required for packaging manufacturing and processing modelling](#)” of PAS 2090, manufacturing waste disposal may be modelled based on its actual end-of-life treatment.

5.7 Administration device manufacturing modelling rules

Overall, the same datasets used for packaging apply to devices. If the device is sterilised by the supplier, a default energy use of 1.5 MJ/kg material can be used (energy use for gamma irradiation from source publication of Table 6 in PAS 2090) can be used, where primary or representative data is not available.

If the device contains electronic components, they can be modelled using the datasets listed in Table 40 unless primary or more accurate data is available. The unspecified datasets can be used if specific knowledge about the composition and production of the sub-components in the electronic component is limited. In this case a weighted average (based on weight) of the unspecified dataset for active/passive components, respectively, can create a reasonable proxy for the electronic component.

Table 40. Recommended datasets for electronic components.

Component production	Recommended dataset
LCD (liquid crystal display)	'Liquid crystal display, unmounted, mobile device'
Integrated circuit (logic or memory)	'Integrated circuit, logic/memory type'
Unspecified/mixed passive components (e.g. connectors, capacitors, inductors, resistors)	'Electronic component, passive, unspecified'
Unspecified/mixed active components (e.g. diodes, transistors, integrated circuits)	'Electronic component, active, unspecified'

Note that the datasets listed in Table 40 are expressed per kg component.

To model the impacts associated with the end-of-life of operational waste arising from administration device manufacturing, the datasets provided in Table 52 may also be applied, following the same methodological principles used for packaging materials.

5.8 Distribution modelling rules

As per PAS 2090, this stage includes transport and storage steps between the secondary packaging factory gate (finished good) and the product delivery site. It also accounts for, as a minimum, weight of tertiary packaging and modelling of production and end-of-life of single-use packaging.

When modelling distribution and transport impacts, actual packaging weight should be used where available, as relying on theoretical weights may underestimate emissions. This distinction is especially relevant for aggregated shipments or when overpackaging occurs. The user can consider modelling the material production and end-of-life for multiuse tertiary packaging, if the packaging is deemed as material-intensive.

5.8.1 Key parameters

The key parameters shown in "Table 13 – Average % of small, medium and large countries in the different regions and worldwide (values compiled using surface area criteria)" of PAS 2090 are used to estimate average transport distances within each region by applying the share of country size distribution percentages. These percentages determine the weighted share of small, medium, and large countries, which are then linked to predefined transport distances (e.g., 700 km for small countries in Europe). An example of how to apply these parameters is provided in the following section.

5.8.2 Transport scenarios (steps, modes and distances)

The recommended datasets indicated in Table 41 should be used to model non-refrigerated, actively and passively refrigerated transport steps for product delivery, excluding product collection and other personal travels to treatment site(s) (section 5.9).

Table 41. Recommended datasets for transport per refrigeration scenario.

	No refrigeration transport mode datasets (referred to as "base dataset" in this table)	Active refrigeration	Passive refrigeration
For all modes: refrigeration process / inputs	N/A	<p>For temperature range 0° to 20°C (specification from ecoinvent): Market for 'Operation, reefer, cooling'.</p> <p>For temperature range -35°C to -18°C (specification from ecoinvent, may be applied to temperatures below zero in general): Market for 'Operation, reefer, freezing' corresponding to 40-foot, high-cube, with mix of R134a & liquid carbon dioxide as refrigerants.</p> <p>Already included in some datasets. Reusable active refrigeration shipping container: the weight of the container can range from 0.25 to 0.75 kg container / kg product depending on their capacity (if unknown, use highest weight ratio as conservative assumption). Their weight must be added to the transportation weight as per PAS 2090 section 5.8.2.</p>	<p>Packaging: See passive cold chain packaging quantities in "Table 12 – Default tertiary packaging components and weight" of PAS 2090 and Table 37 for respective datasets.</p> <p>For all transport modes: To model and add to the base dataset.</p>
Truck	<p>In Europe 'Transport, freight, lorry >32 metric ton, EURO6 {RER}'</p> <p>Elsewhere 'Transport, freight, lorry >32 metric ton, EURO5 {RoW}'</p> <p>Global Market for 'Transport, freight, lorry, diesel, unspecified {GLO}'</p>	<p>Europe or rest of the world: Base dataset + refrigeration process per tkm</p> <p>The quantity of refrigeration process per tkm can be consulted in the respective ecoinvent truck dataset.</p> <p>Global (includes refrigeration process): Market for 'Transport, freight, lorry with refrigeration machine, diesel, cooling, fleet average {GLO}' Market for 'Transport, freight, lorry with reefer, diesel, freezing, fleet average {GLO}'.</p>	

	No refrigeration transport mode datasets (referred to as "base dataset" in this table)	Active refrigeration	Passive refrigeration
Van*	Market for 'Transport, freight, light commercial vehicle'	Base dataset + refrigeration process per tkm. The quantity of refrigeration process per tkm can be consulted in the respective ecoinvent truck dataset.	
Ship	Market for 'Transport, freight, sea, container ship'	Market for 'Transport, freight, sea, container ship with reefer, cooling'. Market for 'Transport, freight, sea, container ship with reefer, freezing'. Refrigeration process included.	
Train	Market for 'Transport, freight train'	Market for 'Transport, freight train with reefer, <i>cooling OR freezing</i> '. Refrigeration process included.	Base dataset + refrigeration inputs considering the allocatable polystyrene packaging fraction per product unit and product weight
Aircraft	Market for 'Transport, freight, aircraft, unspecified' Up to 1 500 km: Market for 'Transport, freight, aircraft, short haul' Between to 1 500 km and 4 000 km distance: Market for 'Transport, freight, aircraft, medium haul' More than 4 000 km distance: Market for 'Transport, freight, aircraft, long haul'	Market for 'Transport, freight, aircraft with reefer, <i>cooling OR freezing</i> '. Refrigeration process included.	

*Compared to trucks, vans have a lower payload and are used for last mile delivery.

An example is provided for better illustration of the key parameters for distribution and recommended datasets.

Example A

Applying parameters and utilizing datasets for transport.

A product from a European manufacturer is distributed all across Europe via wholesalers, under active refrigeration (cooling), without aircraft transport. Following transportation legs need to be modelled:

- Factory to distribution centre (DC)/wholesaler warehouse
- Additional intermediate DC/wholesaler warehouse
- DC/wholesaler warehouse to delivery site

Factory to DC/wholesaler warehouse

Intracontinental supply chain: 3 500 km truck.

To be modelled with Market for ‘transport, freight, lorry >32 metric ton, EURO6 (RER)’. Since the product requires refrigerated conditions, dataset Market for ‘operation, reefer, cooling’ needs to be added in the model. See overview of parameters and recommended datasets [Table 47](#).

Table 42. Example A transport distribution – Application of PAS 2090, Table 14 parameters, for factory to DC.

Supply chain area (from Table 14 in PAS 2090)	Distance by truck [km] (from Table 14 in PAS 2090)	Recommended dataset
Intracontinental (within Europe)	3 500	Market for ‘transport, freight, lorry >32 metric ton, EURO6 (RER)’ with Market for ‘operation, reefer, cooling’



Additional intermediate DCs/wholesaler warehouses

Based on the PAS 2090, the distribution area of country sizes shall be estimated using **Table 13** in the corresponding **section 5.8.1**, which for Europe means Table 43:

Table 43. Example A transport distribution – Application of PAS 2090, Table 13 and Table 14 parameters, for additional intermediate DCs/wholesaler warehouses.

Country size groups (from Table 13 in PAS 2090)	Share in Europe [%] (from Table 13 in PAS 2090)	Distance by truck [km] (from Table 14 in PAS 2090)	Weighted distance by truck [km] (calculated)	Recommended dataset
Small countries	15	700	105	Market for 'transport, freight, lorry >32 metric ton, EURO6 (RER)' with Market for 'operation, reefer, cooling'
Medium countries	65	750	487.5	
Large countries	20	850	170	
Total	100	-	762.5	

DC/wholesaler warehouse to delivery site (pharmacy, HC facility, other)

Based on the PAS 2090, the distribution area shall be estimated using **Table 13**, which for Europe means Table 44:

Table 44. Example A transport distribution – Application of PAS 2090, Table 13 parameters, DC/wholesaler warehouse to delivery site.

Country size groups (from Table 13 in PAS 2090)	Share in Europe [%] (from Table 13 in PAS 2090)	Distance roundtrip by van [km] (from Table 14 in PAS 2090)	Weighted distance by van [km] (calculated)	Recommended dataset
Small countries	15	200	0.75	Market for 'Transport, freight, light commercial vehicle (RER)' with Market for 'operation, reefer, cooling'
Medium countries	65	250	6.5	
Large countries	20	500	3	
Total	100	-	10.25	

5.8.3 Storage scenarios

The storage scenarios of PAS 2090 include default data to estimate energy requirements as well as refrigeration⁶ consumption and leakage of distribution centres (DC), wholesaler warehouses and final delivery sites, which are summarised in “**Table 15 – Default data to use for storage steps modelling according to the refrigeration scenario**” of PAS 2090. The default data applies for storage activities outside of the company’s control or ownership. When applying the parameters, it is important to know the required temperature control:

- Ambient: typically a controlled temperature between 15–25 °C.
- Chilled (refrigerated): generally in the range of +2 to +8 °C.
- Frozen: usually ≤ -18 °C.

The parameters are specific for these temperature-control conditions. While general energy demand is provided for all cases, additional consumption must be accounted for in chilled and frozen storage.

In this section, an application of the default parameters for electricity, natural gas and refrigeration of PAS 2090 is demonstrated for a product.

→ *While general energy demand is provided for all cases, additional consumption must be accounted for in chilled and frozen storage.*



6 In the case of refrigerant, it constitutes the consumption (top-up) as well as the leaked emissions.

Example A

Applying parameters and utilizing datasets for storage.

Following the transport example, it is assumed that the product is chilled (refrigerated) during storage at different stages of the distribution chain in Europe. Assuming that primary data is unavailable, the storage needs to be modelled with the default data from Table 15 of PAS 2090 for following storage steps:

- DC/wholesaler warehouse (first storage step after factory gate)
- DC/wholesaler warehouse (additional intermediate DC/wholesaler warehouse)
- Final delivery site

Table 45 shows the application of the default data for a hypothetical product volume of 200 ml that includes tertiary packaging, in line with a hypothetical declared unit. It is recommended to model the impacts of electricity, heat and refrigerant use at least aggregated at storage step level, for eventual contribution analyses.

Table 45. Default general input and output factors per unit of volume of product applied to 200 ml volume, chilled and distributed in Europe. Default data from Table 15 of PAS 2090.

Storage step	Input/output	Temperature control	Consumption per product volume unit	Unit [-/]	Product volume (example) [l]	Consumption per product	Unit **	Recommended dataset
First DC and wholesaler warehouse*	Electricity	General demand - Chilled	0.14	Wh	0.2	0.028	Wh	Market group for 'Electricity, low voltage {RER}'
	Natural gas		1.7	kJ		0.34	kJ	Market group for 'Heat, central or small-scale, natural gas {RER}'
	Electricity	Additional demand - Chilled	3.1	Wh		0.62	Wh	Market group for 'Electricity, low voltage {RER}'
	Refrigerant		0.00056	g		0.00011	g	Make-up: Carbon dioxide, liquid {RER} market for carbon dioxide, liquid
Additional DC and wholesaler warehouse*	Electricity	General demand - Chilled	0.14	Wh	0.2	0.028	Wh	Market group for 'Electricity, low voltage {RER}'
	Natural gas		1.7	kJ		0.34	kJ	Market group for 'Heat, central or small-scale, natural gas {RER}'
	Electricity	Additional demand - Chilled	3.1	Wh		0.62	Wh	Market group for 'Electricity, low voltage {RER}'
	Refrigerant		0.00056	g		0.00011	g	Make-up: Carbon dioxide, liquid {RER} market for carbon dioxide, liquid
Final delivery site	Electricity	General demand - Chilled	7.7	Wh	0.2	1.5	Wh	Market group for 'Electricity, low voltage {RER}'
		Additional demand - Chilled	37	Wh		7.4	Wh	

* Parameters provided in Table 15 of PAS 2090 are applied to each DC and wholesaler warehouse of the distribution stage.

** Note that in order to apply recommended datasets, quantities should be converted from g, kJ and Wh to kg, MJ or kWh, respectively, by dividing quantities by 1 000. Calculation step not performed to ease readability of numbers and table.

5.9 Modelling rules for product collection and personal travels to administration site(s)

In the lack of primary data, PAS 2090 provides the default transport steps, modes, and distances in “**Table 16 - Default transport steps, modes and distances for product collection and travel to administration site**”, “**Table 17 Default share of mail delivery option use for product collection per (continental) region**”, “**Table 18 – Default patient travel modes per (continental) region**”. In this case It is important to apply default and allocation rules exactly as prescribed:

- When several products are collected or administered per trip, allocate impacts proportionally to the number of products.
 - If no primary data are available, apply the default 25 % allocation factor (average of four products collected per travel).
- Apply the additional 50 % allocation factor to reflect that personal travel may not be fully dedicated to medicine collection.
- Always report the impact of product collection and personal travels.

As a first step, the main administration place of the product should be identified. Where several geographies are relevant, apply weighted shares (default data from PAS 2090 or primary data if available) using available sales or usage data for the product or similar products.

Then, the transport modes and distances are the relevant parameters for modelling. When applying PAS 2090 default data:

- Use the continental-level mode shares from Table 18 (mix of car and public transport) and the default round-trip distances of 5 km / 10 km / 15 km depending on country size (small / medium / large).
- If using car or public transport, represent these as regional mixes of combustion and electric vehicles or bus / tram / subway where applicable.
- Foot or bicycle travel is modelled with no impact.
- Apply mail-delivery shares where relevant: Select the default regional share of mail delivery from [Table 17](#) (e.g. 25 % for Europe) and model mail delivery distances via van transport given in [Table 16](#) (5 km / 10 km / 15 km roundtrip by van, depending on country size).
- When only climate-change impact is assessed, a generic emission factor is provided in the standard (e.g. $4 \times \text{product mass} + 167 \text{ g CO}_2\text{e per roundtrip for product collection; } 1.8 \text{ kg CO}_2\text{e per roundtrip for administration travel}$).

Clearly note that these factors are highly generic and conservative, and that representativeness limitations must be acknowledged in reporting.

In order to model personal travel impacts, the relevant parameters include the distance km (car) or person-kilometre pkm (public transport) using $p = \text{one person}$. To model the impact of car transportation, the share of electric cars for selected regions can be consulted in [Our World in Data](#)⁷ (IEA, 2024) under “Share of cars currently in use that are electric, 2010-2023”. It is recommended to use and document latest year available data. If the region in scope of the study is not available, the ‘transport, passenger car’ dataset can be used. When modelling electric cars, only share of fully electric cars (i.e. not hybrid) should be included. A five-year average of the share of new electric cars that are fully electric, based on the selected data source, can be used to approximate the proportion of fully electric vehicles in circulation.

Table 46. Recommended datasets for product collection and other personal travels to treatment site(s).

Transport mode	Recommended dataset
Van	<p>Ambient temperature Market for 'Transport, freight, light commercial vehicle'.</p> <p>Refrigerated Add refrigeration process per tkm to the impact of ambient temperature (see also Table 41).</p>
Car	<p>Combustion engine Market for 'Transport, passenger car with internal combustion engine'.</p> <p>Electric vehicle Market for 'Transport, passenger car, electric'.</p>
Public transport	Market for 'Transport, regular bus'.



→ A five-year average of the share of new electric cars that are fully electric, based on the selected data source, can be used to approximate the proportion of fully electric vehicles in circulation.

Example A

Applying parameters and utilizing datasets for transport.

A product from all across Europe via wholesalers, refrigerated (cooling), and administered mostly at home (80%) and in hospitals (20%). The product is directly delivered to hospitals when administered there, while for home administration the patient has to pick it up. The patient does not go to the hospital to exclusively have this product administered. Table 47 summarises the application of this example.

Table 47. Example A product collection. Parameters applied for product collection and other personal travels to treatment site(s) in Europe.

Administration site	Pick-up mode	Pharmacy/DC to patient's home via mail delivery	Pharmacy to patient's home via collection (patient travel)	Patient to healthcare facility or other public/private place
	Mail delivery 25%	<p>15% small countries: 5 km roundtrip by van</p> <p>+ 65% medium countries: 10 km roundtrip by van</p> <p>+ 20% large countries: 15 km roundtrip by van</p> <p>modelled per tkm with 1 tkm 'market group for transport, freight, light commercial vehicle (RER)' + 'market for operation, reefer, cooling'</p>	N/A	N/A
Home 80%	Travel to pharmacy 75%	N/A	<p>15% small countries: (44 % by car * 5 km +29% by public transport * 5 km)</p> <p>+ 65% medium countries: (44 % by car * 10 km + 29 % by public transport * 10 km)</p> <p>+ 20% large countries: (44 % by car * 15 km + 29 % by public transport * 15 km)</p> <p>modelled (for each country size) with X km 'transport, passenger car (RER)' + 1*X pkm 'market for transport, passenger coach GLO'</p>	N/A
Hospital 20%	None (direct delivery to facility) 100%	N/A	N/A	0% allocated to the product (no dedicated hospital stay)

5.10 Use stage modelling rules

5.10.1 General

Use-stage modelling requires careful attention to product-specific guidance to ensure that downstream impacts are accurately capture:

- Information in the product leaflet should be reviewed thoroughly, as it often contains critical details on dosing, administration route, and storage requirements.
- The use stage could represent a significant share of the product’s life cycle impact, particularly for hospital-administered therapies involving specialized equipment, energy use, or waste handling.
- When applicable, the daily defined dose (DDD) can be applied as a reference unit, for example, to model the impact for one patient over a one-year treatment period (see 4.2). If such data are unavailable, modelling can be based on the maximum recommended dose to avoid underestimation.

5.10.2 Consumables for use stage

Table 48 includes datasets which can be used to model use stage consumables, which are included if they are indicated in the “instructions for use” of the pharmaceutical product.

The end of life of consumables is modelled in the use stage and recommended datasets listed in section 5.11.2, Table 49 can be used to model the waste treatment. Note that some consumables may require sterilisation, to reflect the impacts of the sterilisation process, a default energy use of 1.5 MJ/kg material can be used (energy use for gamma irradiation from source publication of Table 6 in PAS 2090), which is for consumables in drug substance manufacturing, could be used as an approximation in addition to the recommended datasets.

Table 48. Recommended datasets for consumables at home (H) and/or healthcare provider (HP).

Location (H/HP)	Consumable and use	Recommended production dataset
	Dilution (product-specific)	Product-specific
	Cotton	Market for ‘Fibre, cotton’
	Alcohol or antiseptic for disinfection	Market for ‘Ethanol, without water, in 99.7% solution state, from fermentation’ Market for ‘Ethanol, without water, in 99.7% solution state, from ethylene’
	Syringes	See Table 39 for injection moulding, rubber and PP.
H / HP	Needles	See Table 39 for stainless steel and wire drawing.
	Tape	See Table 39 for plastic film extrusion and PE.
	Cotton swab	See Table 39 for plastic extrusion and PP.
	Water to drink	Market for ‘Tap water’
	Spacer for inhaler (paediatric use)	Approximate silicone to rubber. See Table 39 for injection moulding and rubber.
	Paper tissue	Market for ‘Tissue paper’

Location (H/HP)	Consumable and use	Recommended production dataset
	Disposable cup	Plastic cup: See Table 39 for injection moulding and PP. Paper cup: approximate to kraft paper, see Table 39 for kraft paper
	Dosage spoon or small cup	See Table 39 for injection moulding and PP.
	Sharps disposal container (for needles)	See Table 39 for injection moulding and PP.
HP	IV Catheters IV Tubing Tourniquet Dressing tape IV bag for dilutant	See Table 39 for injection moulding, extrusion, plastic film extrusion, rubber, polyurethane and PVC.
	Wooden stick	Market for 'Sawnwood, hardwood, raw'
	Washing of utensils	Tap water: Market for 'Tap water' Soap: Market for 'Soap' Electricity: see section 5.2.2.2. Heat: see Table 15 for heat sources to be applied
H	Water to wash hands and treated area Energy to heat water (if relevant, see PAS 2090) Soap to wash hands	Tap water: Market for 'Tap water' Soap: Market for 'Soap' Electricity: see Table 18 for datasets and the standard for specific electricity modelling rules. Heat: see Table 15 for datasets, and the standard for specific heat sources.

5.10.3 Storage

Some considerations when modelling storage impact during use stage:

- Verify the products' storage instructions or packaging, to determine the refrigeration requirements.
- Remember to exclude the tertiary packaging: storage volume of the product must include the secondary packaging, as it is the condition in which it is packed and stored in the use stage.
- Account for unused product share if relevant (e.g., doses stored but not administered), when this represents a material additional impact.
- Exclude storage impacts for products used in a single administration.
- Use more representative data (e.g., country-specific storage conditions, passive refrigeration technologies, or product-specific data) when available to improve accuracy.

5.11 End-of-life modelling rules

5.11.1 General

EoL modelling plays a key role in reflecting the environmental implications of waste management. While some waste treatment technologies, such as landfill may lead to a relatively low contribution of EoL in LCA results, this should not overshadow the importance of waste prevention and reduction. It is encouraged to consider these aspects in the interpretation of environmental impact assessments and in the development of broader sustainability strategies.

Waste of formulated DS due to deliberate overfill and overage should be included in this LCS.

5.11.2 Allocation of burdens and credits

The PAS 2090 prescribes the recovered content cut-off approach for recycled content and end-of-life impact, as defined in clause 3.1.35. The product generating the waste is cut off at the point of collection: it bears no recycling or recovery process burdens and receives no end-of-life credits. Recovered materials or energy enter the next product system burden-free, and any burdens associated with the recovery process (e.g. material recycling, incineration for energy recovery) are accounted for in that next life cycle.

In some cases, alternative allocation approaches may offer additional insights, though their results must always be reported separately to remain compliant with PAS 2090. Such methods can be useful for sensitivity or comparative analyses, but the recovered content cut-off approach remains the required method for PAS 2090-compliant LCAs.

5.11.3 Packaging

When modelling the end-of-life stage of packaging, it is helpful to apply a mass balance of both primary and secondary packaging materials. The recommendations in this section can also apply to end of life of devices.

Where possible, country-specific waste management systems should be considered to reflect the actual end-market conditions (local mix as defined in “**Table 22 – Default data on average packaging end-of-life treatment pathways of PAS 2090**”). These systems may differ significantly in terms of recycling rates, incineration practices, and landfill availability, which can influence the environmental profile of packaging materials. Some sources that can be consulted for waste treatment rates include:

- When no country-specific data is available, data from the World Bank can be used (Kaza S., 2018).
- For European countries, Annex C of the PEF (European Commission, 2021) or Eurostat statistics (European Commission, 2023).
- For the USA, US EPA data (U.S. Environmental Protection Agency, 2020).
- For Canada, depending on the materials, the following sources can be used: paper (PPEC, 2011), plastic (Ontario, 2019), steel (SWRC, 2012). For other materials, the World Bank can be used.
- For Australia, APCO data can be used (APCO, 2021).
- For plastic-based materials, the Plasteax database (EA, 2020) can be used, with the World Bank (Kaza S., 2018) as a complement.

It is recommended that impact assessment results from LCA of waste treatment should not be interpreted in isolation but considered alongside the principles of the waste hierarchy (prevention, reuse, recycling, recovery, disposal). For example, a product or material is disposed of in a country where landfill is the prevalent waste treatment method, and the results of modelling this treatment yield relatively low environmental impact in LCA results per functional unit, yet from a waste management perspective, this waste treatment route is the least preferred option. The waste hierarchy reflects broader sustainability priorities, and it is encouraged to inform decisions within that context as well.

Table 49 lists the datasets that can be used to model the impact of packaging EoL depending on the material and treatment. A dataset for transport of waste to the treatment facility is provided in the table, in case it is not already included in the treatment dataset. Note that according to the cutoff approach, the transport of waste for disposal is accounted for at end-of-life phase, however if the product is recycled, the transport should be accounted for when recycled materials are used as input. In the case of specific bio-based plastics, if relevant datasets are not available, approximations using proxy datasets or adjustments of existing conventional plastic datasets may be required, namely, by modifying carbon-based emissions to reflect biogenic rather than fossil origins.

Table 49. Recommended datasets for packaging and device EoL

Packaging waste material	Treatment	Recommended dataset
All	Transport to waste treatment facility	In Europe 'Transport, freight, lorry >32 metric ton, EURO6 {RER}' Elsewhere 'Transport, freight, lorry >32 metric ton, EURO5 {RoW}'
	Recycling	Containerboard, fluting medium containerboard production, fluting medium, recycled
Carton, corrugated board box, folding box board	Incineration	Waste paperboard treatment of waste paperboard, municipal incineration
	Sanitary landfill	Waste paperboard treatment of waste paperboard, sanitary landfill
	Unsanitary landfill	Waste paperboard treatment of waste paperboard, unsanitary landfill, dry infiltration class (100mm)
	Open dump	Waste paperboard treatment of waste paperboard, open dump, dry infiltration class (100mm)
	Open burning	Waste paperboard treatment of waste paperboard, open burning
	Paper	Recycling
Incineration		Waste graphical paper treatment of waste graphical paper, municipal incineration
Sanitary landfill		Waste graphical paper treatment of waste graphical paper, sanitary landfill
Unsanitary landfill		Waste graphical paper treatment of waste graphical paper, unsanitary landfill, dry infiltration class (100mm)
Open dump		Waste graphical paper treatment of waste graphical paper, open dump, dry infiltration class (100mm)
Open burning		Waste graphical paper treatment of waste graphical paper, open burning
Aluminium		Recycling
	Incineration	Scrap aluminium treatment of scrap aluminium, municipal incineration
	Sanitary landfill	Waste aluminium treatment of waste aluminium, sanitary landfill
	Unsanitary landfill	Use Waste aluminium treatment of waste aluminium, sanitary landfill as proxy
	Open dump	Use Waste aluminium treatment of waste aluminium, sanitary landfill as proxy
	Open burning	Use Scrap aluminium treatment of scrap aluminium, municipal incineration as proxy

Packaging waste material	Treatment	Recommended dataset
Glass	Recycling	Market for 'Glass cullet, sorted'
	Incineration	Waste glass treatment of waste glass, municipal incineration
	Sanitary landfill	Waste glass treatment of waste glass, sanitary landfill
	Unsanitary landfill	Waste glass treatment of waste glass, unsanitary landfill, dry infiltration class (100mm)
	Open dump	Waste glass treatment of waste glass, open dump, dry infiltration class (100mm)
	Open burning	Waste glass treatment of waste glass, open burning
HDPE, LDPE, PE	Recycling	Polyethylene, high density, granulate, recycled
	Incineration	Waste polyethylene treatment of waste polyethylene, municipal incineration
	Sanitary landfill	Waste polyethylene treatment of waste polyethylene, sanitary landfill
	Unsanitary landfill	Waste polyethylene treatment of waste polyethylene, unsanitary landfill, dry infiltration class (100mm)
	Open dump	Waste polyethylene treatment of waste polyethylene, open dump, dry infiltration class (100mm)
	Open burning	Waste polyethylene treatment of waste polyethylene, open burning
Nylon (6 or 6-6), ABS, PC, PTFE, SAN, PLA**, other plastic	Recycling	Assume no recycling
	Incineration	Waste plastic, mixture treatment of waste plastic, mixture, municipal incineration
	Sanitary landfill	Waste plastic, mixture treatment of waste plastic, mixture, sanitary landfill
	Unsanitary landfill	Waste plastic, mixture treatment of waste plastic, mixture, unsanitary landfill, dry infiltration class (100mm)
	Open dump	Waste plastic, mixture treatment of waste plastic, mixture, open dump, dry infiltration class (100mm)
	Open burning	Waste plastic, mixture treatment of waste plastic, mixture, open burning
PET (amorphous or bottle grade)	Recycling	Polyethylene terephthalate, granulate, amorphous, recycled
	Incineration	Waste polyethylene terephthalate treatment of waste polyethylene terephthalate, municipal incineration
	Sanitary landfill	Waste polyethylene terephthalate treatment of waste polyethylene terephthalate, sanitary landfill
	Unsanitary landfill	Waste polyethylene terephthalate treatment of waste polyethylene terephthalate, unsanitary landfill, wet infiltration class (500mm)
	Open dump	Waste polyethylene terephthalate treatment of waste polyethylene terephthalate, open dump, dry infiltration class (100mm)
	Open burning	Waste polyethylene terephthalate treatment of waste polyethylene terephthalate, open burning

Packaging waste material	Treatment	Recommended dataset
PP	Recycling	Use 'Polyethylene, high density, granulate, recycled' as proxy
	Incineration	Waste polypropylene treatment of waste polypropylene, municipal incineration
	Sanitary landfill	Waste polypropylene treatment of waste polypropylene, sanitary landfill
	Unsanitary landfill	Waste polypropylene treatment of waste polypropylene, unsanitary landfill, dry infiltration class (100mm)
	Open dump	Waste polypropylene treatment of waste polypropylene, open dump, dry infiltration class (100mm)
	Open burning	Waste polypropylene treatment of waste polypropylene, open burning
PS (general or extruded), EPS	Recycling	Polystyrene foam slab, 100% recycled
	Incineration	Waste polystyrene treatment of waste polystyrene, municipal incineration
	Sanitary landfill	Waste polystyrene treatment of waste polystyrene, sanitary landfill
	Unsanitary landfill	Waste polystyrene treatment of waste polystyrene, unsanitary landfill, dry infiltration class (100mm)
	Open dump	Waste polystyrene treatment of waste polystyrene, open dump, dry infiltration class (100mm)
	Open burning	Waste polystyrene treatment of waste polystyrene, open burning
PU (flexible or rigid)	Recycling	Assume no recycling
	Incineration	Waste polyurethane treatment of waste polyurethane, municipal incineration
	Sanitary landfill	Waste polyurethane treatment of waste polyurethane, sanitary landfill
	Unsanitary landfill	Waste polyurethane treatment of waste polyurethane, unsanitary landfill, dry infiltration class (100mm)
	Open dump	Waste polyurethane treatment of waste polyurethane, open dump, dry infiltration class (100mm)
	Open burning	Waste polyurethane treatment of waste polyurethane, open burning
PVC (bulk or emulsion polymerized)	Recycling	Assume no recycling
	Incineration	Waste polyvinylchloride treatment of waste polyvinylchloride, municipal incineration
	Sanitary landfill	Waste polyvinylchloride treatment of waste polyvinylchloride, sanitary landfill
	Unsanitary landfill	Waste polyvinylchloride treatment of waste polyvinylchloride, unsanitary landfill, dry infiltration class (100mm)
	Open dump	Waste polyvinylchloride treatment of waste polyvinylchloride, open dump, dry infiltration class (100mm)
	Open burning	Waste polyvinylchloride treatment of waste polyvinylchloride, unsanitary landfill, dry infiltration class (100mm)

Packaging waste material	Treatment	Recommended dataset
Steel, stainless steel	Recycling	Waste reinforcement steel treatment of waste reinforcement steel, recycling
	Incineration	Scrap steel treatment of scrap steel, municipal incineration
	Sanitary landfill	Scrap steel treatment of scrap steel, inert material landfill
	Unsanitary landfill	Scrap steel treatment of scrap steel, inert material landfill
	Open dump	Use Scrap steel treatment of scrap steel, inert material landfill as proxy
	Open burning	Use Scrap steel treatment of scrap steel, municipal incineration as proxy, no credits for energy recovery
Synthetic rubber	Recycling	Synthetic rubber
	Incineration	Waste rubber, unspecified treatment of waste rubber, unspecified, municipal incineration
	Sanitary landfill	Waste plastic, mixture treatment of waste plastic, mixture, sanitary landfill
	Unsanitary landfill	Waste plastic, mixture treatment of waste plastic, mixture, unsanitary landfill, dry infiltration class (100mm)
	Open dump	Waste plastic, mixture treatment of waste plastic, mixture, open dump, dry infiltration class (100mm)
	Open burning	Assume as Waste rubber, unspecified, no credit for energy recovery
Wood	Recycling	Assume no recycling
	Incineration	Waste wood, untreated treatment of waste wood, untreated, municipal incineration
	Sanitary landfill	Waste wood, untreated treatment of waste wood, untreated, sanitary landfill
	Unsanitary landfill	Waste wood, untreated treatment of waste wood, untreated, unsanitary landfill, dry infiltration class (100mm)
	Open dump	Waste wood, untreated treatment of waste wood, untreated, open dump, dry infiltration class (100mm)
	Open burning	Waste wood, untreated treatment of waste wood, untreated, open burning
Other materials	All treatments	Use regional/local municipal waste treatment

* The proposed datasets are for the average treatment of specific material. For landfill and open dump, an average technology treatment is not available, therefore this table only proposes dry infiltration class 100mm datasets. The practitioner should choose the infiltration classes which should correspond to the respective technology and geography

** Emissions from incineration of polylactide may lead to an overestimation of climate change impact, since the respective biogenic CO₂ emissions are approximated to an average mixture of plastic waste.

5.11.4 Chemical compounds

5.11.4.1 Drug product-derived compounds

Wastewater (WW) composition and treatment

Based on Table 23 from the PAS 2090, the geographical representativeness of wastewater impacts can be further improved by modelling the share of wastewater treatment and release.

Modelling of wastewater treatment

For the portion of treated wastewater, PAS 2090 requires that the wastewater treatment plant (WWTP) process be modelled using an average municipal WWTP dataset (e.g. ecoinvent market for 'Wastewater, average'). Where possible, the practitioner should adapt the energy-related background datasets to reflect country-specific conditions, if such data are available.

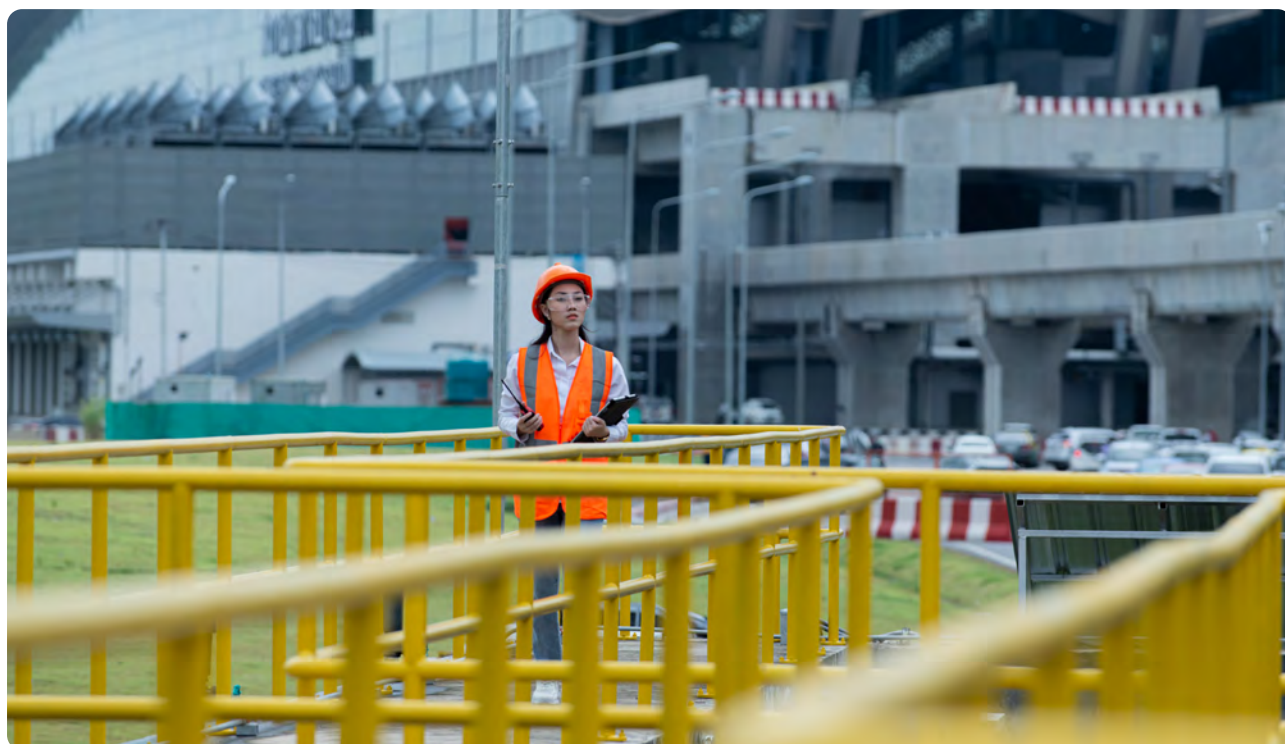
Modelling of untreated wastewater discharge

For the share of wastewater that is discharged into the environment without treatment, the effluent composition can be retrieved from published studies for some regions and potentially consulted in ecoinvent.

5.11.4.2 Carbon dioxide emissions to air

Chemical compounds making up the pharmaceutical product and their derivatives basically end up in two main environmental compartments: water (after wastewater treatment or direct release) and air (via CO₂ and N₂O release).

While the carbon dioxide must be modelled as the fossil carbon content emitted 100% to air according to PAS 2090, the release of nitrogen and phosphorous compounds can be calculated using transfer coefficients from Doka (Doka, 2021) to the respective environmental compartments. This would improve the data quality compared to a generic dataset for wastewater treatment, provided that the untreated wastewater (input to wastewater treatment facility) composition is known.



Emissions to air are calculated as follows (Table 50):

Table 50. Example calculation of emissions to air. Data from Doka (Doka, 2021)

Element	Content in wastewater (mg/L) (A)	Transfer coefficients to air (occurs during secondary treatment) (B)	Emissions to air (mg/L) (C = A · B)	Conversion to emitted substance
N	31	20.7% as N ₂ of which 0.68% is converted to N ₂ O	20.7% x 31mg N/L= 6.4 mg N/L emitted 0.68% x 6.4 mg N/L= 0.044 mg N₂O-N/L	0.44 mg N ₂ O-N/L x 44 mg N ₂ O/28 mg N= 0.69 mg N₂O/L

Emissions to final effluent can be calculated as follows (Table 51):

Table 51. Example calculation of emissions to water. Data from Doka (Doka, 2021)

Element	Content in wastewater (mg/L) (A)	Transfer coefficients to air (occurs during secondary treatment) (B)	Emissions to air (mg/L) (C = A · B)	Conversion to emitted substance
N	31	53% as NO ₃ ⁻	53% x 31mg N/L= 16.4 mg N-NO ₃ ⁻ /L	16.4 mg N ₂ O-N/L x 62 mg NO ₃ ⁻ /14 mg N= 72.8 mg NO₃⁻/L

A similar approach applies to phosphorus emissions to final effluent as phosphate, applying a conversion factor of 3.06 kg PO₄³⁻ / kg P. For further information on wastewater treatment stages and transfer coefficients, see the original publication (Doka, 2021).

6.0 Results interpretation and reporting

6.1 Result interpretation

6.1.1 General

PAS 2090 requires impact assessment interpretation for the impact categories defined in section 4.7. In addition, the model robustness must be evaluated. See the PAS 2090 for further specifications.

In addition, the robustness of the model must be evaluated (see PAS 2090 for detailed requirements).

6.1.2 Product comparisons

The requirements are provided in PAS 2090, which are based on ISO 14044.

6.2 Results reporting

To support the reporting of LCA of pharmaceutical products, a report template is provided in Appendix I – Report template. It is based on the main requirements checklist of PAS 2090 (Annex A, Table A.1).

For public communications, third-party review, self-declared environmental claims and environmental footprint reporting, see the specific standards listed in PAS 2090.

→ *PAS 2090 requires impact assessment interpretation for the impact categories defined in section 4.7.*



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Appendix

Appendix I – Report template

Below is a report template in alignment with PAS 2090 main requirements and based on Table A.1 of PAS 2090.

Goal and scope of the LCA

Goal of the LCA

Define the goal of the study. The goal of the study must be set according to BS EN ISO 14044:2006+A2 and should match the purpose of which it is intended.

Make sure to state:

- a) the intended application;
- b) the reasons for performing the study;
- c) the intended audience for the communication of results; and
- d) whether comparative assertions resulting from the study are intended to be publicly disclosed.

Scope of the LCA

Declared unit

A declared unit, corresponding to “manufacturing of one product unit” must be used as per PAS 2090 requirements. Clearly report the product unit(s) evaluated.

Reference flow: The reference flow must equal the product unit(s).

For chronic disease, report the period of application of the treatment.

Functional unit

If product comparison is in scope of the study, the same functional unit must be defined and applied as per PAS 2090 considerations (sections 4.2 to 4.6).

System boundaries

Select and report the boundaries in alignment with the goal of the LCA, specifying the gate. Remember that all attributable activities, inputs, and outputs within the system boundary must be included.

When non-attributable activities are included due to its relevant for the goal and scope of the study, clearly document them and list them (also in the inventory documentation). This also applies for capital goods included in the analysis (foreground data).

Clearly indicate if product collection is included in the system boundaries and intentionally excluded with appropriate justification. Results including this impacts still must be separately reported using default data.

Recommended: provide as much information as possible of the system in scope for transparency.

Geographical scope

Report the geographical area(s) where each LCS occurs, whether single or multiple.

Cut-off criteria

If cut-off rule is applied, report and explain the selected threshold.

When data collection or modelling is limited by a selected cut-off rule, the significance threshold shall be reported and justified. Remember that no cut-off shall be applied to the BOM used for DS and DP manufacturing modelling, except for starting materials for biological drug substance (master or working cell bank).

Impact categories

PEF impact assessment methods must be used. Impact categories must be selected based on the goal and scope of the study.

Life cycle inventory

Report non-confidential life cycle inventory data.

Report the fossil and biogenic carbon content of the drug product.

Report any non-attributable activities included.

For manufacturing stages report:

- Whether energy data of manufacturing stages includes energy for water treatment.
- Total amount of waste considered hazardous.
- Amount of consumables in units/pieces or weight (kg).

Report storage site locations for the distribution stage, product volume, and refrigeration requirements.

Specify for which data points or datasets, default data of PAS 2090 has been used when primary data was not available (and in alignment with PAS 2090 requirements).

Recommended: disclose foreground and background data per functional unit.

Data sources

Collect data for all processes under the company's ownership or control.

Disclose and justify the use of supplier-specific data. Report any limitations identified. Make sure that all documentation is provided.

Secondary data sources

Use the relevant clauses to obtain secondary data.

Recommended: report database utilized. Databases in use must meet criteria of section 5.1.3. of PAS 2090.

Data quality requirements

Specify the data quality requirements needed to meet the goal and scope of the LCA.

Report whether the activity and background data are primary, secondary or proxy data for each first impact driver per life cycle stage, in each environmental impact category assessed.

For comparative assertions intended for public disclosure, address data quality in terms of time, geographical and technological representativeness, precision, completeness, consistency, reproducibility, data sources, and uncertainty.

Data quality assessment

If the study is to be used for comparative assertions made publicly, include the data quality assessment as per PAS 2090 5.1.2 requirements, and in compliance with the data quality requirements set.

Method

Recommended: report general methodological approaches. Example: description of allocation of utilities at product level, if applicable.

Allocation rules

Multi-output processes are modelled following the decision tree in Figure 2. For transparency, it is recommended to describe the allocation approach applied for each multi-output process within the system boundaries, especially if it is deemed to have a significant influence in the results. Alternative allocation approaches (example, CFF for EoL) must be included in this section. Note that results must be reported with cut-off approach, and results using alternative methods are reported separately.

Result reporting and interpretation

Conduct interpretation of the impact categories selected in accordance with Section 4.7 Impact categories of PAS 2090.

Include assessment of model robustness through completeness check, sensitivity check and consistency check.

Report results including product collection and personal travels to administration site(s), if it is part of the system boundaries. If the stage is within the system boundaries but deliberately excluded from the goal and scope, results must still be reported in the annex.

Report the name, nature, and composition of the primary API metabolite, as systematically identified during product development.

If contractual instruments are included in the scope of the study: Report results under market-based and location-based approach.

Report overall limitations of the study.

Separately report results with approaches alternative to the PAS 2090 requirements, for example (not limited to):

- Results where recycled content cut-off is not applied
- Results calculated using other impact assessment methods
- Results with alternative allocation methods (sensitivity analysis, etc.)
- Results including impact of capital goods and infrastructure modelled in the foreground
- Results without product collection impact
- Results including fossil carbon uptake and emissions
- Results including biogenic CO₂ uptake and emissions

In case of comparison, follow the ISO 14044.

Annex

List any modified dataset.

Include results of product collection (when deliberately excluded from goal and scope of the study and the system boundaries include the stage).

Appendix II – Modelling single use items

Modelling single-use items is crucial when conducting LCAs for the manufacture of biologics, large molecules and vaccines, given their extensive use in these processes. Ideally, such data should be obtained directly from suppliers; however, there are often hundreds of different items sourced from numerous suppliers, making data collection resource intensive.

Where supplier-specific LCA data cannot be obtained, it is recommended to follow the steps outlined below. PAS 2090 provides a simplified method for estimating consumable weight, assuming it represents 5% of the total process water plus the attributable material weight, as outlined in Note 5 of “**Table 5 – Minimum inventory data required for drug-substance manufacturing modelling**”. The approach described here allows further differentiation by incorporating actual bill-of-materials (BOM) data and grouping items according to their type, material, processing method and cost.

Gather BOM Items

Compile the bill of materials and identify the single-use items that require modelling. Collect any available data, such as the material of construction (which may sometimes be indicated in the item name) and the cost of each item.

Identify item groupings

Group items into the following non-exhaustive list of categories:

- Connector
- Filter
- Assembly
- Manifold
- Bottle
- Bag
- Cap
- Tubing
- Plastic
- Bioreactor

→ *Modelling single-use items is crucial when conducting LCAs for the manufacture of biologics, large molecules and vaccines, given their extensive use in these processes.*



Where assemblies consist of multiple individual components, the drawing specification can be used to break out all items; otherwise, the overall assembly impact may be underestimated.

Groups may be further disaggregated to improve modelling detail by defining simple and complex versions of each item type and using the median price of consumables to distinguish subcategories.

Ancillary items used for activities outside the scope of the LCA (for example, laboratory testing) may be excluded.

Groups can be further disaggregated to improve modelling detail by deriving simple and complex versions of each of the items and using the median price of consumables to group consumables into the subcategories.

An example of possible item groupings and indicative grouping rules is provided in Table 52.

Table 52. Example of item groupings and indicative grouping rules.

Item type	Item group	Grouping rule
Connector	Simple connector	Low cost, based on cost threshold for connectors
	Complex connector	High cost, based on cost threshold for connectors
Filter	Simple filter	Low cost, based on cost threshold for filters
	Complex filter	High cost, based on cost threshold for filters
Assembly	Simple assembly	Low cost, based on cost threshold for assemblies
	Complex assembly	High cost, based on cost threshold for assemblies
Manifold	Simple manifold	Low cost, based on cost threshold for manifolds
	Complex manifold	High cost, based on cost threshold for manifolds
Bottle	Glass bottle	Any bottle made of glass
	Plastic bottle	Any bottle made of plastic
Bag	Bag	All bag items
Cap	Cap	All cap items
Tubing	Tubing	All tubing
Plastic	Plastic	All plastic items
Bioreactor	Bioreactor	All bioreactors

Identify representative items to collect primary data

Collecting data for all individual items can be impractical. Within each group, identify representative items, for example, based on quantity, cost or relevance. These items should be modelled using primary data to approximate the total number of items in that group. Either a single representative item can be selected, or multiple items can be modelled and their results averaged to obtain a representative value.

Fill primary data gaps

For the identified representative items, gather the following data by reaching out to suppliers, measuring the data:

- Primary material of construction; breakdown % mass of materials of construction
- Mass of item
- Main processing method
- Price of item

An example of how such data can be organised is provided in Table 53.

Table 53. Example primary data collection sheet.

Component number	Material name	Supplier	Manufacturing location	Main material of construction	Mass (kg/unit)	Processing type	Unitary price of item (currency/unit)
ID of component	Bioreactor 500L	Supplier 1	Country 1	PE	32	Extrusion	100

Model emission factor data

Using these data, an emission factor can be calculated. The mass, material composition, and processing type are first used to estimate the baseline emissions of each item. However, manufacturing of these components involves additional requirements, such as cleanroom conditions, HVAC operation and sterility controls, which increase energy use and overall impact beyond that of the basic processing step (e.g. injection moulding or extrusion). To capture this, a complexity factor is introduced, calculated as the ratio of the item cost to the cost of the main commodity material.

$$EF_{item} = ([m_{item} \times EF_{material}] + [m_{item} \times EF_{processing}]) \times \left(\frac{P_{item}}{P_{material}} \right)$$

Where:

EF_{item} = total emission factor for the item in kg CO₂e/kg

m_{item} = mass of the item in kg

$EF_{material}$ = emission factor of the material in kg CO₂e/kg

$EF_{processing}$ = emission factor for processing in kg CO₂e/kg

P_{item} = price of the item (currency/unit)

$P_{material}$ = price of the main commodity material (currency/unit)

This complexity factor can be significant, in these cases, an upper cap of 5 is applied based on expert judgement.

For the purpose of this illustration, the calculation focuses on the climate change indicator (kg CO₂e). However, the same approach can be applied more broadly within the LCI model to quantify other environmental flows and impact categories, in line with a complete life cycle assessment.

Calculate total impacts per item group

Multiply the modelled emission factor by the number of items in each group to calculate the total impact per item type. Repeat this step for all item categories. An example of the resulting calculations is provided in Table 54.

Table 54. Example of aggregated results for consumable item groups.

Item type	Item group	Number of units per batch	Unit	Carbon footprint per unit [kg CO ₂ e/piece]	Total carbon footprint [kg CO ₂ e]
Connector	Simple Connector	32	piece	0.1	3.20
	Complex Connector	19	piece	11.8	224.20
Filter	Simple Filter	40	piece	12.3	492.00
	Complex filter	24	piece	35.1	842.40
Manifold	Simple Manifold	28	piece	12.1	338.80
	Complex Manifold	0	piece	33.2	0
Bottle	Glass Bottle	83	piece	2.05	170.15
	Plastic Bottle	100	piece	0.03	3.00
Bag	Bag	14	piece	21.1	295.40
Cap	Cap	50	piece	0.09	4.50
Tubing	Tubing	112	piece	2.1	235.20
Plastic	Plastic	201	piece	0.02	4.02
Bioreactor	Bioreactor	1	piece	253	253.00

Appendix III – Modelling of injection needles

The following table provides indicative data to support the modelling of needles used in syringe and pen systems. These represent configurations for different administration routes: subcutaneous, intramuscular, and intravenous injections, as well as pen needles used for devices such as insulin pens.

This classification is not exhaustive and serves as an indication of typical gauge, length, material composition, and component mass ranges observed in common medical applications. Values are based on data from consortium members, the Apiject LCA report (Eckelman & Litan, 2024), and manufacturer specifications (e.g. Sigma-Aldrich).

Table 55. Configurations and component data for needles used in syringe and pen systems.

Needle type			Pen Needles (subcutaneous)	Hypodermic needles (subcutaneous injections)	Hypodermic needles (intramuscular injections)	Hypodermic needles (intravenous injections)	References
Gauge/Length			29 - 32 G / 4 - 8 mm	25 -27 G / 13 - 25 mm	18 - 23 G / 25 - 40 mm	18 - 25 G / 25 - 40 mm	Obtained from Sigma Aldrich
Device components	Material	Unit / needle					
Needle (hub + cannula)	-	-	-	-	-	-	-
Needle plastic hub	Plastic (PP or PE)	g	0.1 - 0.2	0.4-0.6	0.4-0.6	0.4-0.6	Pen needles: Provided by members of the consortium Other needles: Based on Apiject report (Eckelman & Litan, 2024)
Steel cannula (SS SUS 304) Density 8.02 g/cc	Stainless steel	g	0.004 - 0.008	0.018 - 0.044	0.066 - 0.287	0.044 - 0.287	
Safety cap/ cover	-	-	-	-	-	-	-
Safety cap (inner and outer cap)	Plastic (PP)	g	1	1	1	1	Apiject LCA report (Eckelman & Litan, 2024)
Consumption	-	-	-	-	-	-	-
Assembly energy	Electricity	kWh		0.006-0.012			Apiject LCA report, Appendix B (Eckelman & Litan, 2024)
Sterilization (EtOH)	EtOH	mg		50-100			Provided by members of the consortium

Technical Guidance

Supplementary document to the PAS
2090:2025, Pharmaceutical products – Product
category rules for environmental life cycle
assessments – Specification

Prepared by



Contributors



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