Life Cycle Assessment of Industrial Chemical Production Processes

An Analysis using openLCA and the Ecoinvent Database

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Outline

Project Overview and Objectives

Primary Goal

To perform a comprehensive Life Cycle Assessment (LCA) for three distinct industrial processes:

- **Paracetamol Production** (1 kg functional unit)
- **Ammonia Production** (1 Ton functional unit)
- **Cement Production** (1 Ton functional unit)

Core Objectives

- To quantify the environmental impacts across various categories for each process.
- To identify the primary environmental "hotspots" within each life cycle.
- To utilize openLCA software and the Ecoinvent database for a standardized and transparent analysis.

Standardized LCA Methodology

All three assessments were performed following a consistent and robust methodology to ensure comparability and scientific validity.

LCA Software & Database

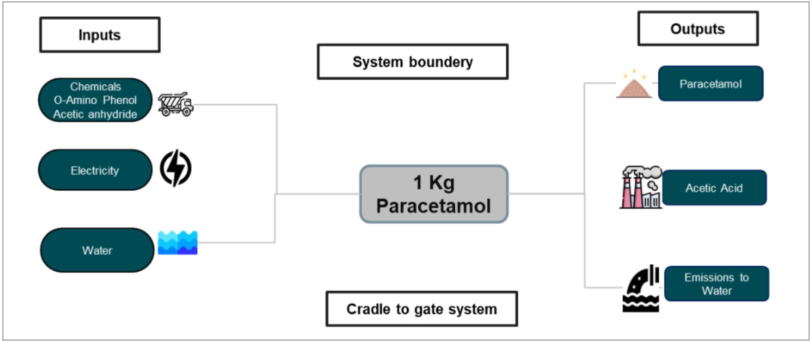
- **Software:** openLCA (v1.11)
- **Database:** Ecoinvent (v3.8)
- **Rationale:** Ecoinvent is a globally recognized, comprehensive, and transparent LCI database, making it a standard choice for credible LCA studies.

Impact Assessment Method

- **LCIA Method:** ReCiPe Midpoint (H)
- **Description:** This method provides a wide range of well-documented impact categories, allowing for a detailed and multi-faceted environmental analysis.

System Boundary

- **Boundary:** Cradle-to-Gate
- **Scope:** Includes raw material extraction, transportation, and final product


Inputs
System boundery
Outputs
Chemicals
O-Amino Phenol
Acetic anhydride
Electricity
Water
1 Kg
Paracetamol
Paracetamol
Acetic Acid
Emissions to Water
Cradle to gate system

LCA of Paracetamol (1 kg)

Goal and Scope

To assess the environmental impacts of producing 1 kg of Paracetamol, focusing on identifying hotspots in the upstream supply chain.

Table: Inventory Data for 1 kg Paracetamol Production

Inputs	**Amount**	**Unit**
4-Nitrophenol	0.92	kg
Pd/catalyst	0.92	kg
Acetic acid	0.69	kg
Water (Demineralised)	1.38	kg
Energy	19.9	MJ

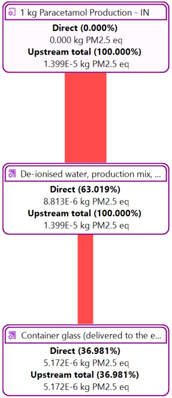


Figure: Sankey for paracetamol

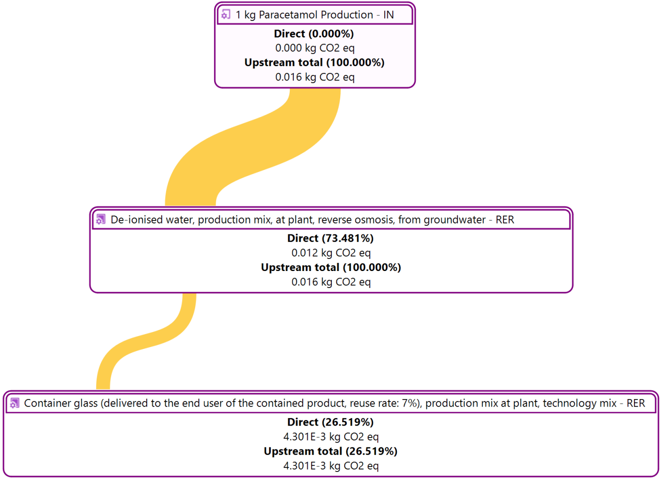


Figure: Sankey for paracetamol

Paracetamol: Hotspot Analysis (PM2.5)

Key Finding

The direct manufacturing process of Paracetamol has a negligible direct impact. The environmental hotspots are located in the upstream supply chain, specifically related to auxiliary inputs and packaging.

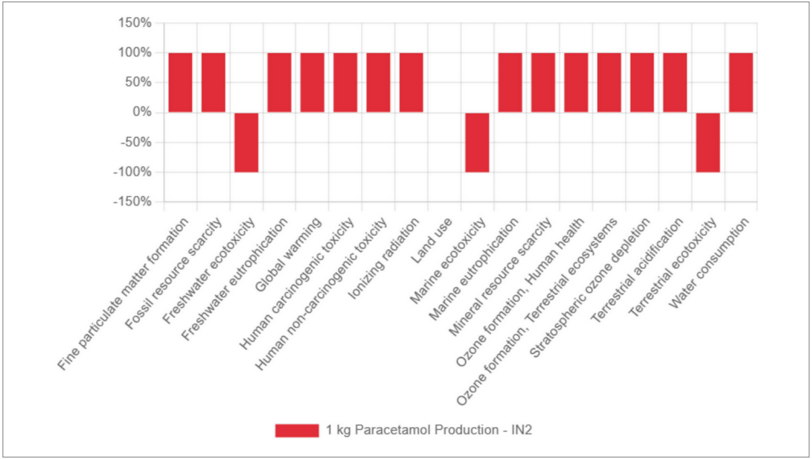


Figure: Process contribution for Fine Particulate Matter (PM2.5). Hotspots are clearly identified as de-ionised water production (63%) and container glass manufacturing (37%).

Paracetamol: Final Impact Assessment Results

Table: Key Impact Indicators for 1 kg Paracetamol

Indicator	Result	Unit
Global warming	**1.622e-2**	**kg CO2 eq**
Mineral resource scarcity	3.937e+3	kg Cu eq
Human non-carcinogenic toxicity	5.871e-2	kg 1,4-DCB
Fine particulate matter formation	1.398e-5	kg PM2.5 eq
Freshwater ecotoxicity	-2.557e-2	kg 1,4-DCB
Marine ecotoxicity	-2.368e-3	kg 1,4-DCB
Terrestrial ecotoxicity	-5.971e+1	kg 1,4-DCB

Key Observations

- The global warming impact is relatively small at 0.016 kg CO2 eq.
- Mineral resource scarcity remains the most significant positive impact.
- The final results confirm the **negative values** for multiple ecotoxicity categories.

Paracetamol: Impact Assessment Results

Table: Key Impact Indicators for 1 kg Paracetamol

Indicator	Result	Unit
Mineral resource scarcity	3.93760e+3	kg Cu eq
Human non-carcinogenic toxicity	5.87131e-2	kg 1,4-DCB
Global warming	1.62202e-2	kg CO2 eq
Fine particulate matter formation	1.39851e-5	kg PM2.5 eq
Freshwater ecotoxicity	-2.55751e-2	kg 1,4-DCB
Terrestrial ecotoxicity	-5.97107e+1	kg 1,4-DCB

Notable Results

- **Mineral Resource Scarcity** is overwhelmingly the largest impact, likely due to the use of catalysts (e.g., Palladium).
- Several ecotoxicity categories show **negative values**. This is a significant finding that requires explanation.

Relative Impact Profile and Discussion

Relative Contribution Across All Categories

This chart shows the relative impact for each category, with the largest impact set to 100%. It provides an excellent overview of the environmental profile.

- It visually confirms that impacts like Mineral Resource Scarcity and Human Toxicity are significant positive contributors.
- It clearly displays the "environmental credit" or **avoided burden** in the ecotoxicity categories, shown as negative bars.

Explaining Negative Ecotoxicity: The "Avoided Burden" Principle

Observation

The results for Freshwater and Terrestrial Ecotoxicity are negative. This seems counter-intuitive but is a valid outcome in LCA.

Explanation: Avoided Burden

- Negative values typically represent an "avoided burden" or environmental credit.
- This occurs when a process within the system boundary (e.g., an input's production) includes co-production of a recycled material or has an advanced waste treatment process.
- The environmental benefit of this co-process (e.g., avoiding the production of virgin material or treating waste that would otherwise be released) is credited to the system, resulting in a negative impact value.
- **Our Case:** The specific data flow chosen for one of the inputs likely contained an internal waste management or recycling process. This flow was selected after careful review, as it was the most representative option available in the Ecoinvent database for the specified chemical input.

Case Study 2: Ammonia Production

LCA of Ammonia (1 Ton)

Goal and Scope

To assess the environmental impacts of producing 1 Ton of Ammonia via the Haber-Bosch process, including the upstream production of hydrogen via steam reforming.

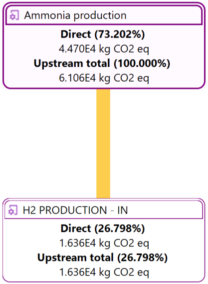
Phase I: H Production (Inputs)

- Water: 4.9 Ton
- Energy: 5.7 MWh
- Methane: 2.2 Ton

Phase II: Ammonia Synthesis (Inputs)

- Hydrogen (from Phase I): 3 Ton
- Nitrogen: 1 Ton
- Energy: 8.1 MWh

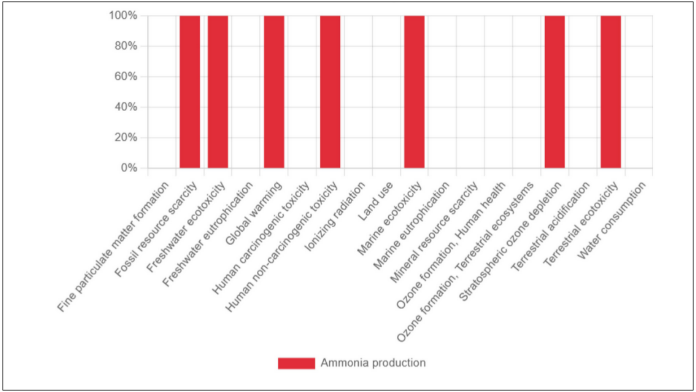
Sankey for Amomonia (Global Warming)



Ammonia: Hotspot Analysis (Global Warming)

Key Finding

Ammonia production is a major contributor to global warming. Both the direct synthesis and the upstream hydrogen production are significant hotspots.



Ammonia: Impact Assessment Results

Key Impact Indicators for 1 Ton Ammonia

Indicator	Result	Unit
Global warming	**2.65e+5**	**kg CO2 eq**
Human non-carcinogenic toxicity	1.25e+5	kg 1,4-DCB
Terrestrial ecotoxicity	6.94e+4	kg 1,4-DCB
Fossil resource scarcity	1.23e+3	kg oil eq
Stratospheric ozone depletion	1.65e+0	kg CFC11 eq

Analysis

The extremely high Global Warming Potential (GWP) is expected and aligns with literature values. This is due to the high energy demand (primarily from natural gas for both heat and as a feedstock) of the steam reforming and Haber-Bosch processes.

Case Study 3: Cement Production

LCA of Cement (1 Ton)

Goal and Scope

To assess the environmental impacts of producing 1 Ton of cement, with a focus on energy consumption and raw material inputs.

Table: Key Inventory Data for 1 Ton Cement Production

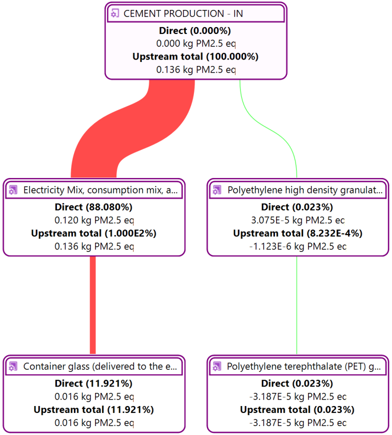
Inputs	**Amount**	**Unit**
Limestone	1.37	Ton
Electricity	120	kWh
Clay	0.0597	Ton
Gypsum	0.0616	Ton
Water	0.752	m^3

Cement: Hotspot Analysis (PM2.5)

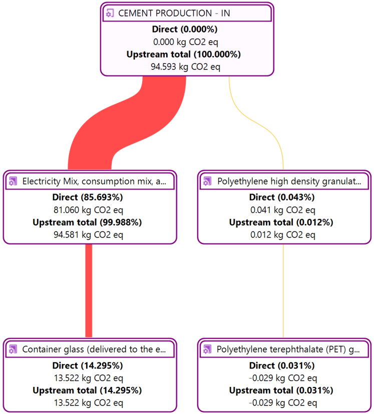
Key Finding

For fine particulate matter formation, the primary hotspot is not the cement process itself, but the upstream generation of electricity required to power the plant.

Sankey for Cement (PM 2.5)



Sankey for Cement Global Warming



Cement Impact Factor

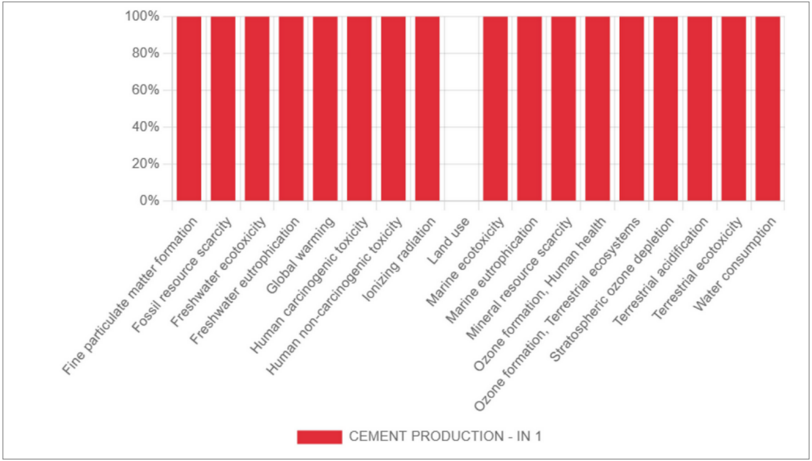


Figure: All Impact Factors for Cement

Cement: Impact Assessment Results

Key Impact Indicators for 1 Ton Cement

Indicator	Result	Unit
Global warming	9.46e+1	kg CO2 eq
Mineral resource scarcity	2.81e+1	kg Cu eq
Fossil resource scarcity	2.37e+1	kg oil eq
Terrestrial ecotoxicity	1.92e+1	kg 1,4-DCB
Fine particulate matter formation	1.36e-1	kg PM2.5 eq

Analysis

While the GWP is significant (due to both energy use and calcination of limestone), the hotspot analysis reveals the critical importance of the electricity source. A transition to cleaner electricity would drastically reduce the PM2.5 impact.

Data Selection and Addressing Discrepancies

Our Commitment to Data Quality

The credibility of an LCA heavily relies on the quality and relevance of the Life Cycle Inventory (LCI) data. We undertook a rigorous process for data selection.

Data Selection Process

- **Multiple Checks:** For each input in our inventory, multiple data flows within the Ecoinvent database were reviewed for relevance.
- **Best Fit Principle:** We selected the dataset that most closely matched the process in terms of technology, geography (where applicable), and system boundary.
- **Use of Proxies:** In cases where an exact match was not available (a common challenge in LCA), we used a proxy dataset. This involves selecting a flow for a similar chemical or process. This choice was made transparently and based on the best available data.
- **Documentation:** All data selections and justifications were documented internally to ensure transparency and reproducibility of our results.

Summary of Key Findings

This analysis successfully quantified the environmental impacts and identified key hotspots for three industrial processes using openLCA.

Paracetamol Production

The primary environmental burdens are not from the direct synthesis but from **upstream processes**, namely the production of de-ionised water and glass packaging. This highlights the importance of a full life-cycle perspective.

Ammonia Production

The process is a major contributor to **global warming**, driven by the high energy intensity of both steam reforming for H and the subsequent Haber-Bosch synthesis.

Cement Production

Energy consumption is the dominant driver of several impact categories. Specifically, the **electricity grid mix** is the single largest hotspot for fine particulate matter formation.

Thank You

Questions?