



GreenDelta

sustainability consulting + software



# Rethinking Additives in Plastic LCA: Predictive openLCA Workflows for an underrepresented Material Class

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Picture: Julia Cilleruego Palomero

# Motivation

≡ CNN Health

## Millions of preterm births and thousands of infant deaths linked to plastic chemical

Two chemicals used to make plastic more flexible are linked to nearly 2 million **premature births** and the deaths of 74,000 newborns worldwide in 2018, according to a new study.



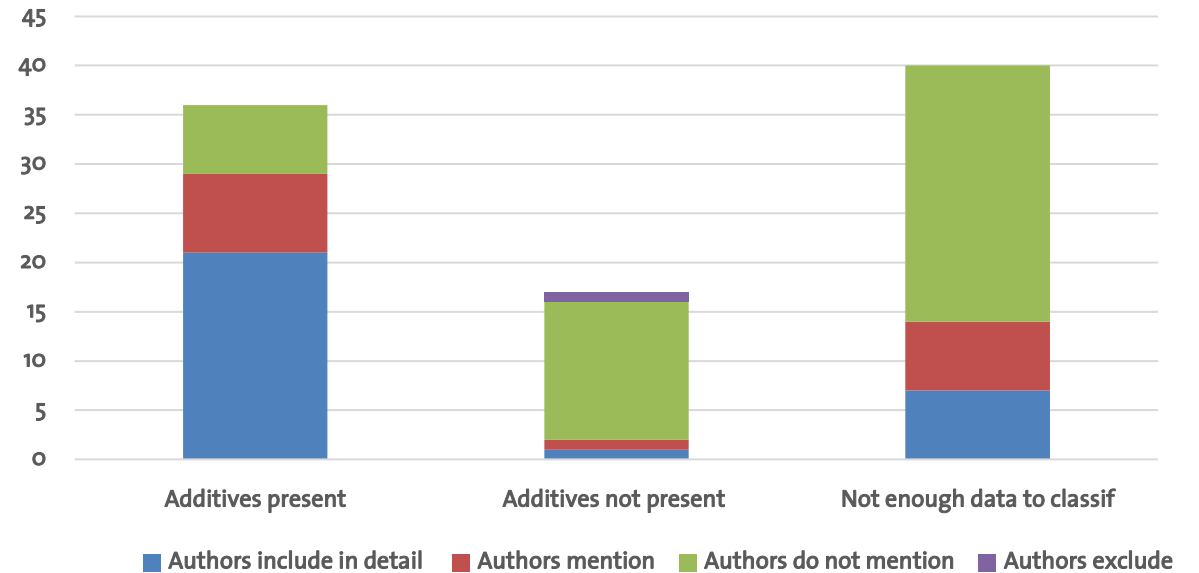
(Jennifer Brückner/picture alliance/Getty Images)

“This is a dangerous class of chemicals,” said Dr. Leonardo Trasande, senior author of the new study and the Jim G. Hendrick, M.D., Professor of Pediatrics at NYU Langone’s Grossman School of Medicine in New York City.

“In the context of all the efforts that we’re taking to have more babies born in the United States, we should also make sure that babies are born healthy,” said Trasande, who is also a professor of population health and director of the Division of Environmental Pediatrics and the Center for the Investigation of Environmental Hazards at NYU Langone Health.

<https://edition.cnn.com/2026/03/31/health/phthalates-infant-death-prematurity-wellness> (10.04.26)

## Additives in LCI data



However, if data was present in 40% of the datasets, aggregated additives or utilized generic proxy data (generic disclosures) to model additives. Further, generic disclosures of additives limit what can be understood about their environmental and human health impacts

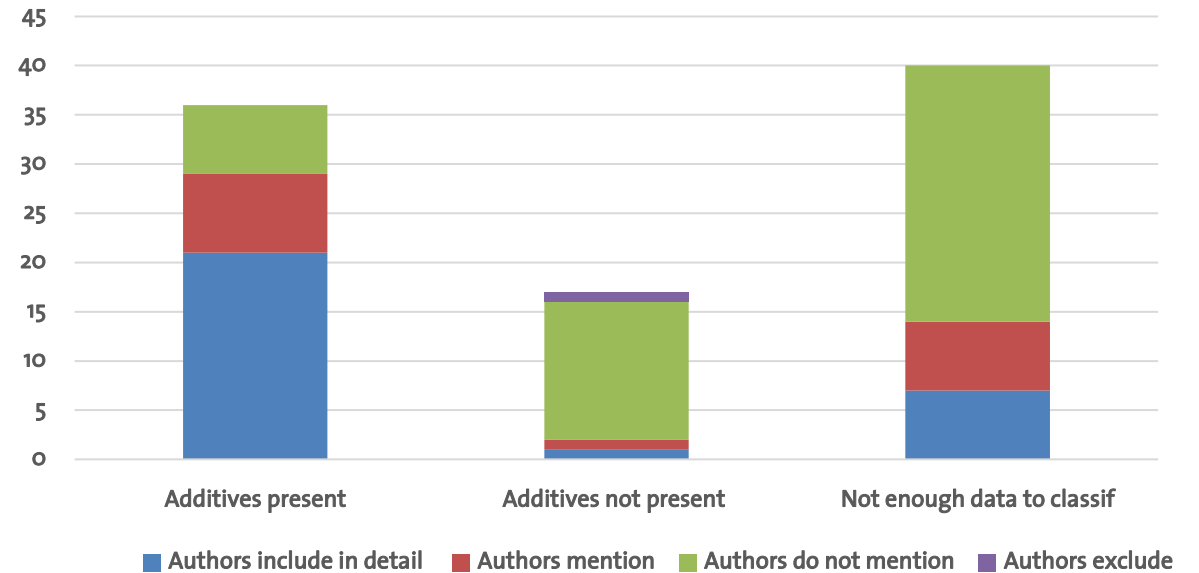
Logan et al., J. Ind. Ecol. 2024 Aug 16;28(6):1582–1597.

# Motivation

| Additive classification term         | Source for classification term | Examples of additives (OECD, 2019)   |
|--------------------------------------|--------------------------------|--|
| Additives for processability         | OECD (2019)                    | Plasticizers, lubricants, blowing agents   |
| Surface protector / modifier         | OECD (2019)                    | Antistatic agents, antifriction agents, adhesion-improving agents, anti-fog agents |
| Material protectants                 | OECD (2019)                    | Antioxidants, light stabilizers, ultraviolet-absorbing agents, thermostabilizers   |
| Physical–chemical property improvers | OECD (2019)                    | Flame retardants, fillers / reinforcement materials                                |
| Functionalization agents             | OECD (2019)                    | Coloring agents  |

OECD (2019). Complementing document to the emission scenario document on plastic additives: Plastic additives during the use of end products [OECD Series on Emission Scenario Documents No. 38].

Additives in LCI data



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## Plastic Functional Units

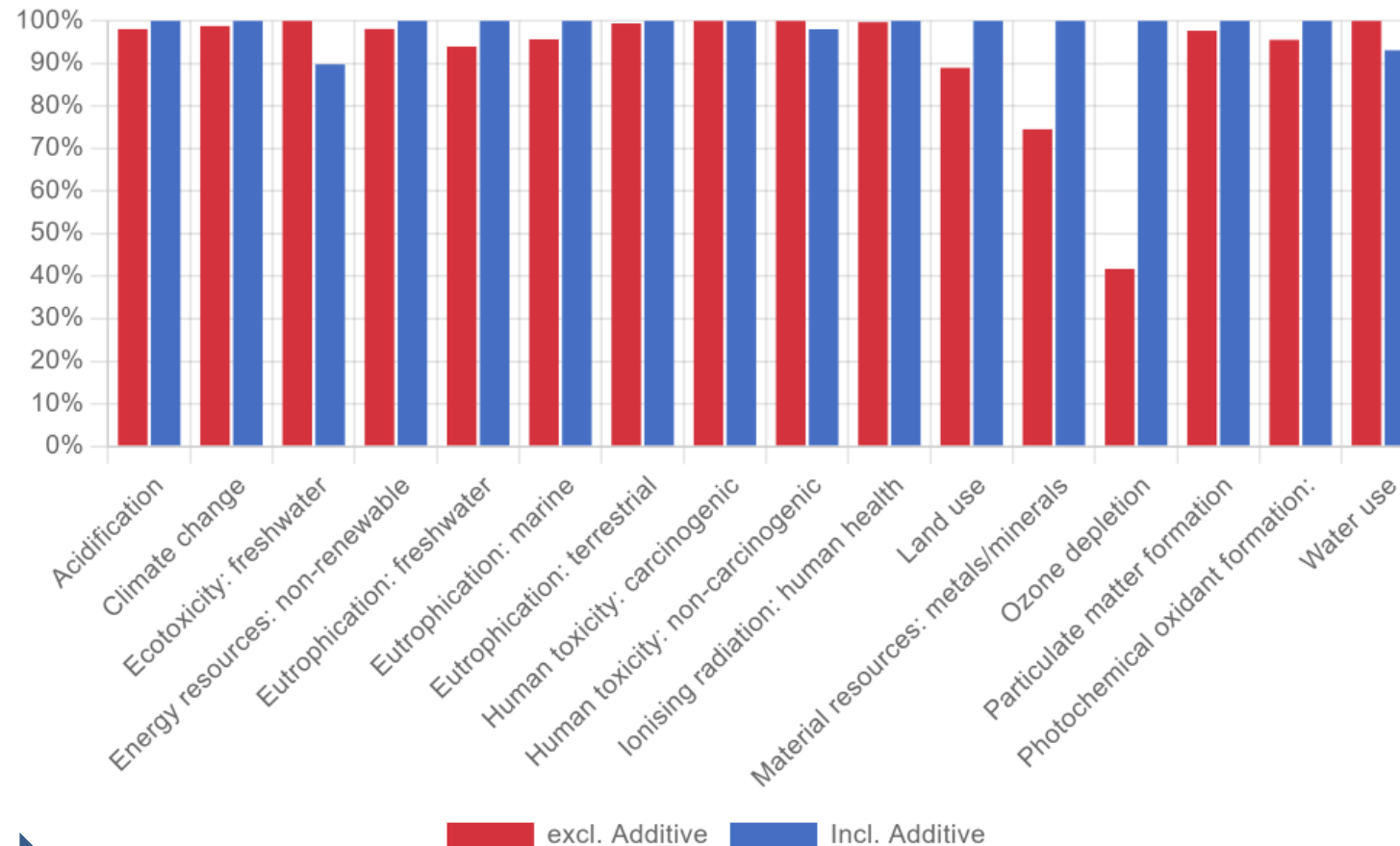
| Author, Year                   | Product  | functional unit   | Scope           | Reference   | Additive, Scope                             |
|--------------------------------|--|---|-----------------|---|---|
| JRC, plastic case study (2022) | Agricultural mulching films (LDPE, starch, PLA)                            | To provide mulching and associated agronomic functions to 1 hectare of agricultural land cultivated in the EU for one growing season  | Cradle-to-grave | Amount of mulching film required to fulfil the functional unit                  | Excluded production, influence EoL (direct) |
| JRC, plastic case study (2022) | Beverage bottles (HDPE, PET, PEF)  | To contain and deliver 1000 L of beverage to the final consumer in Europe, with product-specific bottle systems sized to provide that service   | Cradle-to-grave | Amount of bottles and packaging components needed to fulfil the functional unit | No  |
| JRC, SSbD case study (2023)    | PVC gasket with different additives  | To provide an airtight seal between one glass jar and its metal cap, able to last for the whole shelf-life of the food content of the jar, and which is suitable for the contact with oily food | Cradle-to-grave | 1 kg of PVC   | Yes (stoichiometric), Production            |
| PRIMUS D6.3 (2025)             | Interior (rABS, rPC), Cooling (rEPDM/rPP), Fridge (rHIPS), Sealing (rEPDM) | a plastic part at factory gate, performing the usual functionality of the same plastic part with no recycled content  | Cradle-to-gate  | Mass of plastic part  | Yes, stoichiometric                         |



**What are the impacts of additives? It depends!**

## JRC, plastic case study (2022) on mulching films

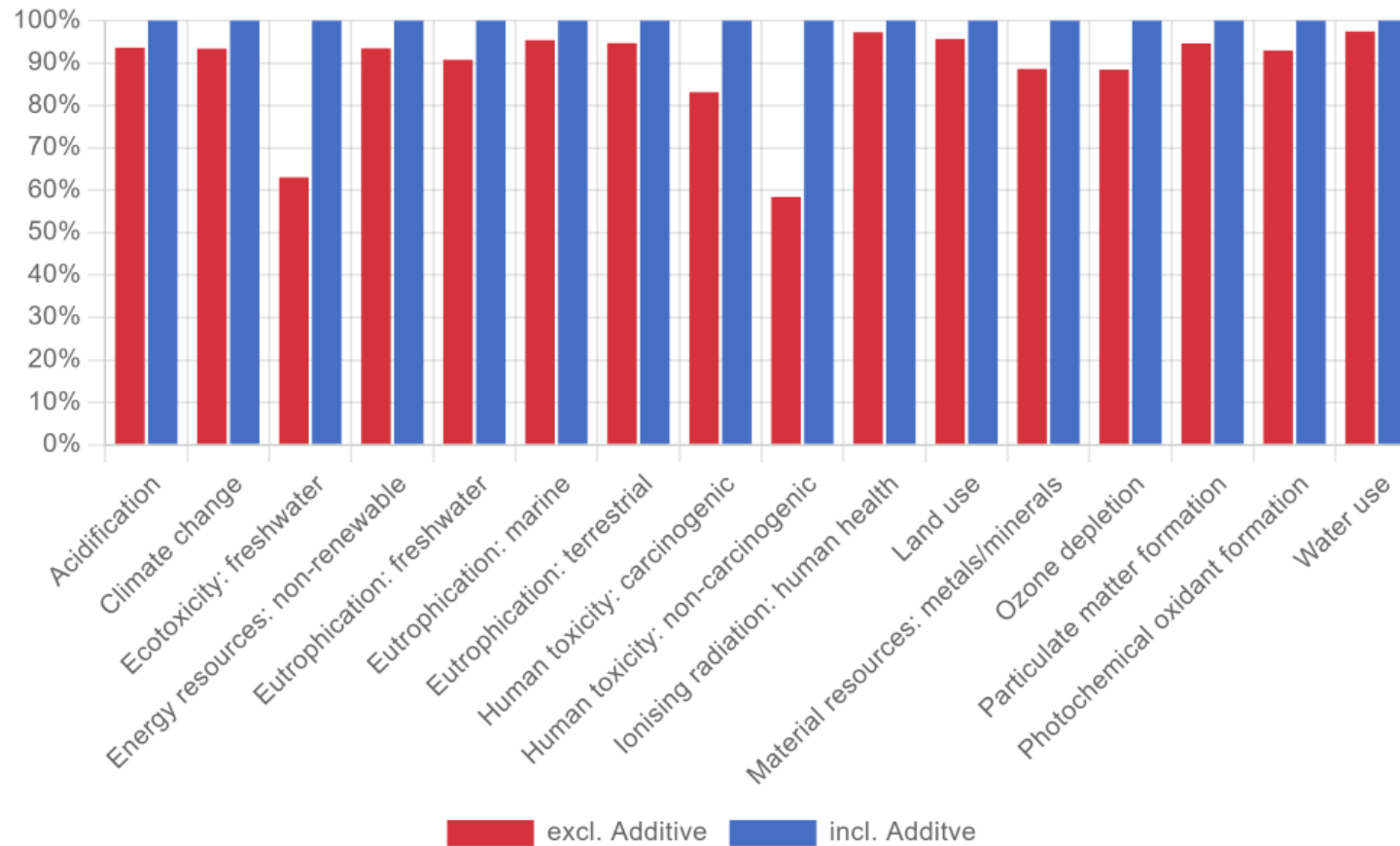
This sensitivity analysis evaluates the effects of excluding additives (mainly plasticisers) from the composition [...]. This choice was made considering the uncertainties and approximations performed in the modelling of additives [...]. For the purpose of simplicity, the exclusion was limited to the **Polymer Production stage** [...] while for **End of Life modelling the composition was not changed**.



“Additives (25w%) holds rather small overall contribution”

## PRIMUS, case study on rHIPS for fridge

A hidden environmental-burden hotspot of the system is the production of the antioxidant. Only 2% is used to make the plastic part, however the model suggests that it can have very high contributions, i.e. around 40% of contribution to Ecotoxicity (freshwater) and Human Toxicity.



“Additive (2w%) holds significant contribution”

# How to fill the data gap for the organic antioxidant?

<ecoinvent v3.11

> chemical, organic

| Flow               | Category           | Amount  | Unit |
|--------------------|--------------------|---------|------|
| urea               | C:Manufacturing... | 0.05015 | kg   |
| acetic acid, wi... | C:Manufacturing... | 0.05000 | kg   |
| methyl t-butyl...  | C:Manufacturing... | 0.05000 | kg   |
| styrene            | C:Manufacturing... | 0.05000 | kg   |
| vinyl acetate      | C:Manufacturing... | 0.05000 | kg   |
| ethylene glycol    | C:Manufacturing... | 0.04715 | kg   |
| ethylene           | C:Manufacturing... | 0.04569 | kg   |
| propylene          | C:Manufacturing... | 0.04561 | kg   |
| ethylene dichl...  | C:Manufacturing... | 0.04438 | kg   |
| xylene, mixed      | C:Manufacturing... | 0.04421 | kg   |

>ecoinvent v3.11

- chemical, organic, alcohols
- chemical, organic, aromatics
- chemical, organic, carboxylic acids
- chemical, organic, esters
- chemical, organic, unspecified



Selecting the right proxy is an art itself!

With ecoinvent v3.12 molality of >9000 chemicals:

- Production details from Ullmann or public sources
- Create a process with the flow and „mol“
- Add inputs in stoichiometric fashion (CAS search)

LCA

Irganox 1010 Production - RER

Inputs/Outputs - Irganox 1010 Production - RER

Inputs

| Flow             | Category          | Amount  | Unit | Costs/... | Uncert... | Avoid... | Provider |
|------------------|-------------------|---------|------|-----------|-----------|----------|----------|
| 2,6-di-tert-b... | C:Manufacturin... | 4.00000 | mol  |           | none      |          | ma...    |
| methyl meth...   | C:Manufacturin... | 4.00000 | mol  |           | none      |          | ma...    |
| pentaerythritol  | C:Manufacturin... | 1.00000 | mol  |           | none      |          | ma...    |

Outputs

| Flow        | Category | Amount   | Unit | Costs/... | Uncert... | Avoid... | Provider |
|-------------|----------|----------|------|-----------|-----------|----------|----------|
| Irganox1010 |          | 1.000... | mol  |           | none      |          |          |

General information | Inputs/Outputs | Documentation | Parameters | Allocation | Social aspects | Direct in

- This can be adapted to yield and energy demand but also direct emissions (mol)

## Plastic Functional Units

| Author, Year                   | Product  | functional unit   | Scope           | Reference   | Additive, Scope                             |
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**Additives often alter the technical performance!**

## Plastic Functional Units

| Author, Year                   | Product  | functional unit   | Scope           | Reference   | Additive, Scope                             | Comparative? Performance? |
|--------------------------------|--|---|-----------------|---|---|---------------------------|
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| JRC, SSbD case study (2023)    | PVC gasket with different additives  | To provide an airtight seal between one glass jar and its metal cap, able to last for the whole shelf-life of the food content of the jar, and which is suitable for the contact with oily food | Cradle-to-grave | 1 kg of PVC   | Yes (stoichiometric), Production            | Yes, same performance     |
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Additives are incorporated into plastic materials to modify and enhance specific properties such as durability, processability, stability, and functionality during use. → How to quantify?

## JRC, plastic case study (2022), bottle case study

- “According to the suggestions of a relevant stakeholder, the improved barrier and mechanical properties of PEF should approximately allow for an overall 20% reduction in material usage”

| Material | Bottle mass (g) | Reference flow (kg/FU) |
|----------|-----------------|------------------------|
| PET      | 24              | 48                     |
| HDPE     | 26.5            | 53                     |
| PEF      | 24 x 80%        | 38.4                   |

The amount of polymer required to fulfil the function of the bottle was **calculated based on the gas permeability values** [...]. These calculations resulted in bottle masses of 13 g for PEF and 24 g for the reference PET bottle. Bottle masses were confirmed as being appropriate under the assumptions used by industry experts - PEF – A Sustainable Packaging Material for Bottles – Nova Institute 2022

How is better performance even taken into account using LCA methods?



- Here, the FU was „ensuring a minimum of 12 weeks CO<sub>2</sub> shelf life”
- However, barrier properties of PEF, which are ~10x better for O<sub>2</sub> , ~15x better for CO<sub>2</sub>, and ~2.5x better for water than PET

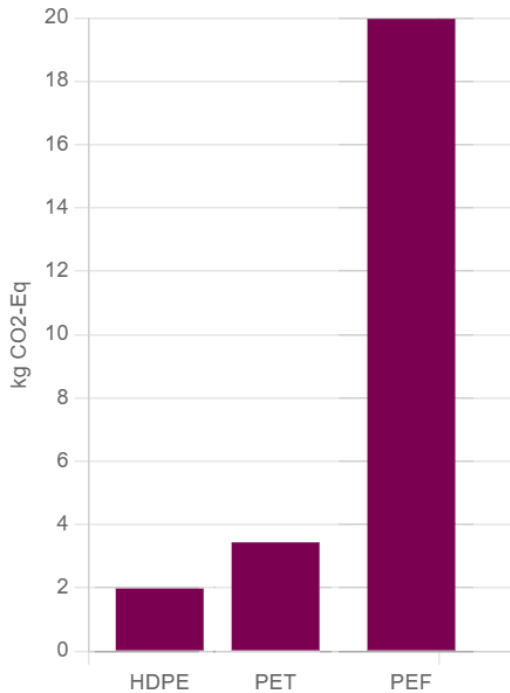
## Defining Functional Units in Comparative Scenarios

|  | Reference flow functional unit   | Property functional unit  | Performance functional unit   |
|--|--|---|---|
| Description                                | Represents a certain amount of material  | Represents the main relevant properties of the material for a certain application area                | Represents the performance of the material in a specific end product          |
| Typical goal                               | Generic comparison of environmental impacts of materials, e.g., for ecodesign purposes | Comparison of environmental impacts of materials based on relevant properties for an application area | Comparison of the environmental impacts of materials in specific end products |
| Typical example                            | 1 kg material  | 1 kg material with certain properties   | 1 end product with a certain performance                                      |
| Procedure for functional unit construction | Equal to the LCA reference flow  | Relevant properties are combined in some way  | Performance data is estimated from, e.g., experiments                         |

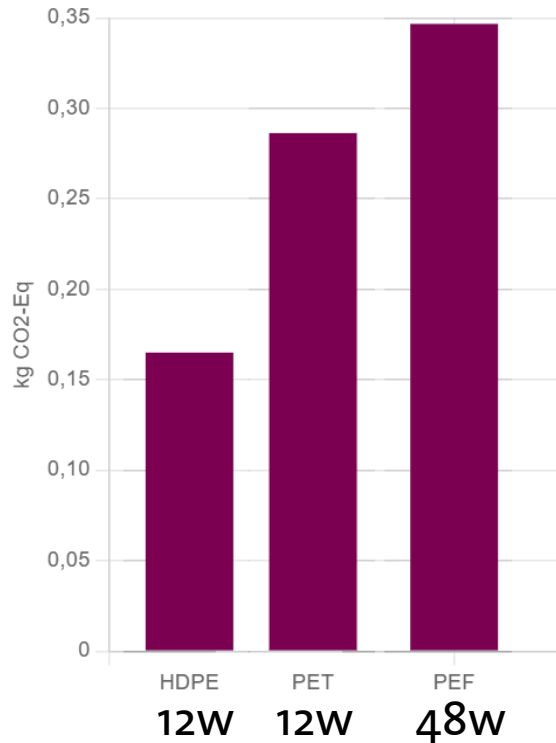
# Defining Functional Units in Comparative Scenarios

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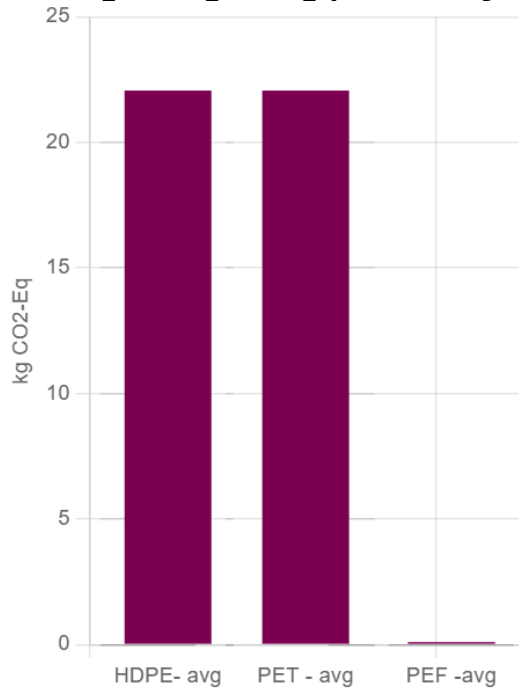
per kg of material (cradle-to-gate)



per property-scaled kg (weeks of storage adj.)

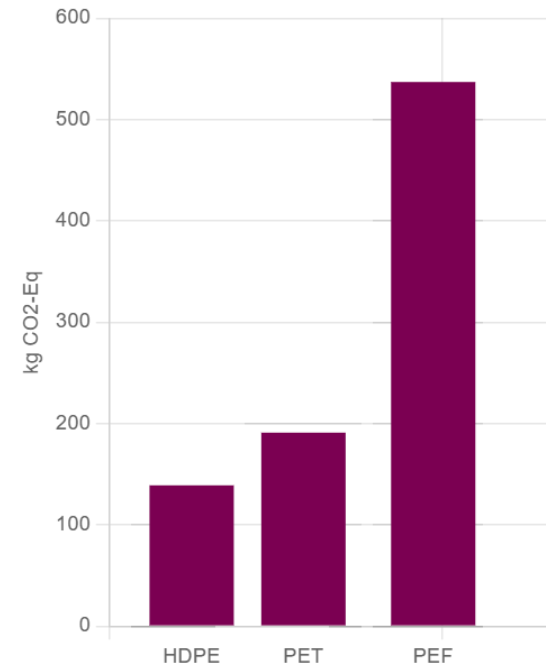


per property-scaled kg (H<sub>2</sub>O/O<sub>2</sub>/CO<sub>2</sub> perf. adj.)



Very subjective!

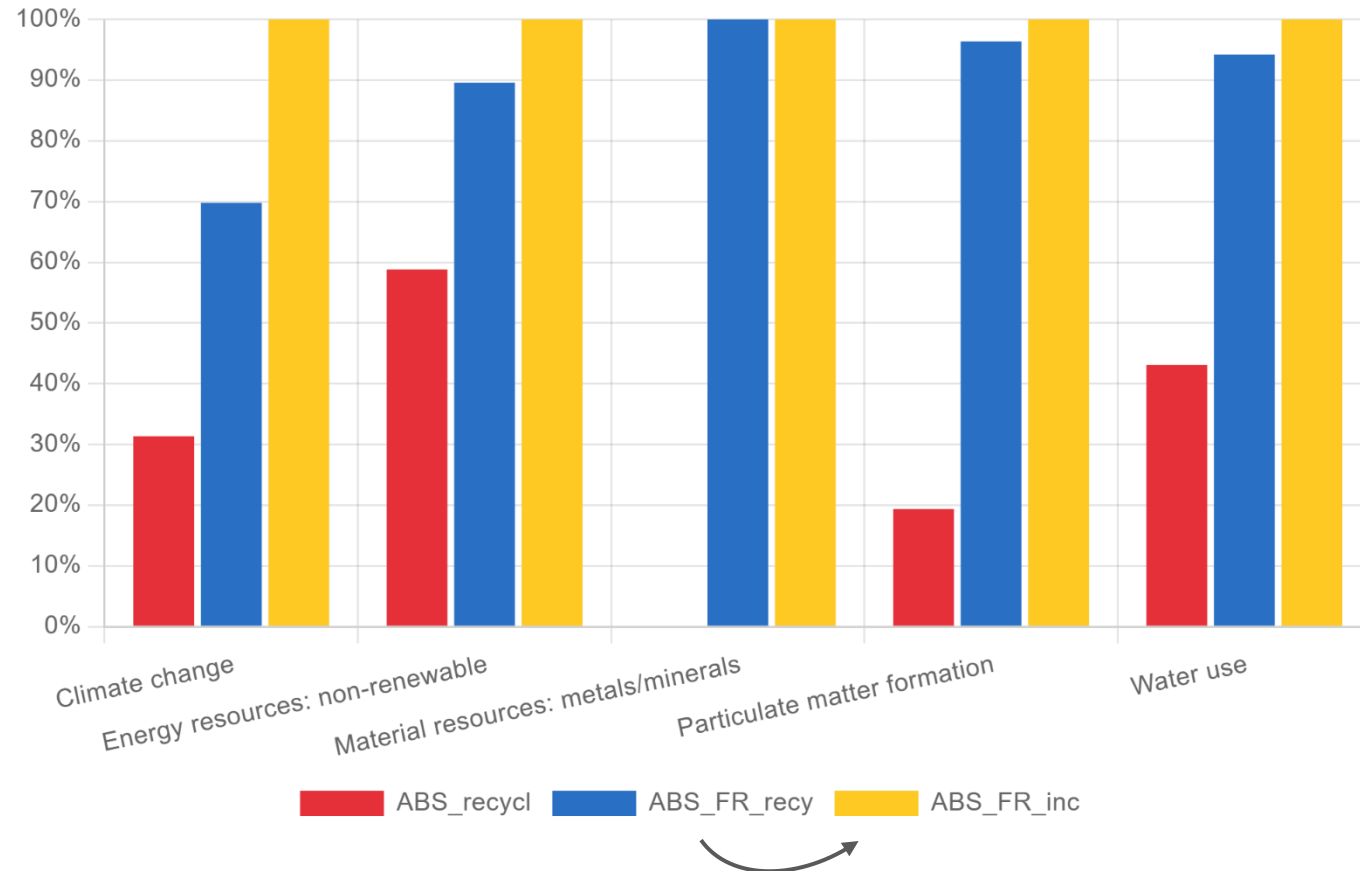
per 1000 litres of beverage delivered



Using property-based functional unit can be misleading

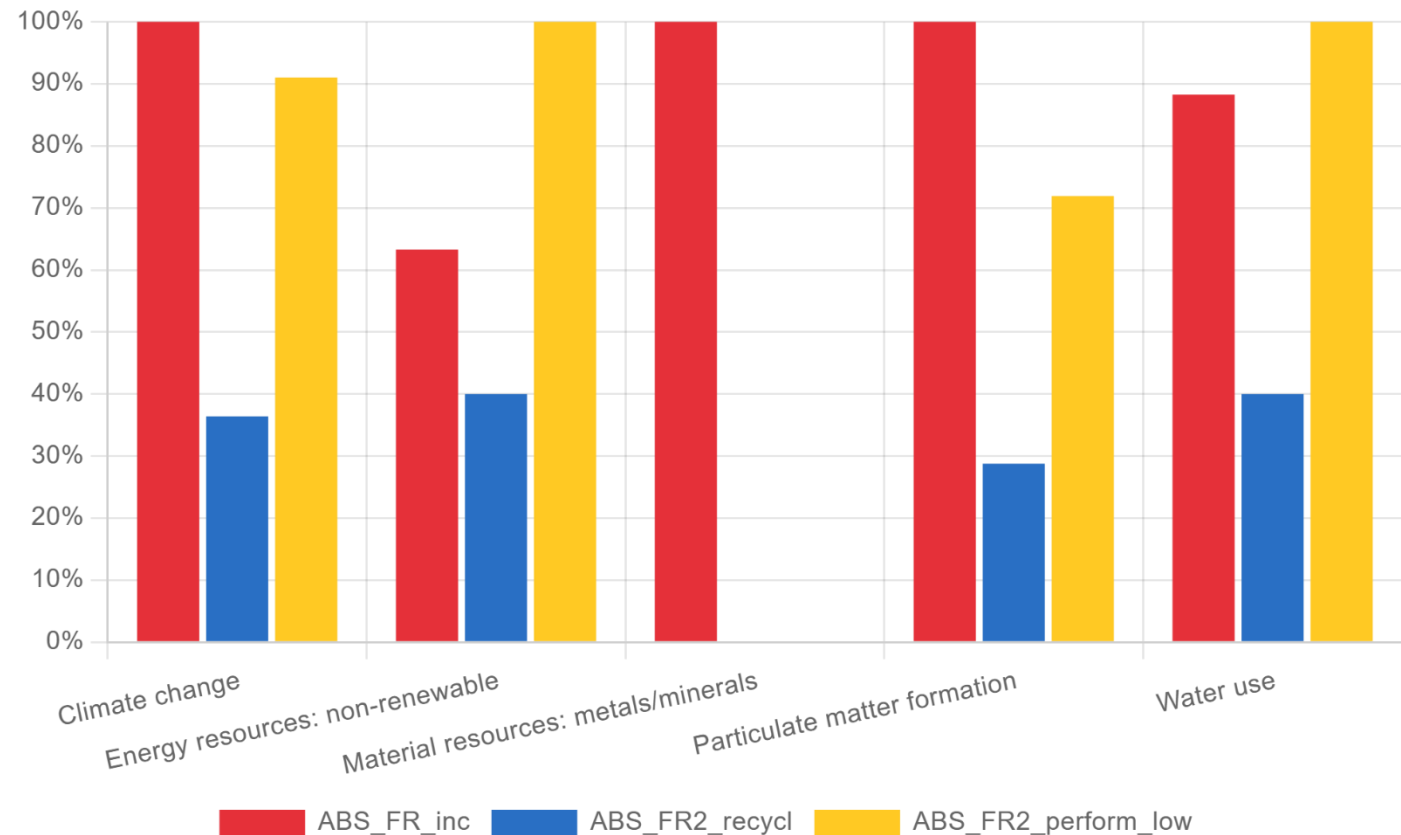
# Systems level thinking

- However, we have also system related dimensions: If we add an additive to a material, its EoL pathway might differ (FR is DecaBDE and Sb<sub>2</sub>O<sub>3</sub>)!



## Systems level thinking

- However, we have also system related dimensions: If we add an additive to a material, its EoL pathway might differ (FR is DecaBDE and Sb<sub>2</sub>O<sub>3</sub>; FR2: Al(OH)<sub>3</sub>; with 2.5 worse performance)



## Conclusion

- Please consider **implementation of additives** in your products life cycle
  - It can have strong implications to environmental impacts besides small mass
  - openLCA supports implementation of stoichiometric pathways
  - The whole product's life cycle can be effected by it (system thinking)
  - Also the performance **might be improved and can influence impacts:**  
Reference flow functional unit | Property functional unit | Performance functional unit
- **Do not limit the scope to the production of additives:**
  - Integrate it in the **Use phase** (see performance but also direct emissions)
  - Investigated if the **EoL** if changed with present additives (recyclability)



**Visit Max presentation on how additives can change EoL pathway!**

# GreenDelta

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## Thank you!

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Picture: Julia Cilleruego Palomero