



Sustainability & Materials

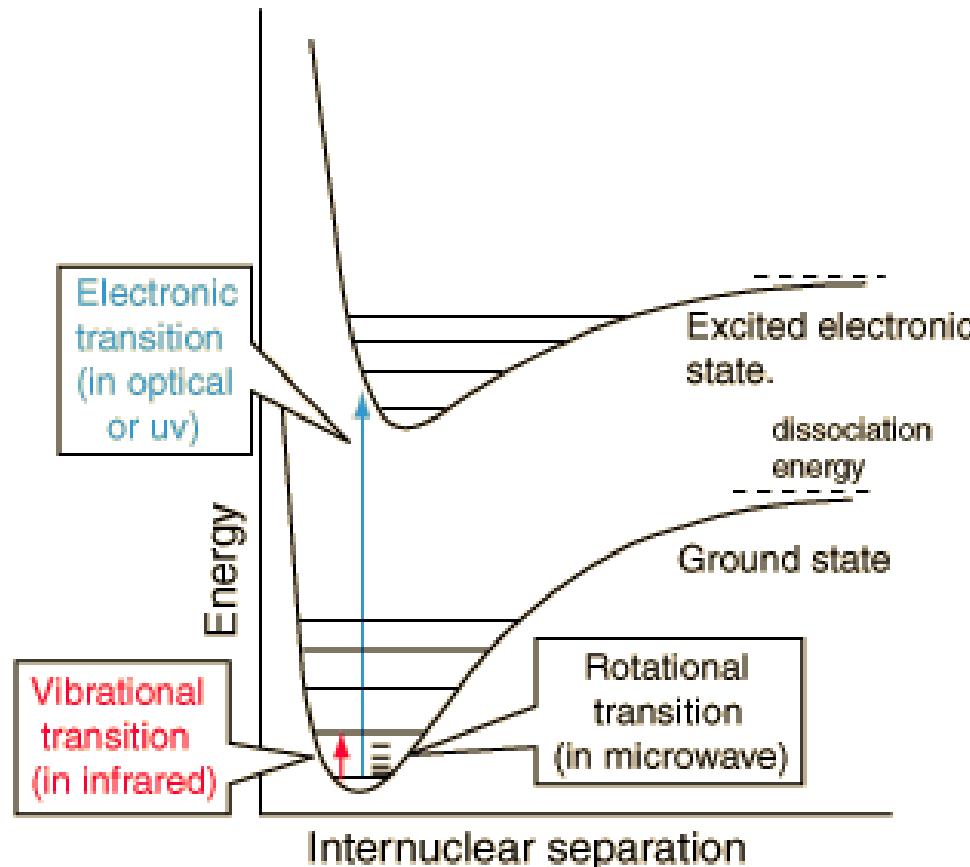
Prof. Tiffany Abitbol
2025

Recap

- **New:** Assignment deadline extended until Mar 24 at 17
- **Update:** Glencore guest lecture on May 14 (please prioritize)
- Last week we discussed circularity and how recycling fits in
- If we ranked according to circularity
reuse/share/refurbish>recycle>bioenergy> landfill
- Closed and open-loop recycling – which is more circular? Can you explain what circularity is? Is it possible to be fully circular in a growing economy?
- What's in store for today: some metrics that can be used to assess sustainability

But before that....

- We looked at a lot of spectra of different gas molecules, some of which (GHG) absorb IR light
- What is a spectra of a molecule? Where does it come from? Why is it sometime called a “fingerprint” of a molecule?



- Potential energy curves of a molecule in ground and excited state
- Internuclear distance is the distance between the nuclei of 2 atoms in a molecule
- Electronic > Vibrational > Rotational (energy scale)
- Electronic – excited states (UV-Visible)
- Vibrational – molecular bond vibrations (IR)
- Rotational – rotational modes (microwave)

IR absorbance (43 s)

<https://youtu.be/AF1JPg20amY>

MSJChem
Tutorials for IB Chemistry

IR absorbance

Asymmetrical stretching and bending produce a change in the dipole moment of the CO_2 molecule.

The diagram illustrates the CO_2 molecule with a central carbon atom (C) bonded to two oxygen atoms (O). In the first part, labeled 'asymmetrical stretching', arrows above the molecule indicate the movement of the oxygen atoms towards the center, creating a more polar structure. In the second part, labeled 'bending', arrows show the oxygen atoms moving upwards and downwards from the horizontal axis, further increasing the dipole moment.

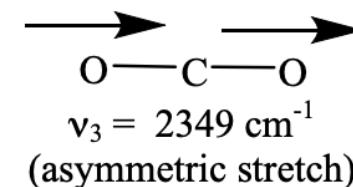
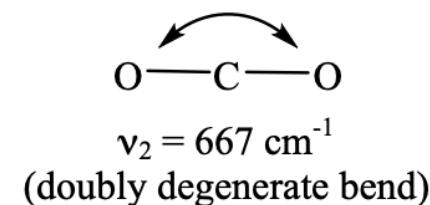
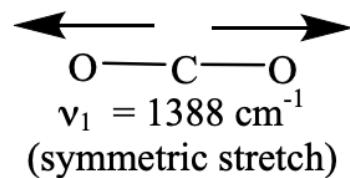
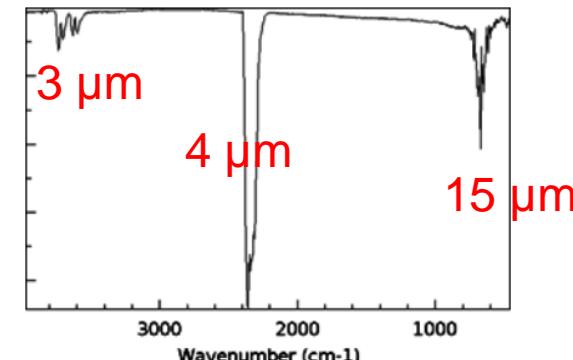
- In order to absorb IR radiation, there must be a change in the dipole moment of the molecule as the bonds undergo asymmetrical stretching or bending.

Assigning the IR Spectra of Polyatomic Molecules

Model 1: CO₂

The IR spectrum of CO₂ from 600 – 4000 cm^{-1} is shown opposite and contains three bands.

The bands at 667 cm^{-1} and 2349 cm^{-1} are due to the bend, ν_2 , and asymmetric, ν_3 , vibrations respectively.



Different vibrational modes:

No IR absorption for ν_1 = symmetric, no dipole

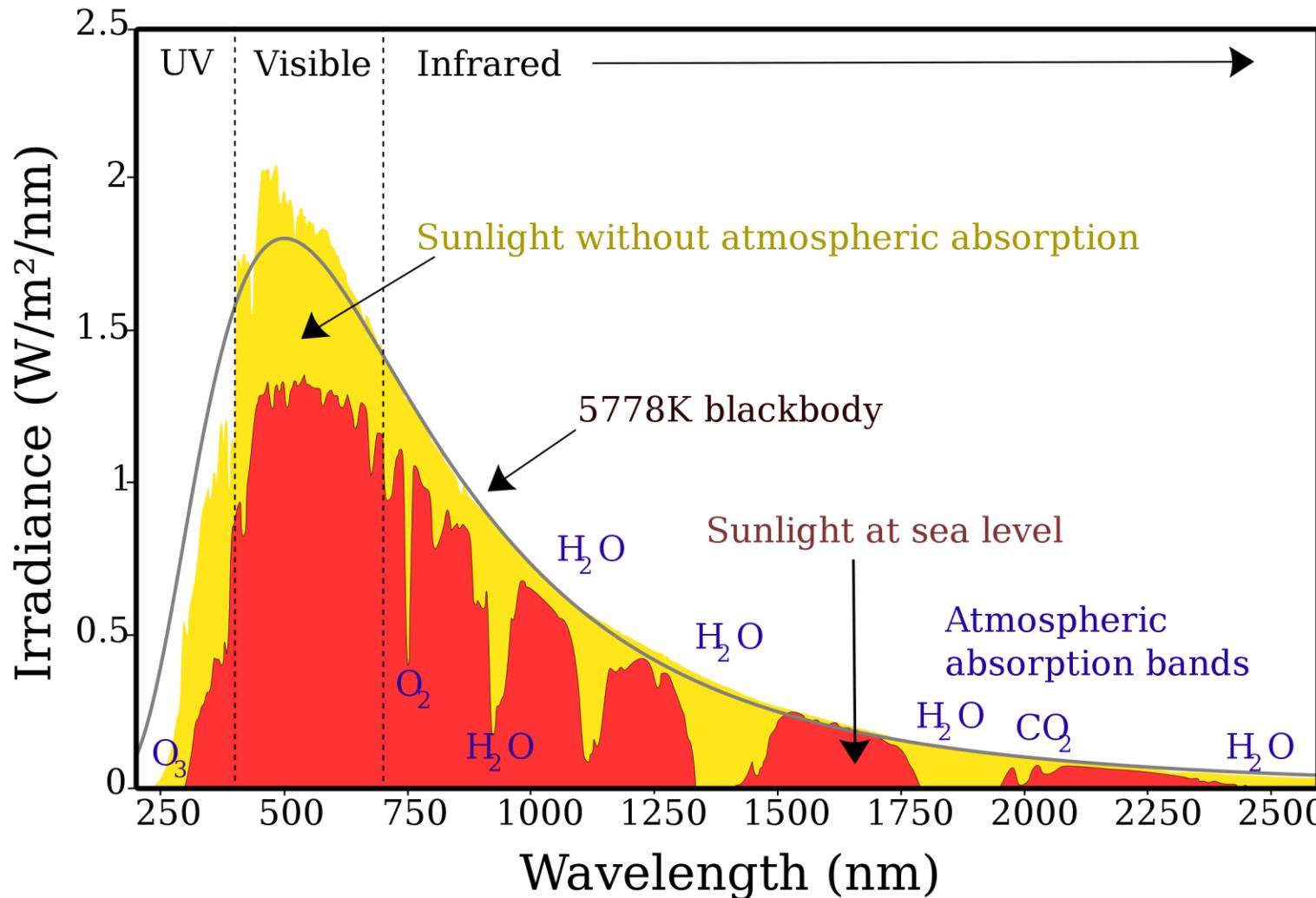
$\nu_2 = 667 \text{ cm}^{-1}$, asymmetric bends

$\nu_3 = 2349 \text{ cm}^{-1}$, asymmetric stretches (425 μm)

Why 3 clusters of peaks?

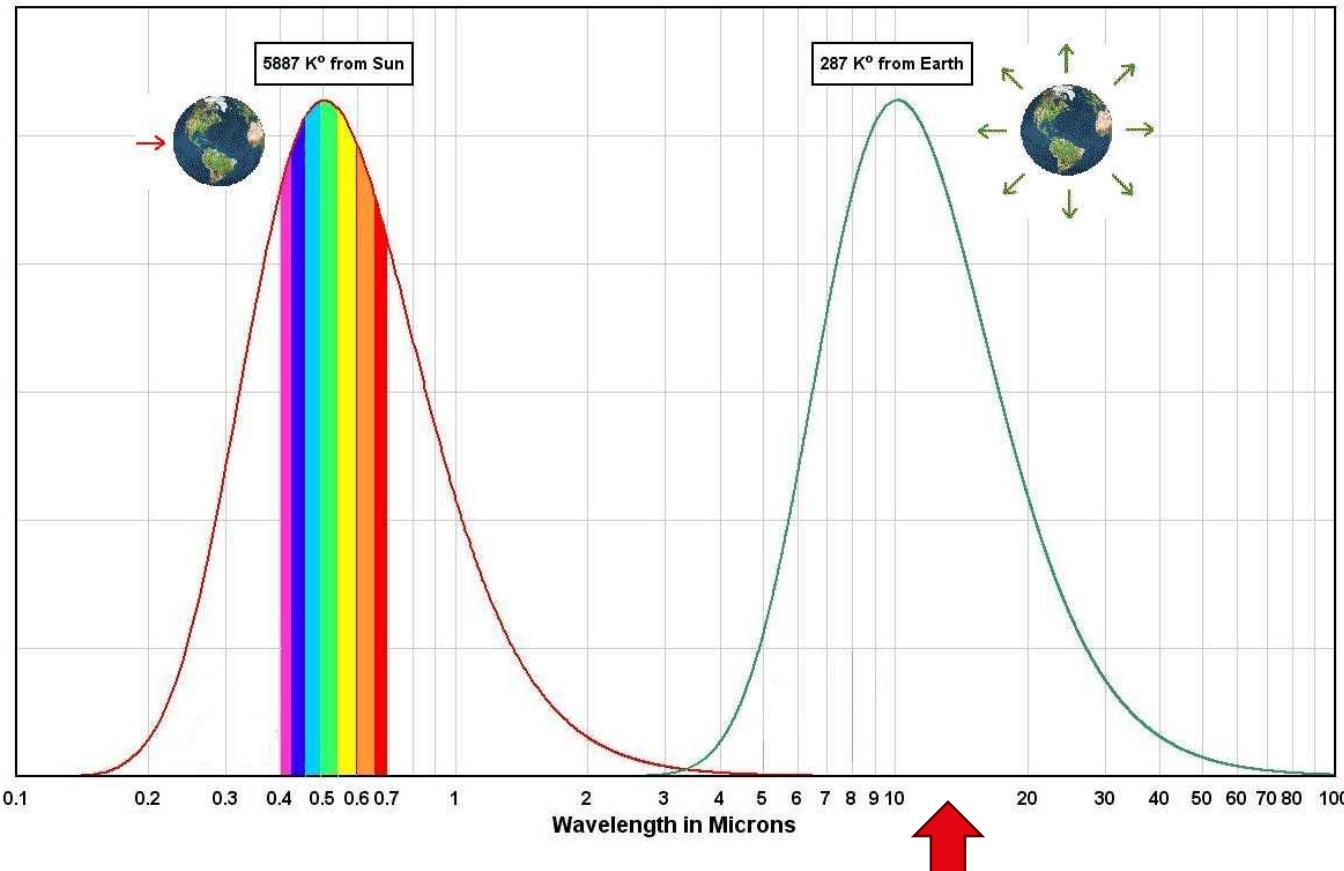
Light emitted from the sun toward us

Spectrum of Solar Radiation (Earth)



- Recall: Sunlight is mostly visible energy
- Visible spectrum: 400-800 nm
- CO₂ and other GHGs are transparent to visible light
- So, it can pass through our atmosphere to the earth's surface, where it can enable neat stuff like photosynthesis

Now add in the Earth's emission back out to space



- Both approximated as blackbodies
- Intensities are normalized in this graph
- As the IR emitted from the Earth hits our atmosphere it is blocked by GHGs that absorb IR radiation
- These GHGs emit the IR in all directions, some of it coming back toward the Earth, heating the planet (IR is heat)
- This is the GH effect (good thing) and why we have global warming (bad thing)

Materials life cycle

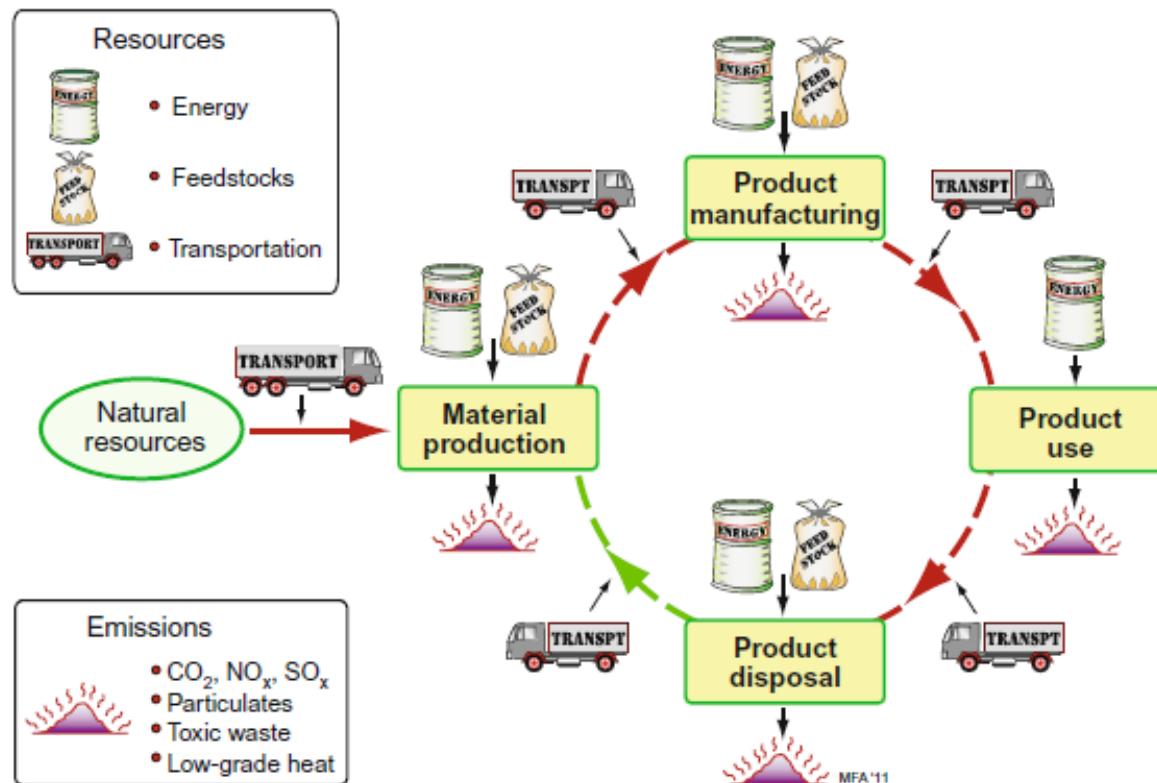


FIGURE 3.2 The material life cycle. Ore and feedstock are mined and processed to yield a material. This is manufactured into a product that is used and, at the end of its life, discarded, recycled, or, less commonly, refurbished and reused. Energy and materials are consumed in each phase, generating waste heat and solid, liquid, and gaseous emissions.

- Unwanted by-products often exceed the capacity of the earth to absorb them (recall: Overshoot Day)
- Emissions/environmental costs at every stage
- *Internalized environmental cost* = local damage, responsibility of emitter to fix
- *Externalized environmental cost* = global damage, burdens all of society

SDGs implicated in the materials life cycle



★ less obvious link

★★ clear, direct link

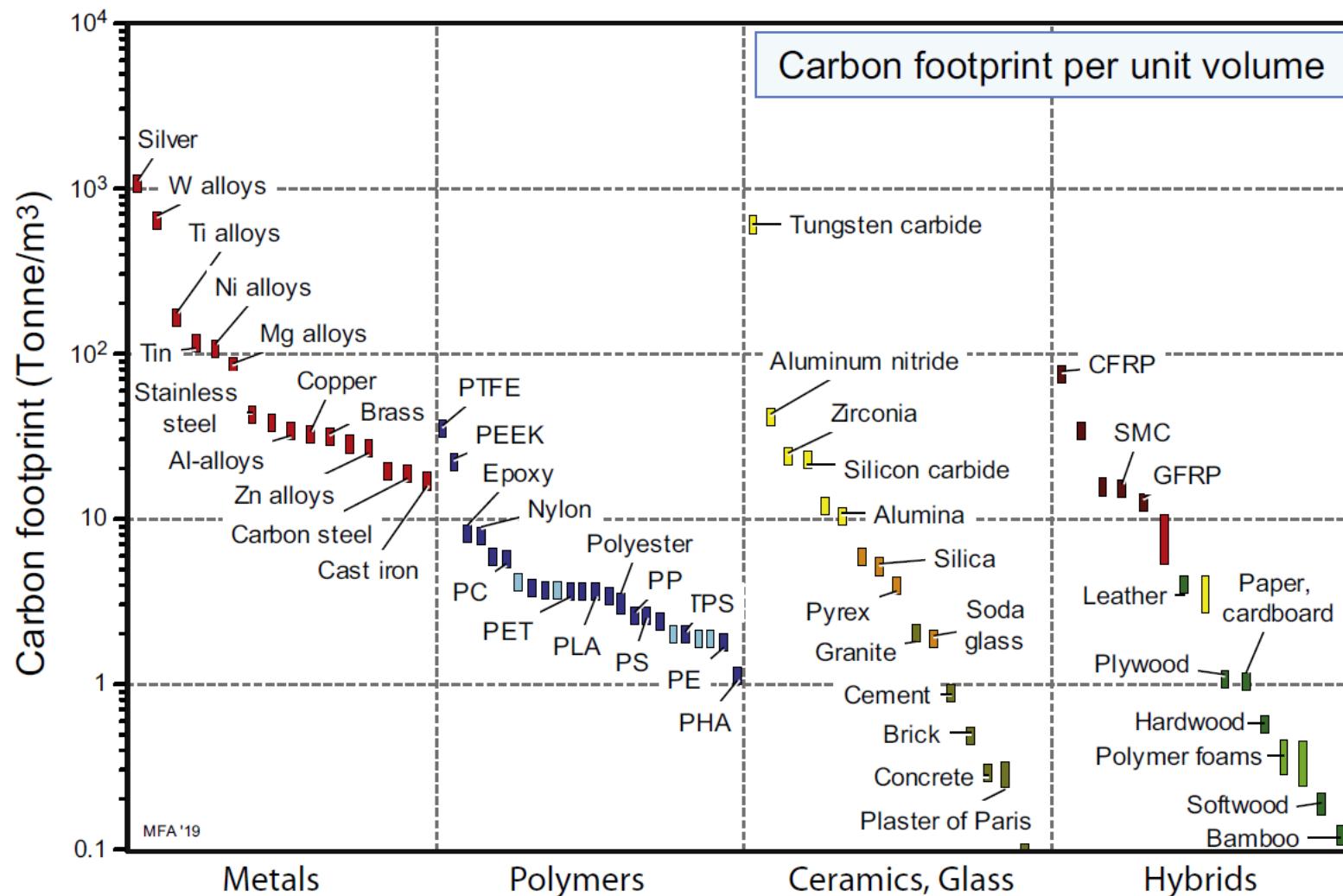
Carbon footprint of a material

- CO₂ footprint – mass of CO₂ released into the atmosphere per 1 kg of any given material, can be expressed in CO₂ equivalents
- CO₂ footprint (as defined above) is not a fair parameter to assess a material's environmental impact
- To evaluate the real emission burden of a specific material, global carbon release from material production must be considered
- E.g., concrete has a relatively low carbon footprint, but being one of the most used construction materials, its global carbon impact is extremely high
- ***Broad category that considers the negative impacts of products, persons, companies, nations... (the unit needs to make sense...we will discuss “scope” in the coming slides)***



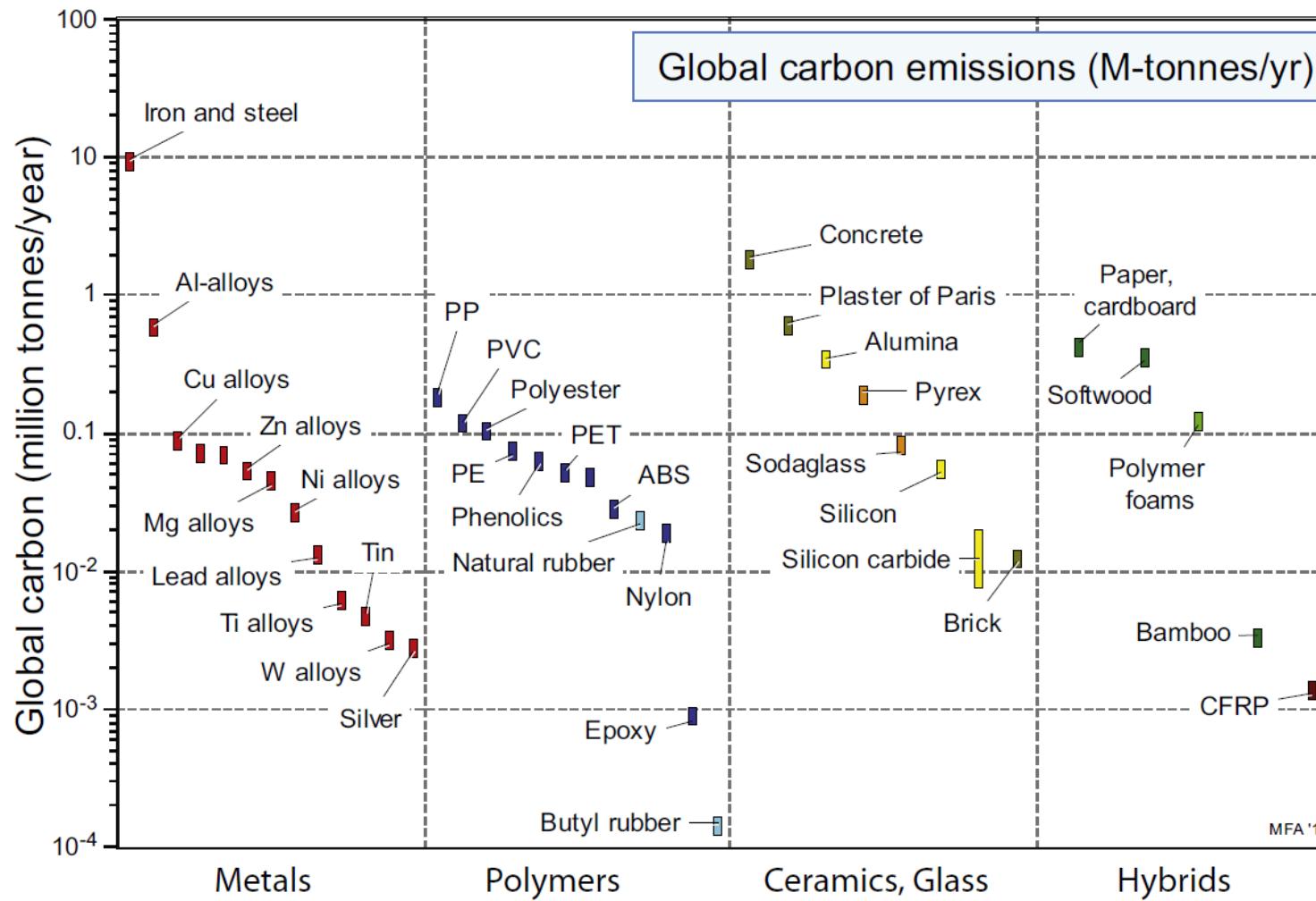
The Carbon Footprint

Carbon footprint for materials



- Per unit volume or mass, concrete has a low carbon footprint

Carbon footprint for materials



- But when we look at the global carbon emitted by concrete, we see that it is very high because it is used so much

Concept of footprint/handprint

- “Footprints” are framed to tell us about negative impacts, e.g., the GHG emissions associated with our flights
 - *A carbon footprint of 1T CO₂ is better than a footprint of 2T CO₂*
 - *Want our footprint as close to zero as possible*
- “Handprints” are a positive reframing – aim to grow our handprint and shrink our footprint
 - *A carbon handprint of 2T CO₂ is better than handprint of 1T CO₂*
 - *Want to increase our handprint, which quantifies our positive impacts (e.g., beneficial impacts of a product when used by a customer)*

- Apparently motivating
- A way to spread wins

Concept of footprint/handprint



A handprint refers to the beneficial environmental impacts that organizations can achieve and communicate by providing products that reduce the footprints of customers.

A carbon handprint is the reduction of the carbon footprint of a customer or customers.



- Can you just subtract your handprint from your footprint?

- “Positive impact that helps others reduce their footprint”
- Accomplished “by providing new technologies, energy solutions”, etc.,
- Numerical value that represent how many kg of CO₂ you help someone else to cut
- Having a handprint does not reduce your footprint: why?
- A footprint is a measure of actual reductions in emissions, whereas a handprint measures emissions that were avoided
- No standards for measuring handprints
- Why do companies do it? To communicate their progress...

- Is this a tool for greenwashing?
- I haven't found tons of companies reporting a handprint...



About offsetting How to offset UN certification Projects Contributors FAQ

EN ▾

Search for Project ID, industry, co-benefits

Search

UN carbon footprint calculator

Household

Transport

Lifestyle

ABOUT YOUR HOUSEHOLD

Number of people in the household

4

Country of residence

Select country

Size of housing (m²)

100

Type of housing

Detached

ENERGY CONSUMPTION

Electricity consumption

KWh/month



I don't know the KWh/month

...from a clean energy source

0

%

Heating energy source

Coal

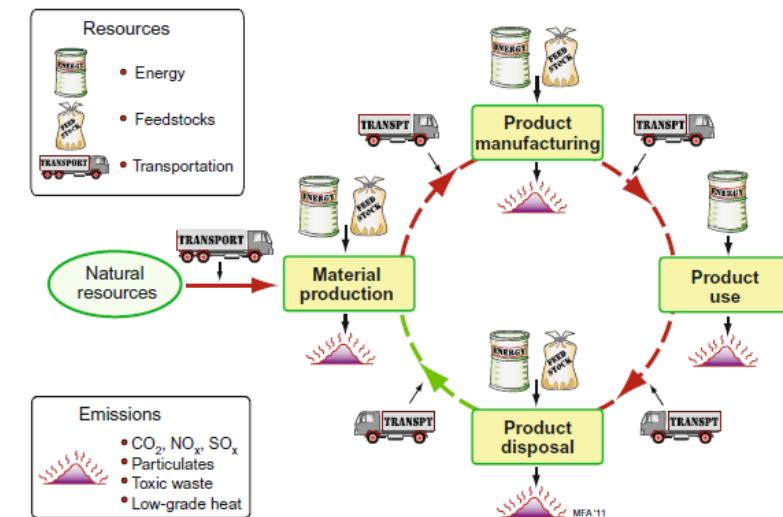
Nice tool from UN to calculate:

1. Personal carbon footprint
2. Organization carbon footprint

[footprintcalc](#)

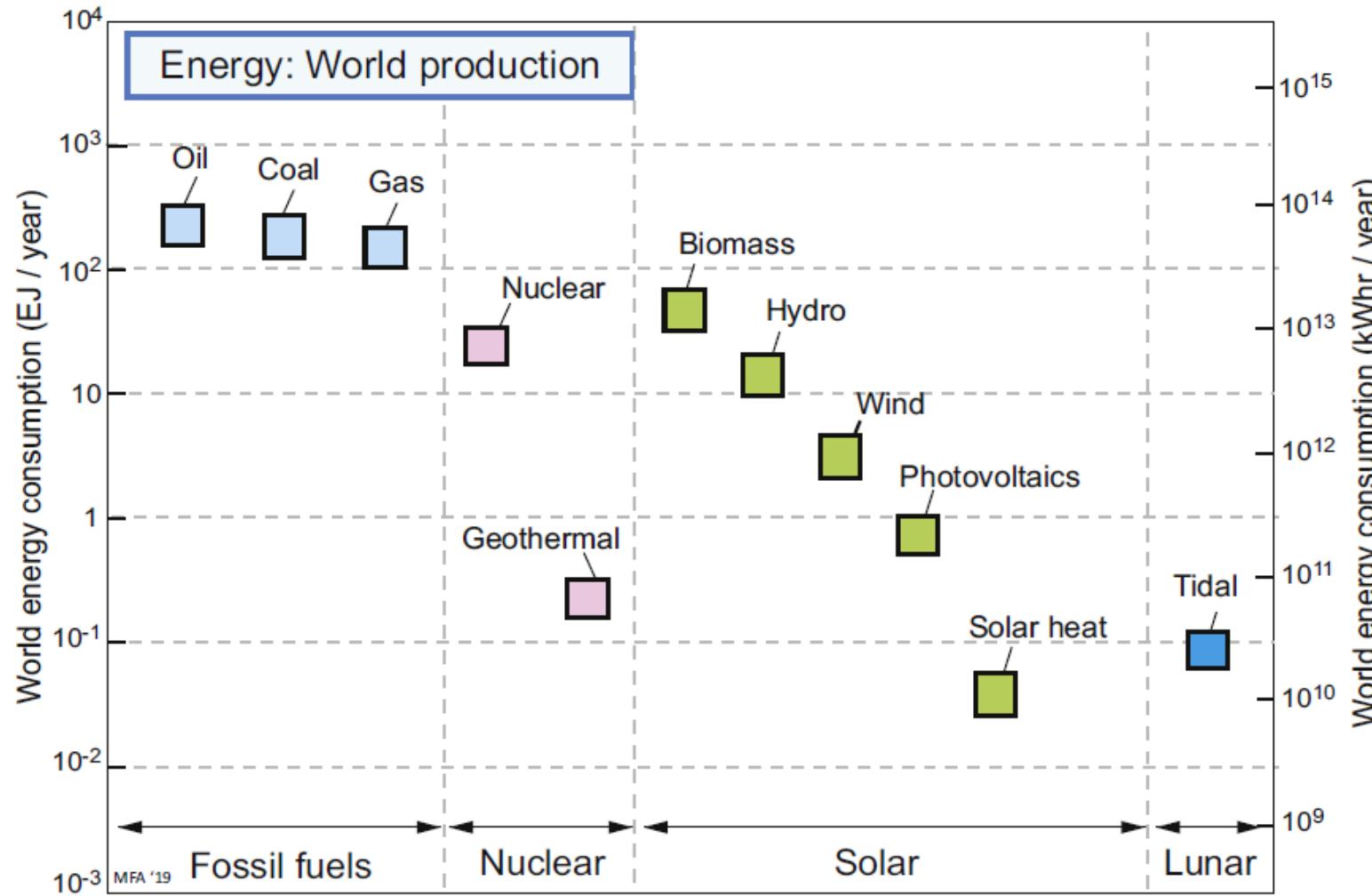
What else goes into materials?

- Two weeks ago: we saw that we need: raw materials, energy, water & that all of this can contribute to GHG emissions
- For the life cycle of a material, we need to consider all inputs to making a material (as well as emissions associated with material lifetime and end of life)
- Metrics like **embodied energy**, **water usage**, and **embodied carbon** can help define the production phase
- Embodied energy is the sum of all the energy required to produce any goods or services, considered as if that energy were incorporated or 'embodied' in the product itself (analogous metric for embodied carbon)



Steps of a material's life cycle, with emissions along the way

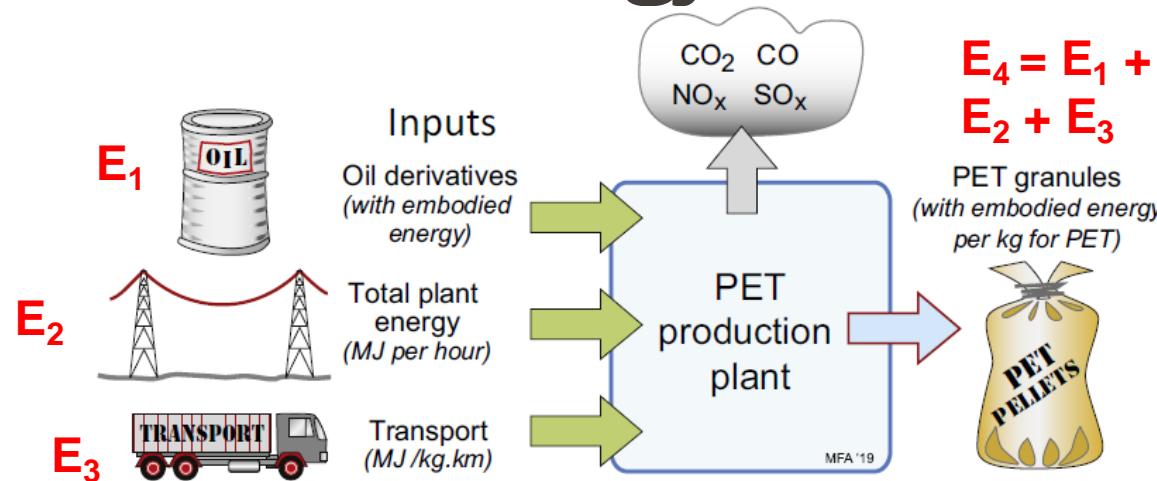
What else goes into materials? Energy



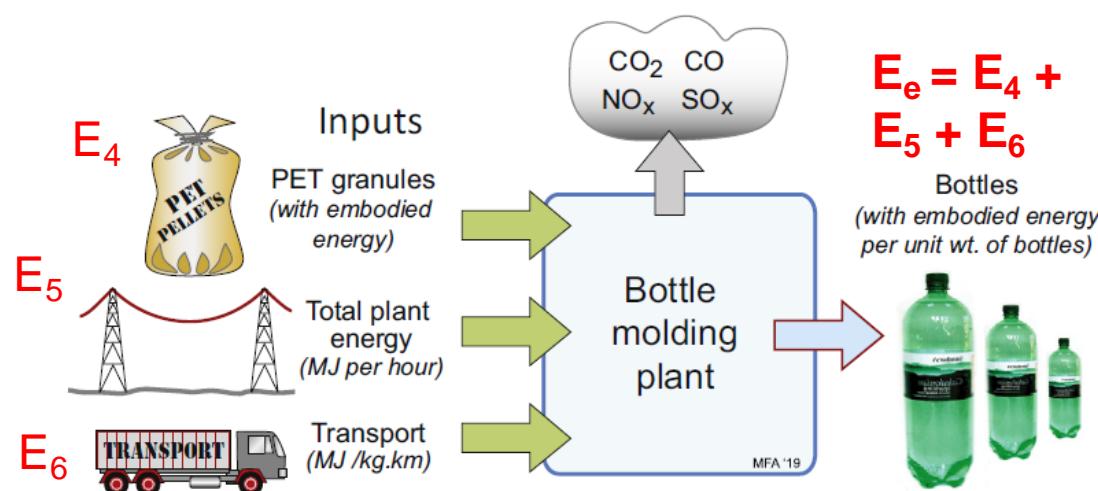
Recall:

- Many energy systems are inefficient (losses in conversion)
- Material production accounts for about 15% of global energy use and carbon emissions

Embodied energy

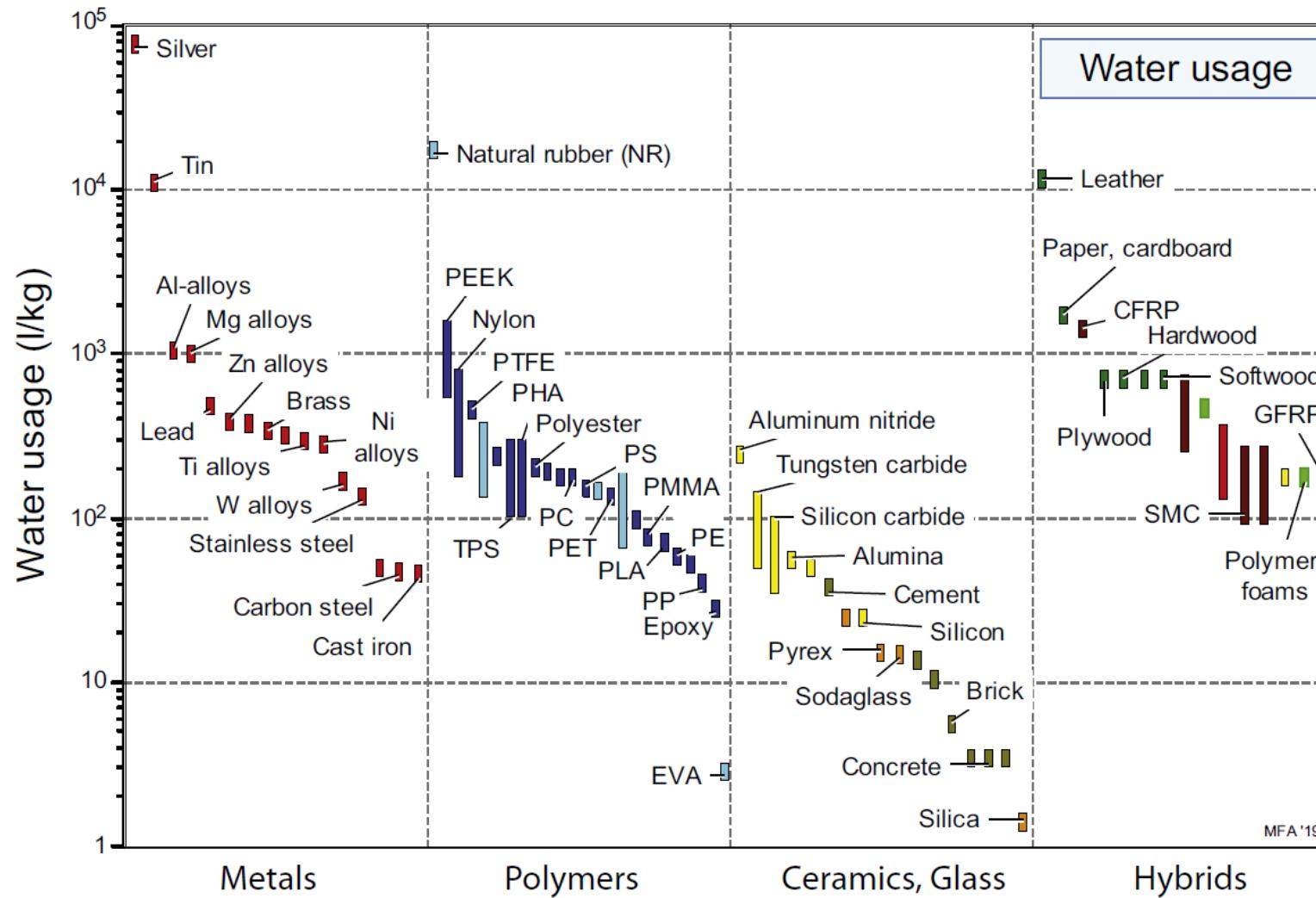


Embodied energy to produce PET pellets (E_4) is the determined from the sum of all inputs



Total embodied energy to produce PET bottles (E_e) is the determined from the sum of all inputs

What else goes into materials? Water

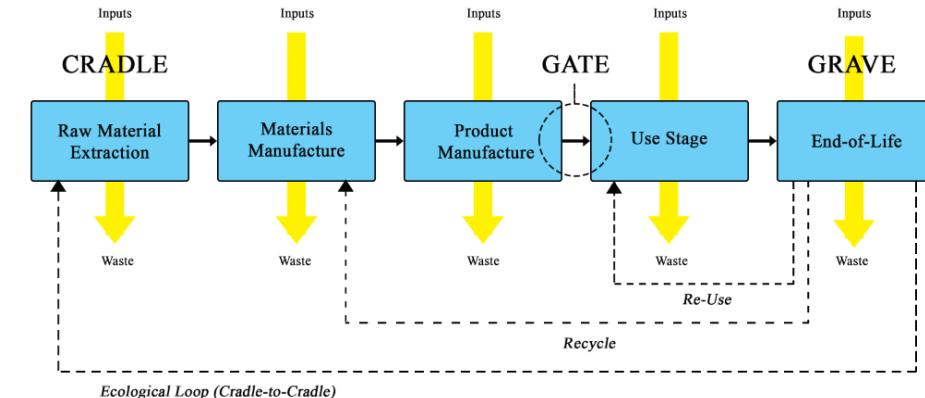


Recall:

- Even though water is renewable, high consumption can lead to scarcity

Lifecycle of a material

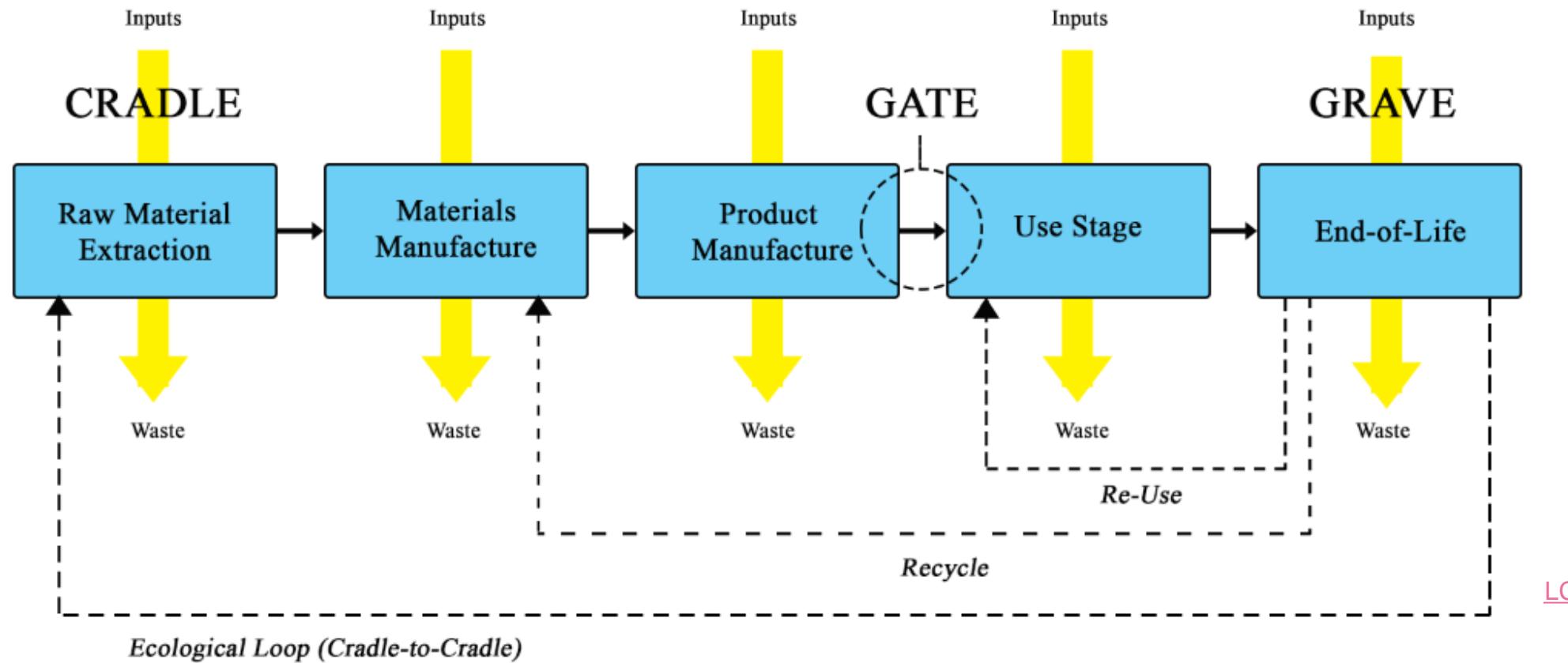
- Imagine materials and products as a "living" entity, moving through its lifespan from birth to death (and beyond!)
- Where does the "stuff of life" come from?
- What happens when at death, when utility is over?
- In most cases materials can't just be buried in the earth to regenerate...
- When you describe impact of a product/or person/or a service/ or an activity, where do you focus? The entire lifespan? Hotspots? What is the **scope** of our analysis?
- These decisions need to be made so we can quantify impact!



LCA

What are the scopes that we consider in a materials lifecycle?

- Cradle-to-gate (production)
- Cradle-to-grave (full lifecycle)
- Gate-to-grave (operational impacts)
- Gate-to-gate (manufacturing impacts)
- Cradle-to-cradle (we will see more of this later)

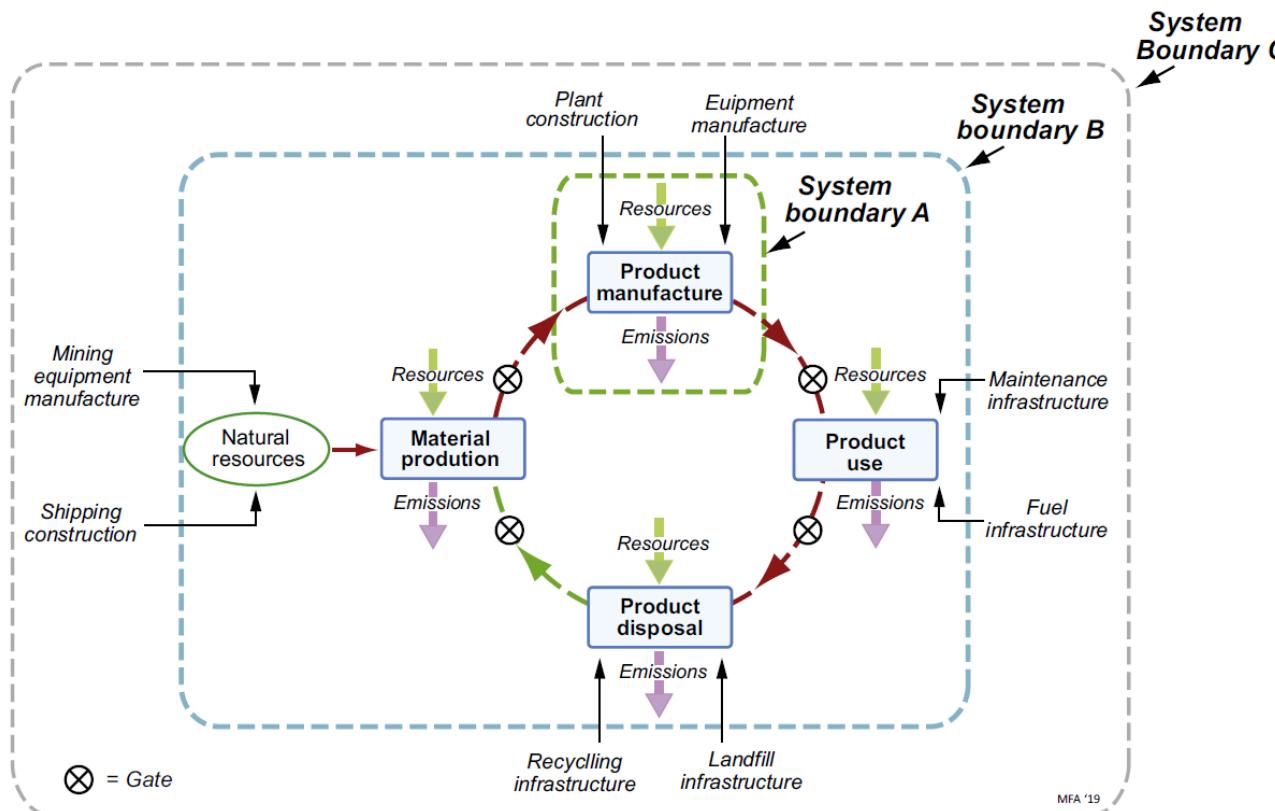


More on the topic of “scope” and embodied metrics and footprint metrics

- Sometimes in this class (and sometimes in the textbook), embodied metrics are usually **cradle-to-gate**, not considering use-related emissions or end-of life related emissions; this definition is not universal, and, in some cases, embodied metrics consider the entire lifecycle (**cradle-to-grave**)
- A carbon footprint of a person or company or nation or product is the sum of emissive activities (direct, indirect) over a certain timeframe, usually defined annually, but this is arbitrary, it can be determined to cover the duration of an event or project
- The metric you report depends on scope!

Life cycle assessment (LCA)

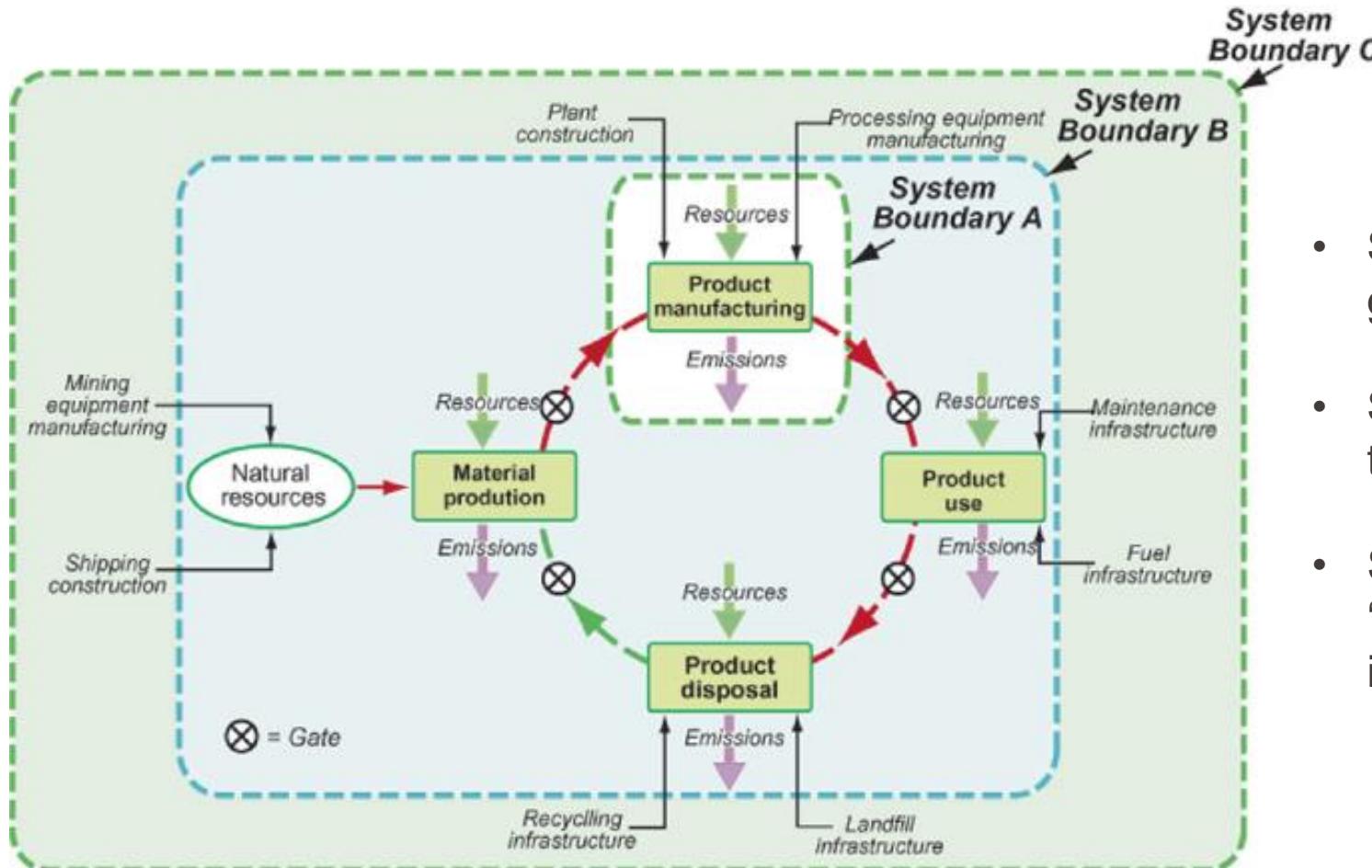
“...because of its limited capacity to absorb the effects of human activities, the environment sets a limit to society’s development.”



- Energy and material flows across the materials life cycle
- LCA helps to select the least impactful options
- Accounts in a scope-dependent way on resource consumption, emissions, and environmental impacts
- Regulated by a set of standards in 1997 (ISO 14040, and subsections 14041, 14042, and 14043)

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 Environmental Life Cycle Assessment, Jolliet et al., CRC Press, 2016.

Life cycle assessment (LCA)



- System boundary A = 'gate to gate'
- System boundaries B = 'cradle to gate', or 'cradle to grave'
- System boundary C = beyond 'cradle to grave'; considering infrastructure, recycling, etc.,

- Is a decision-making tool
- Can cover the entire life cycle, avoiding that local improvements shift the impact elsewhere
- Includes assumptions, simplifies complex systems
- Is not bias-proof, requires critical analysis along the way
- If comparative, do we compare to state of the art or the worst player? Can LCA or similar be a tool of greenwashing?

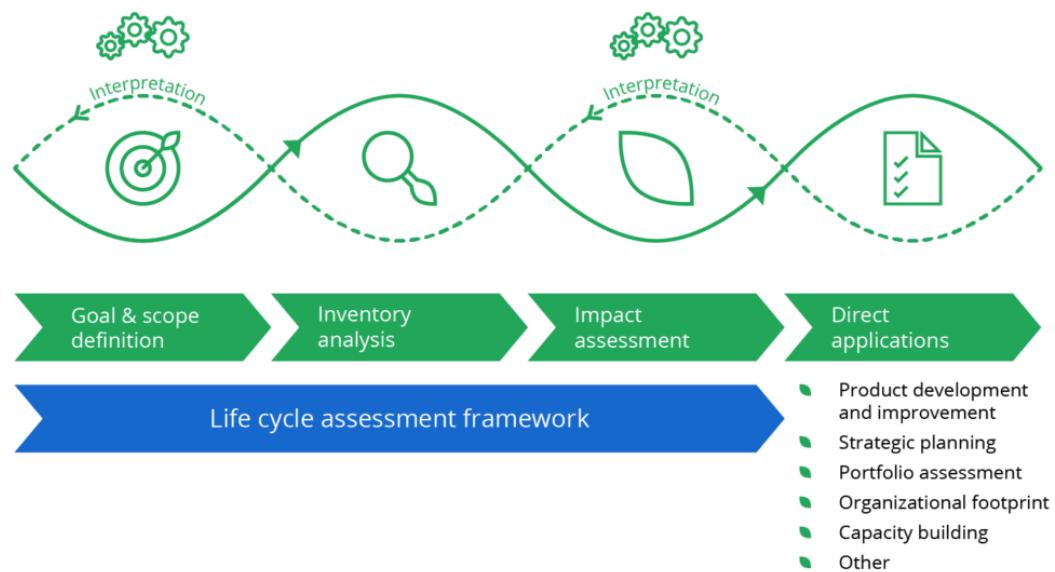


From: Environmental Life Cycle Assessment, Jolliet et al., CRC Press, 2016.
life-cycle-assessment-lca-basics/

Is an iterative process in **4 phases**, so you can refine assumptions, data sets, interpretations, etc.

Two-step LCA recommended:

- Step 1 – screening, “quick and dirty” identify the main processes and impacts (eco-audit)
- Step 2 – detailed analysis



4 phases:

1. Goal & scope
2. Inventory analysis
3. Impact assessment
4. Interpretation

From: Environmental Life Cycle Assessment, Jolliet et al., CRC Press, 2016.
life-cycle-assessment-lca-basics/

Phase 1. Goal and scope

- Most important part (but subjective and often simplified)

- Defines key aspects of the study (both what is included and what is not included)

- May need iteration

- Goal: defines the purpose, audience, intended application of the LCA study

- Scope: defines the boundaries, data requirements, and system

- Curran, M.A. (2017). Overview of Goal and Scope Definition in Life Cycle Assessment. In: Curran, M. (eds) Goal and Scope Definition in Life Cycle Assessment. LCA Compendium – The Complete World of Life Cycle Assessment. Springer, Dordrecht. https://doi.org/10.1007/978-94-024-0855-3_1life-cycle-assessment-lca-guide/

Goal & Scope of a Life Cycle Assessment



Phase 1. Goal and scope – Example

- **Goal:** "To compare the environmental impact of plastic and paper packaging for beverage bottles and determine which has a lower carbon footprint."

Tells you what is being measured and why

- **Scope:** "This LCA will assess the **carbon footprint, water usage, and air emissions** of plastic and paper beverage bottles from raw material extraction to disposal (**Cradle-to-Grave**). The **functional unit** is 1 liter of packaged beverage."

Tells you the boundaries (C2G), data requirements (C-footprint, water use, and emission), and system that will be studied (1 liter of a packaged beverage)

More on the functional unit (system that will be studied)

- Describes the quantity of a product or product system based on the performance it delivers in its end-use application
- Convenient and physically meaningful quantity
- A well-defined functional unit **allows comparisons** of different products or services that have the same function (functional equivalence)
- A functional unit does not contain product system inputs and outputs (e.g., based on CO₂ emissions)



Quantitative
and precise



Expressed in terms of
application-specific
performance requirements



Defined broadly
enough to encompass
competing technologies

Another way to look at it is by considering the following questions:

What? How much? For how long / how many times? Where? How well?

Functional unit examples

- *A measure of the performance of the functional outputs of a product system (ISO, 2006)*
- ***Allows comparison of different products and technologies that provide the same end function***

Don't compare 1 bar of soap to 1 bottle of liquid soap

Do compare the amount of product needed for given number of hand washings

Don't compare 1 ton of catalyst

Do compare the quantity of catalyst needed to obtain a defined amount of product

Don't compare the amount of sorbent needed to capture a defined amount of CO₂

Do the amount of sorbent needed to capture a defined amount of CO₂ over a fixed time period

Don't compare different food types

Do compare the amount of a given food type needed to obtain a fixed amount of nutrition (e.g., protein)

Examples of good functional units (ChatGPT)

- 1 "1,000 liters of clean drinking water supplied by a filtration system over its lifetime."
 -  **Why it's good?**
 - Clearly defines **quantity** (1,000 L).
 - Focuses on the **service provided** (clean water, not just the filter).
 - Ensures comparability between different filtration systems.
- 2 "1,000 km of passenger transport by a mid-size electric vehicle."
 -  **Why it's good?**
 - Specifies **distance** (1,000 km).
 - Focuses on **transport function, not just the car itself**.
 - Can be compared to other transport modes (e.g., diesel cars, buses, trains).
- 3 "1 m² of wall insulation providing a thermal resistance of R-5 for 50 years."
 -  **Why it's good?**
 - Defines **area** (1 m²) and **performance** (R-5 insulation value).
 - Includes **lifetime (50 years)** for long-term impact assessment.
 - Allows fair comparison between insulation materials.

Examples of good functional units (ChatGPT)

- 1 "One water filter."
-  **Why it's bad?**
 - Doesn't specify **how much water it filters**.
 - Can't compare different filters (one might last longer or filter more).
 - Focuses on the product, not the service it provides.
- 2 "A car."
-  **Why it's bad?**
 - Too **generic**—doesn't specify type, size, or purpose.
 - **No functional measure** (e.g., distance traveled, number of passengers).
 - Can't compare against other transport options like buses or bikes.
- 3 "An insulation material."
-  **Why it's bad?**
 - **No defined area or performance** (R-value, thickness, or lifespan).
 - Doesn't specify how well it insulates or for how long.
 - Makes comparison with other insulation types meaningless.

Challenges in defining the functional unit

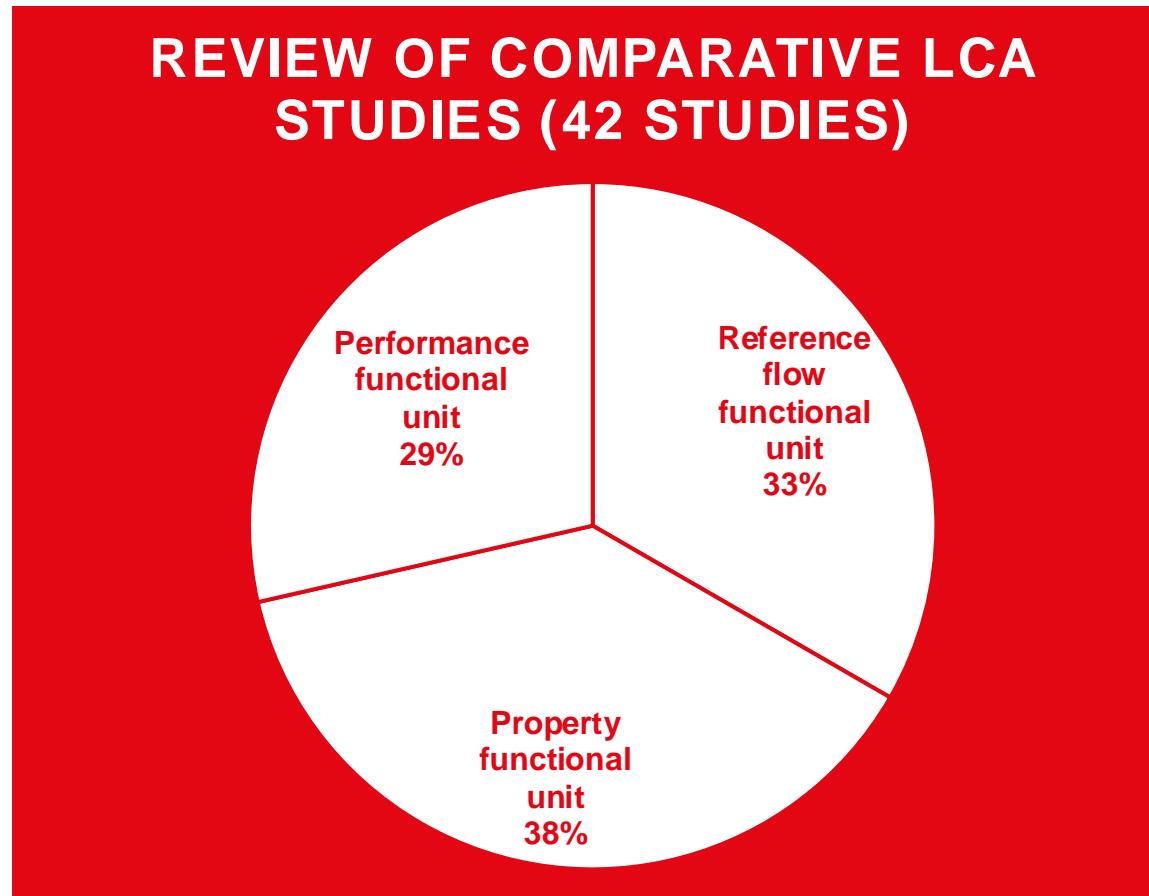
- Some functions can be difficult to quantify
- How to represent products with multiple functions?
- How to represent emerging technologies with functions that are not yet fully known?

Functional equivalence is more or less required, otherwise how can we compare?!

Realistically, most materials have at least some degree of:

- Different properties
- Different performances
- Additional functions

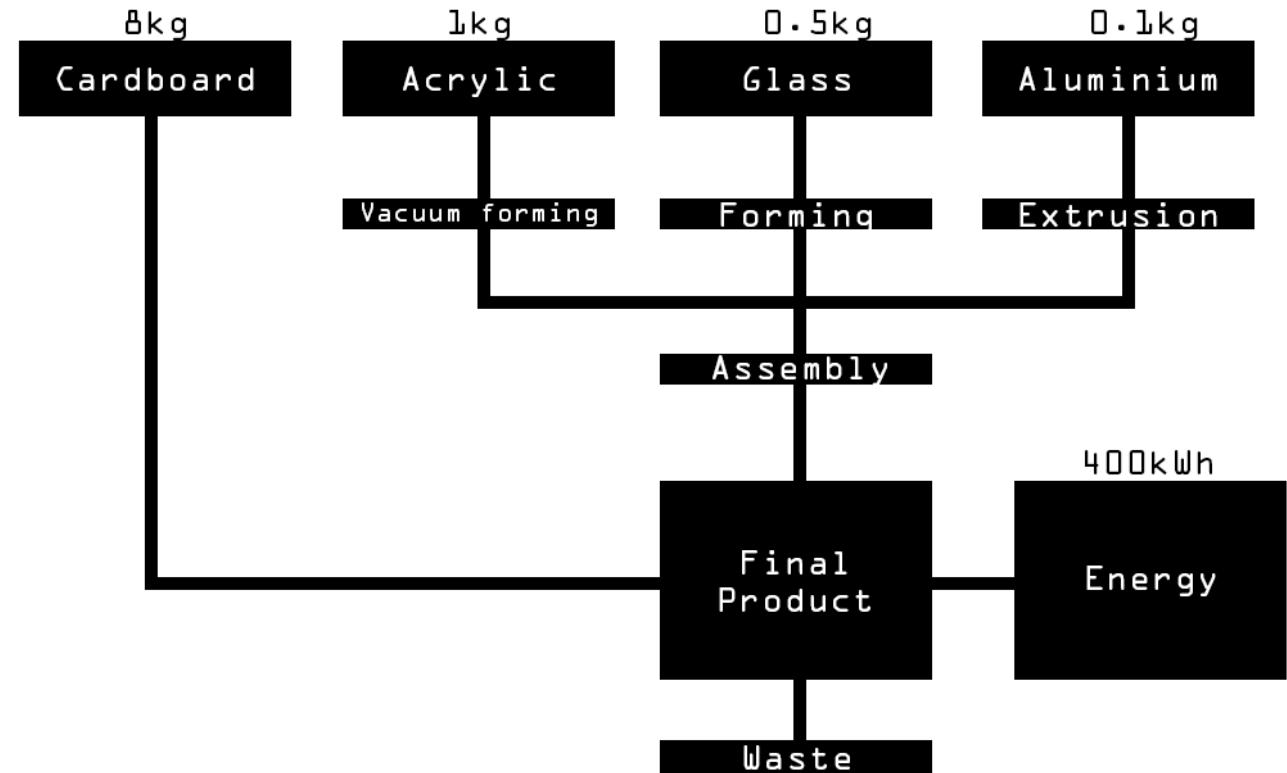
Functional units in the LCA literature



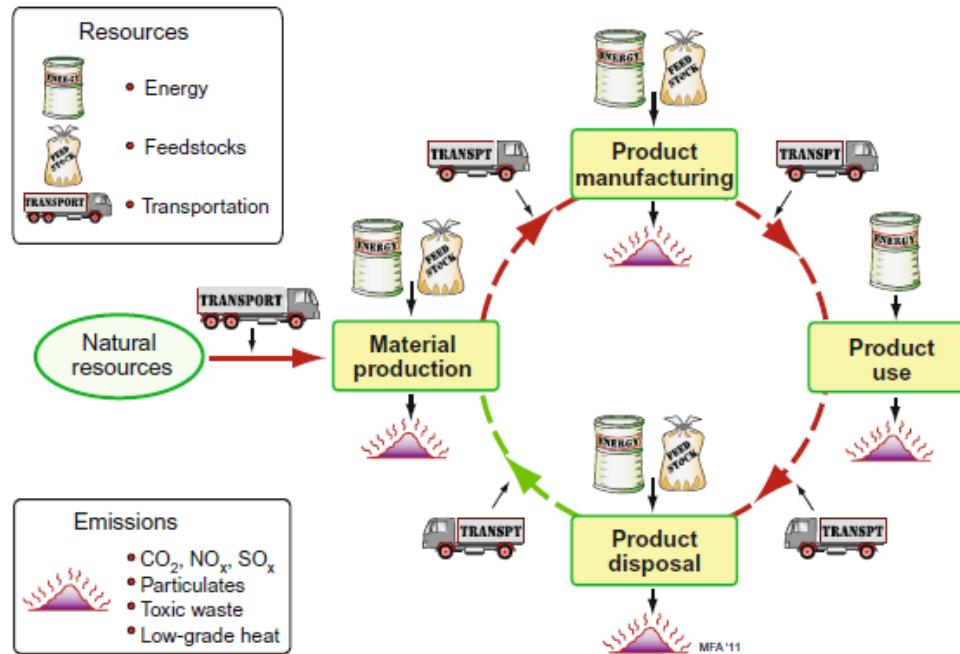
- Reference flow functional unit
 - Usually kg of material
 - Non-compliant for comparative studies
 - Environmental profile of a single product
- Property functional unit
 - e.g., mass of material needed to achieve a certain property
 - Non-compliant to LCA guidelines, function of the material in a specific product is not considered
- Performance functional unit
 - e.g., 1 disposable cup for serving 180 ml of a hot drink in comparing cups from different materials
 - Compliant

Phase 2. Life cycle inventory (LCI)

- LCI sums up environmental inputs (resources) and outputs (emissions, waste)
- Goal is to quantify these inputs and outputs
- Most time-consuming step



Phase 2. Inventory



- Collect different categories of data along lifecycle, according to defined scope/boundaries of the study
- Examples: inputs/outputs related to raw material extraction, production, transportation, use phase, end of life
- Data can be primary (more reliable, harder to get) or secondary (less reliable)
- Primary data originates from manufacturers, suppliers, field studies
- Secondary data originates from average or estimated from data bases
- Challenges: data gaps, inaccurate data

Environmental Life Cycle Assessment, Jolliet et al., CRC Press, 2016.
life-cycle-assessment-lca-basics/

Image from: https://en.wikipedia.org/wiki/Life-cycle_assessment

Phase 2. Inventory

Example of the kinds of data you can get from the LCI of a 1 L, single-use plastic bottle (generated by ChatGPT*)

Input/outputs	Amount per 1 bottle
Crude oil input	0.05 kg
Water used	0.2 L
Electricity in production	1.5 MJ
CO ₂ emissions	0.15 kg CO ₂ -eq
Transport fuel use	0.02 L diesel
Waste to landfill	5 g plastic

- But what do you do with data?
- Phase 3. Assessment!

*disclaimer, this data is only for illustrative purposes, do not trust AI blindly to give you correct data

3. Impact Assessment

- Classify environmental impacts into themes, e.g., global warming, health
- Converts all impacts into a common unit for comparison, e.g., CO₂-e

The amount in tonnes of CO₂ equivalent is the mass (in metric tonnes) of F gas multiplied by the GWP of that F gas.

For example the global warming potential of HFC 404A is 3,922. Therefore the tonnes CO₂ equivalent of 10kg of hydrofluorocarbon (HFC) 404a is calculated as follows:

1. Mass (in metric tonnes) of F gas multiplied by GWP of F gas
2. $= (10/1,000) * 3,922$
3. $= 39.2$ tonnes CO₂ equivalent

Conversion factors can be used to convert flows to CO₂ equivalents

Environmental Life Cycle Assessment, Jolliet et al., CRC Press, 2016.

[life-cycle-assessment-lca-basics/](#)

<https://www.gov.uk/guidance/calculate-the-carbon-dioxide-equivalent-quantity-of-an-f-gas>

LCA of single use PET bottle

Impact category	%
Ecological damage	
Acidification	2.9
Ecotoxicity	5.15
Eutrophication	5.2
Global warming	20.76
Ozone depletion	0.01
Resource depletion	
Fossil fuel depletion	20.1
Human health damage	
Carcinogenics	36.36
Non carcinogenics	4.92
Respiratory effects	2.4
Smog	2.19

Example of LCIA of single-use PET bottle in all the impact categories

- How is this type of data given in % and compared?
- Impact categories have their own units; e.g., global warming potential is in kg CO₂-eq, eutrophication is in kg N-eq, acidification in kg SO₂-eq, water use in m³, possible resource depletion in MJ
- Direct comparison is not possible
- So, data is **normalized** to give a unitless value and **weighted** by multiplication of a weighting factor based expert opinion, policies, etc.,

Normalized impact

Normalized Impact =

Impact value/ Reference Value (e.g., per person per year)

- If your product results in **2 kg N-eq eutrophication**, and the average eutrophication per person per year is **10 kg N-eq**
- Then the normalized impact of your product is $2/10 = 0.2$ (or 20% of a person's annual impact)
- Now you need to weight this impact to compare its importance relative to the other impacts of your product

Weighted impact

*Made up data in table

Impact Category	Normalized Value	Weighting Factor	Final Score	Final score in %
Global Warming	0.5	40%	$0.5 \times 0.4 = 0.2$	61
Eutrophication	0.2	30%	$0.2 \times 0.3 = 0.06$	18
Acidification	0.3	20%	$0.3 \times 0.2 = 0.06$	18
Water Use	0.1	10%	$0.1 \times 0.1 = 0.01$	3
SUM	1	100%	0.33	100

- Weighted value for eutrophication = $0.2 \times 30\% = 0.06$ (final score)
- Final score on % for eutrophication = $0.06 / 0.33 \times 100\% = 18\%$

4. Interpretation

- Systematic check that conclusions are substantiated (ISO 14043)
- Use results to identify alternatives that mitigate environmental impacts – action prioritization

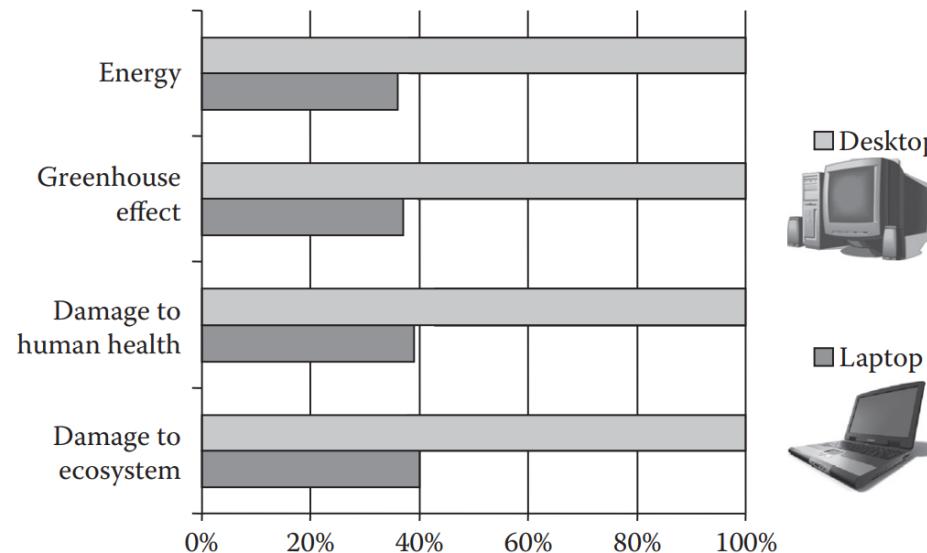
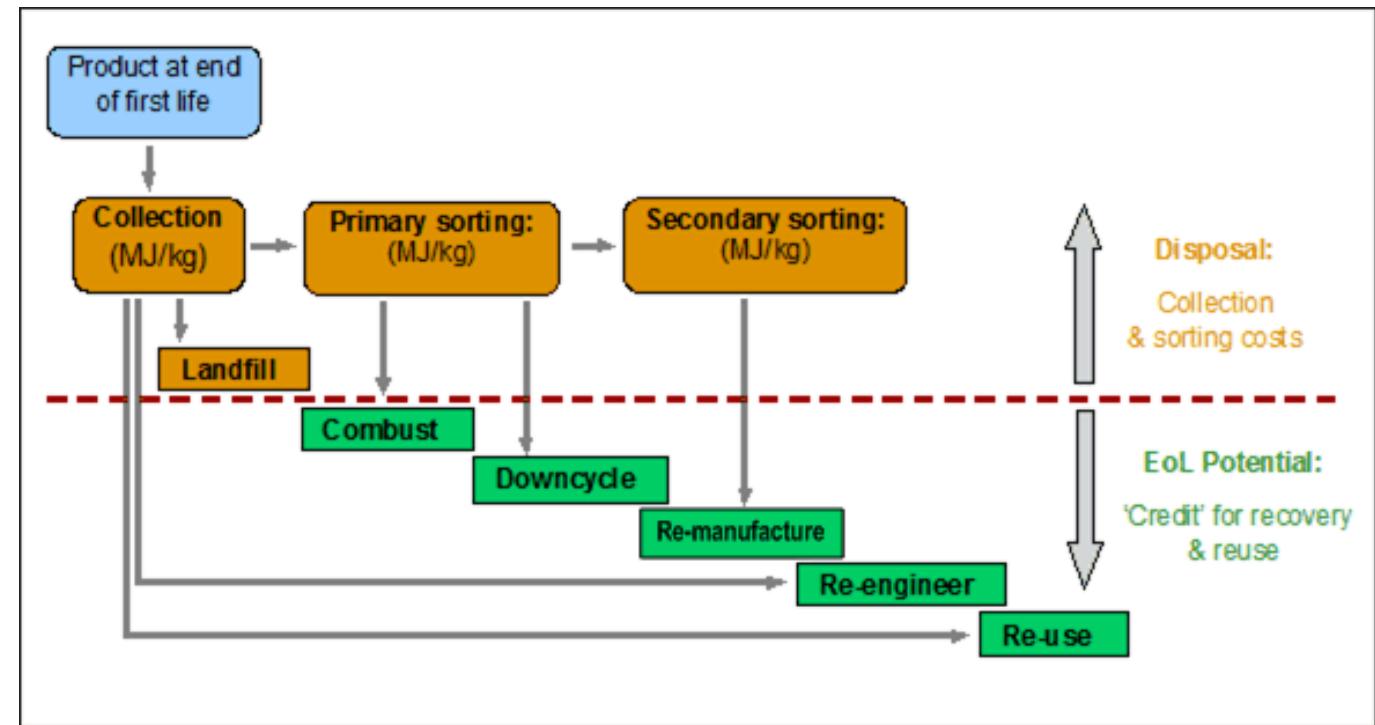


FIGURE 6.4 Impact assessment based on the critical surface-time method. Results are normalized to the desktop PC scenario.

- Useful impact quantification tool
- Did you ask a good question and define a relevant scope (goal, scope, functional unit?)
- Do you have quality data?
- Are your assumptions founded?
- Are you confident with the weighting of different impacts and the interpretation of the data? Are other interpretations possible?
- What will you do with this assessment? Change a process, change a raw material, use it to market your own product or research?

- Streamlined assessment of energy demands and carbon emissions
- Aims to identify life phase(s) with greatest negative impact and to use this info for improvements and redesign
- *EoL* (end-of-life) potential or credit gives the end-of-life savings or 'credits' that can be realized in future life cycles by using the recovered material or components



From: Materials and the Environment, Michael F. Ashby, Copyright 2021 Elsevier, chapter 7.

[EoL potential](#)

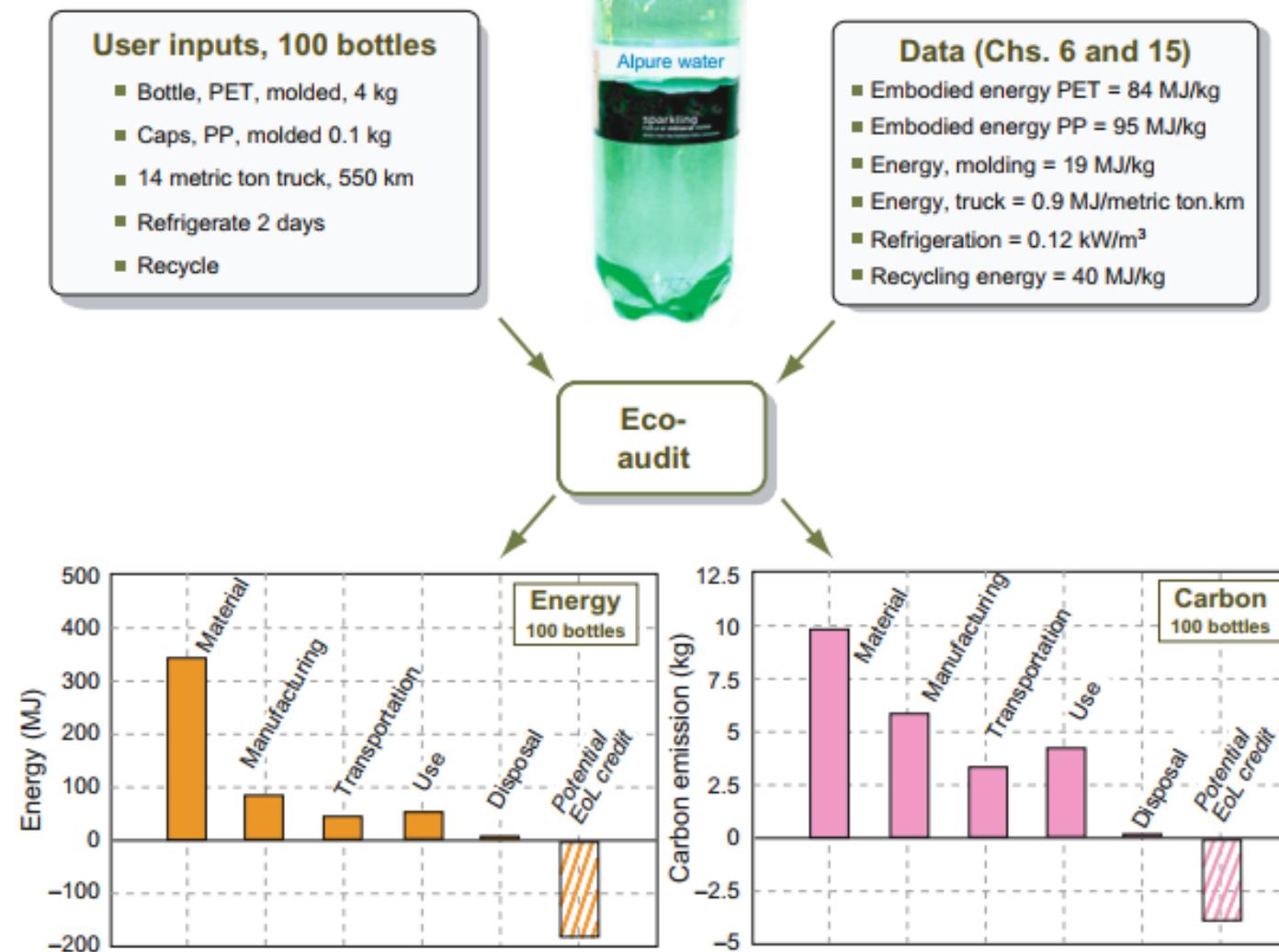


FIGURE 7.2 The eco-audit of a 1-liter PET water bottle, filled in France, trucked to England, and refrigerated for 2 days

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EoL potential

- Clear that the material is the hotspot & that EoL credits through recycling can be used to offset impact

Take aways

- Last time we look at CO₂ spectra (I promise!)
- Carbon footprint/handprint
- Embodied metrics
- Four phases of an LCA (and challenges)
- How do we actually compare the importance of different impacts?
- Eco-audit