ETH zürich

Energy & Process
Systems Engineering

Introduction to Modeling and Optimization of Sustainable Energy Systems:

Life cycle assessment

André Bardow
Energy and Process Systems Engineering

After this lecture, you will be able to…

- ✓ employ basic **solution methods** for **mixed-integer linear** (MILP) & **nonlinear programming** (MINLP) problems.
- ✓ find optimal heat-exchanger networks and near-optimal solutions with **integer cuts**
- discuss **(dis)advantages** of optimization problem classes

Optimization problem classes

constraints \ variables	continuous	continuous & discrete
linear	linear program (LP)	mixed-integer linear program (MILP)
nonlinear	nonlinear program (NLP)	mixed-integer nonlinear program (MINLP)

Problem types and problem size

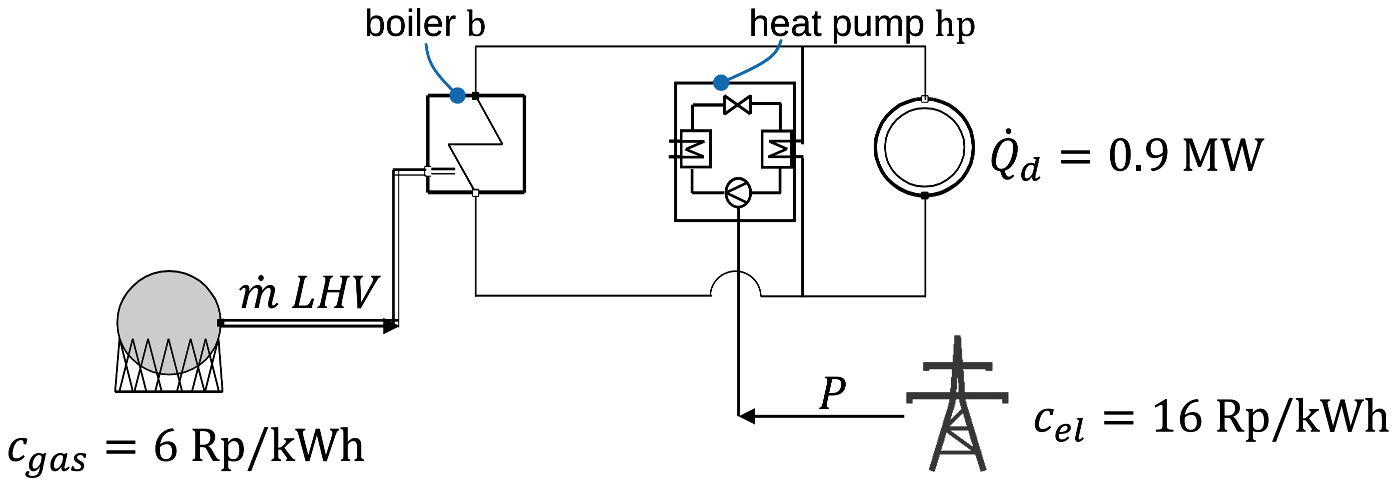
Leyffer-Linderoth-Luedtke (LLL) Complexity

Assuming a problem of type X with a number of Y decision variables:

LLL = The largest number of decision variables Y, for which at least one of the Professors Leyffer, Linderoth or Luedtke is willing to bet $50 that the problem of type X can be solved using a state-of-the-art solver.

	convex	non-convex
MINLP	500	100
NLP	$5 \cdot 10^4$	100
MILP	$2 \cdot 10^4$	-
LP	$5 \cdot 10^7$	-

Structural optimization of a heating system: Boiler or heat pump?



LINEAR

objective function

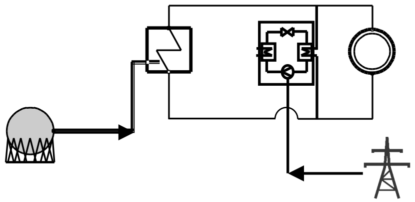
$$\min_{\substack{y_c, \dot{Q}_c,\\ c \in \{b,hp\}}} \text{TAC} = \underbrace{\sum_c y_c\, I_c \frac{(1+i)^n\, i}{(1+i)^n - 1}}_{\text{annualized capital cost}} + \underbrace{\int_{t=0}^{T} \left[c_{\text{gas}} \frac{\dot{Q}_b}{\eta_b} + c_{\text{el}} \frac{\dot{Q}_{hp}}{\eta_{hp}} \right] dt}_{\text{cost of energy consumption}}$$

variables

$\dot{Q}_c \in \left[0, \dot{Q}_c^N\right], \forall\, c \in \{b, hp\}$ heating output of component i

$y_c \in \{0,1\}, \quad \forall\, c \in \{b, hp\}$ component i is purchased ($= 1$) or not ($= 0$)

Structural optimization of a heating system: Boiler or heat pump?



$\dot{Q}_c \in [0, \dot{Q}_c^N], \forall\, c \in \{b, hp\}$ heating output of component i

$y_c \in \{0,1\}, \quad \forall\, c \in \{b, hp\}$ component i is purchased $(= 1)$ or not $(= 0)$

objective function

$$\min_{\substack{y_c, \dot{Q}_c,\\ c\in\{b,hp\}}} \ \mathrm{TAC} \ = \sum_c y_c\, I_c \frac{(1+i)^n\, i}{(1+i)^n - 1} + \int_{t=0}^{T} \left[c_{\mathrm{gas}} \frac{\dot{Q}_b}{\eta_b} + c_{\mathrm{el}} \frac{\dot{Q}_{hp}}{\eta_{hp}} \right] dt$$

MINLP

constraints

$$s.t. \qquad 0 \le \dot{Q}_c, \qquad \forall\, c \in \{\mathrm{b}, \mathrm{hp}\}$$

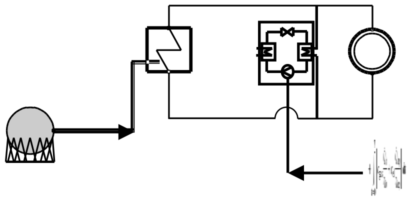
$$\dot{Q}_c \le \dot{Q}_c^N, \qquad \forall\, c \in \{\mathrm{b}, \mathrm{hp}\}$$

$$\sum_c y_i\, \dot{Q}_c = \dot{Q}_d,$$

A single nonlinearity turns the whole problem into an MINLP!

Product of two variables is nonlinear!

Structural optimization of a heating system: Boiler or heat pump?



$\dot{Q}_c \in [0, \dot{Q}_c^N], \forall\, c \in \{b, hp\}$ heating output of component i

$y_c \in \{0,1\}, \quad \forall\, c \in \{b, hp\}$ component i is purchased $(=1)$ or not $(=0)$

objective function

$$\min_{\substack{y_c, \dot{Q}_c,\\ c \in \{b,hp\}}} \ \mathrm{TAC} = \sum_c y_c\, I_c \frac{(1+i)^n\, i}{(1+i)^n - 1} + \int_{t=0}^{T} \left[c_{\mathrm{gas}} \frac{\dot{Q}_b}{\eta_b} + c_{\mathrm{el}} \frac{\dot{Q}_{hp}}{\eta_{hp}} \right] dt$$

MINLP

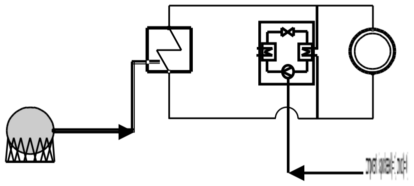
constraints

$$\begin{aligned} s.t. \quad & 0 \le \dot{Q}_c, && \forall\, c \in \{\mathrm{b}, \mathrm{hp}\} \\ & \dot{Q}_c \le \dot{Q}_c^N, && \forall\, c \in \{\mathrm{b}, \mathrm{hp}\} \\ & \sum_c y_i\, \dot{Q}_c = \dot{Q}_d, && \end{aligned}$$

$$\begin{aligned} & 0 \le \dot{Q}_c, && \forall\, c \in \{\mathrm{b}, \mathrm{hp}\} \\ & \dot{Q}_c \le y_i\, \dot{Q}_c^N, && \forall\, c \in \{\mathrm{b}, \mathrm{hp}\} \\ & \sum_c \cancel{y_i} \dot{Q}_c = \dot{Q}_d, && \end{aligned}$$

Alternative formulation with $\dot{Q}_c^N$ as big-M parameter results in linear constraints.

Structural optimization of a heating system: Boiler or heat pump?



$\dot{Q}_c \in [0, \dot{Q}_c^N], \forall\, c \in \{b, hp\}$ heating output of component i

$y_c \in \{0,1\}, \quad \forall\, c \in \{b, hp\}$ component i is purchased $(= 1)$ or not $(= 0)$

objective function

$$\min_{\substack{y_c, \dot{Q}_c,\\ c \in \{b,hp\}}} \ \mathrm{TAC} \ = \sum_c y_c\, I_c \frac{(1+i)^n\, i}{(1+i)^n - 1} \ + \int_{t=0}^{T} \left[c_{\mathrm{gas}} \frac{\dot{Q}_b}{\eta_b} + c_{\mathrm{el}} \frac{\dot{Q}_{hp}}{\eta_{hp}} \right] dt$$

MILP

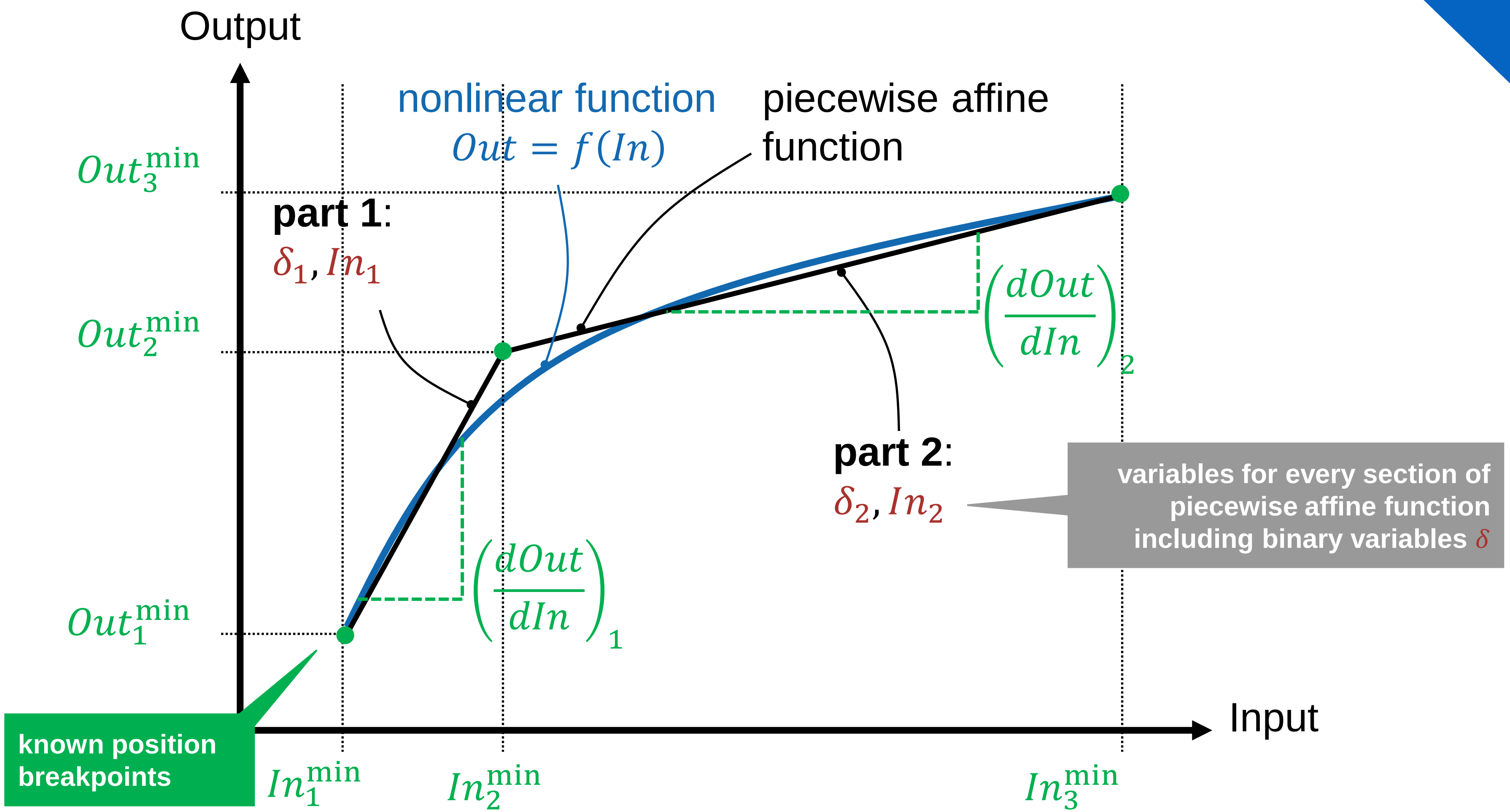
constraints

$$
\begin{aligned}
s.t. \qquad & 0 \le \dot{Q}_c, && \forall\, c \in \{\mathrm{b}, \mathrm{hp}\} \\
& \dot{Q}_c \le y_i\, \dot{Q}_c^N, && \forall\, c \in \{\mathrm{b}, \mathrm{hp}\} \\
& \sum_c \cancel{y_c}\, \dot{Q}_c = \dot{Q}_d, &&
\end{aligned}
$$

Exact linearizations allow to transform nonlinear to linear problems ☺

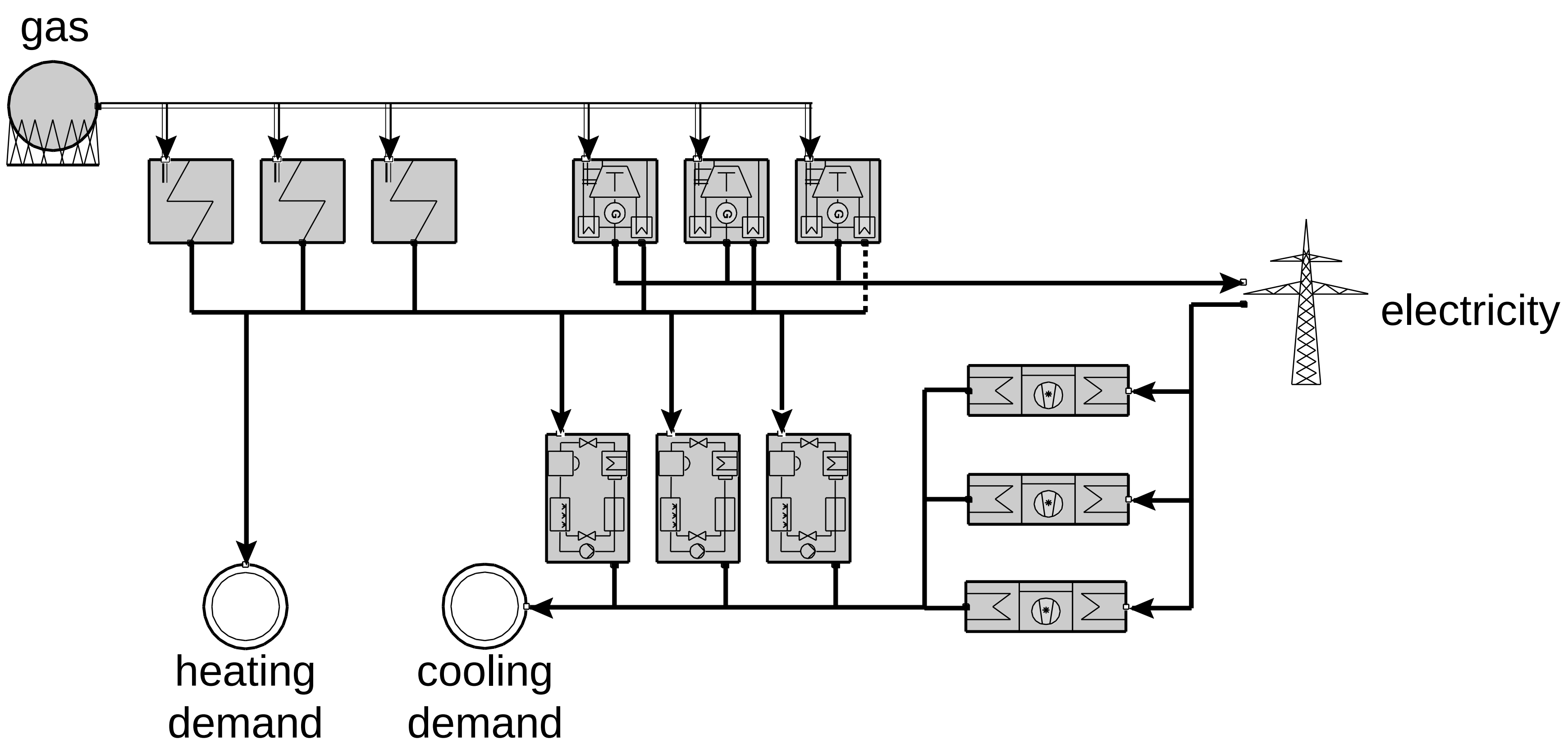
Approximating NLPs with MILPs – Piecewise affine formulation

More details on MILPs in Lectures 10!

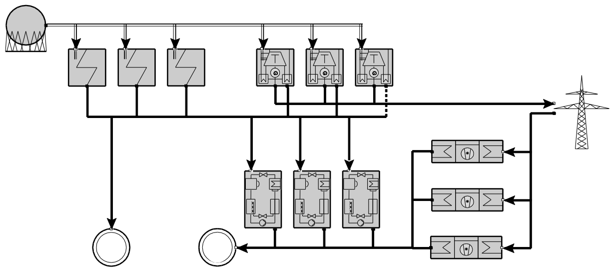


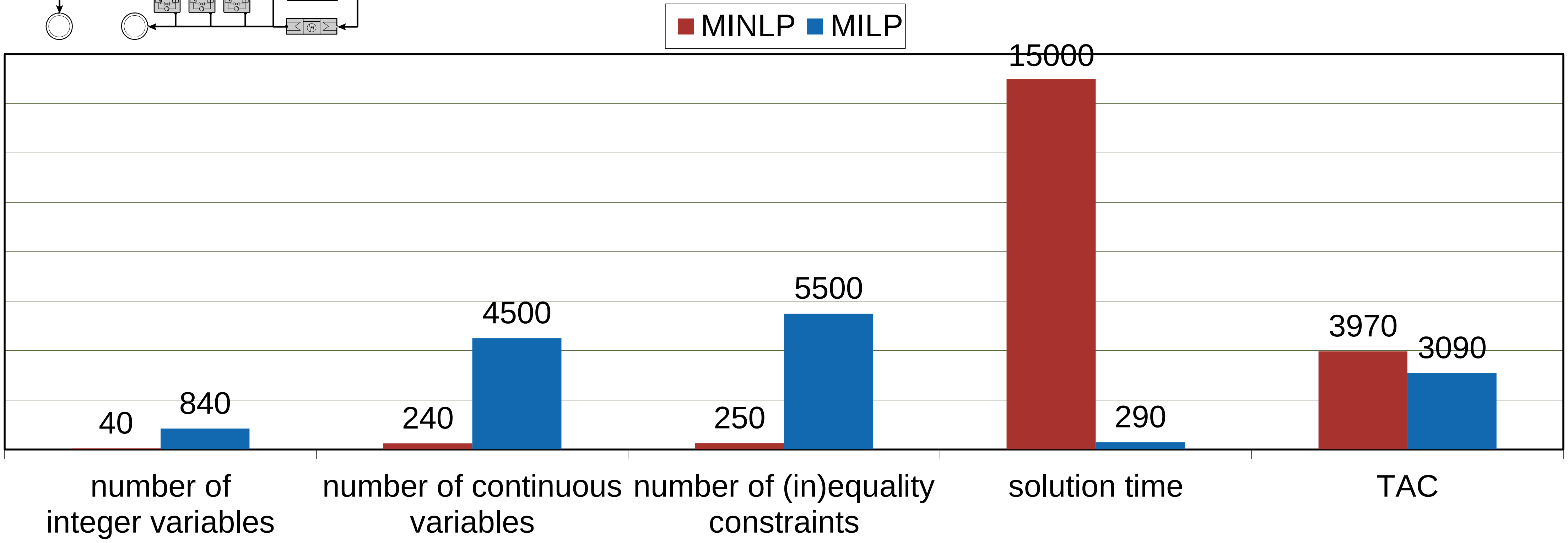
Nonlinear function can be approximated by piecewise-affine functions
$\Rightarrow$ no longer exact
$\Rightarrow$ usually introduces binary variables (but not always)

Solving MINLP vs. MILP – Piecewise linearization in practice



Solving MINLP vs. MILP – Piecewise linearization in practice





Problem class much more important than number of variables & equations

After this lecture, you will be able to…

- ✓ employ basic **solution methods** for **mixed-integer linear** (MILP) & **nonlinear programming** (MINLP) problems.
- ✓ find optimal heat-exchanger networks and near-optimal solutions with **integer cuts**
- ✓ discuss **(dis)advantages** of optimization problem classes

Lecture plan

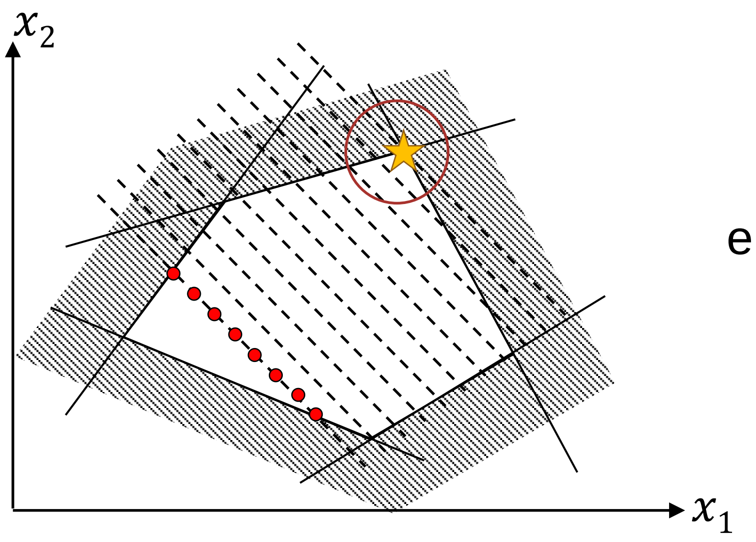
No.	Date	Content	
1	29.09.	Introduction & Models	
2	06.10.	Heat integration	Applications
3	13.10.	Continuous Optimization	Methods
4	20.10.	Heat exchanger networks	Applications
5	27.10.	Discrete Optimization	Methods
6	03.11.	Life Cycle Assessment (LCA)	Metrics
7	10.11.	Thermoeconomics	Metrics
8	17.11.	Risk Key Performance Indicators for Security	Metrics
9	24.11.	Multi-energy dimension: introduction	Methods & Applications
10	01.12.	Design dimensions: technology modelling	
11	08.12.	Space dimensions: energy networks	
12	15.12.	Uncertainty in energy systems	
13	22.12.	Recap (online)	

Optimization problem: The objective function is key

$$\min_{\boldsymbol{x}} \quad z = f(\boldsymbol{x})$$

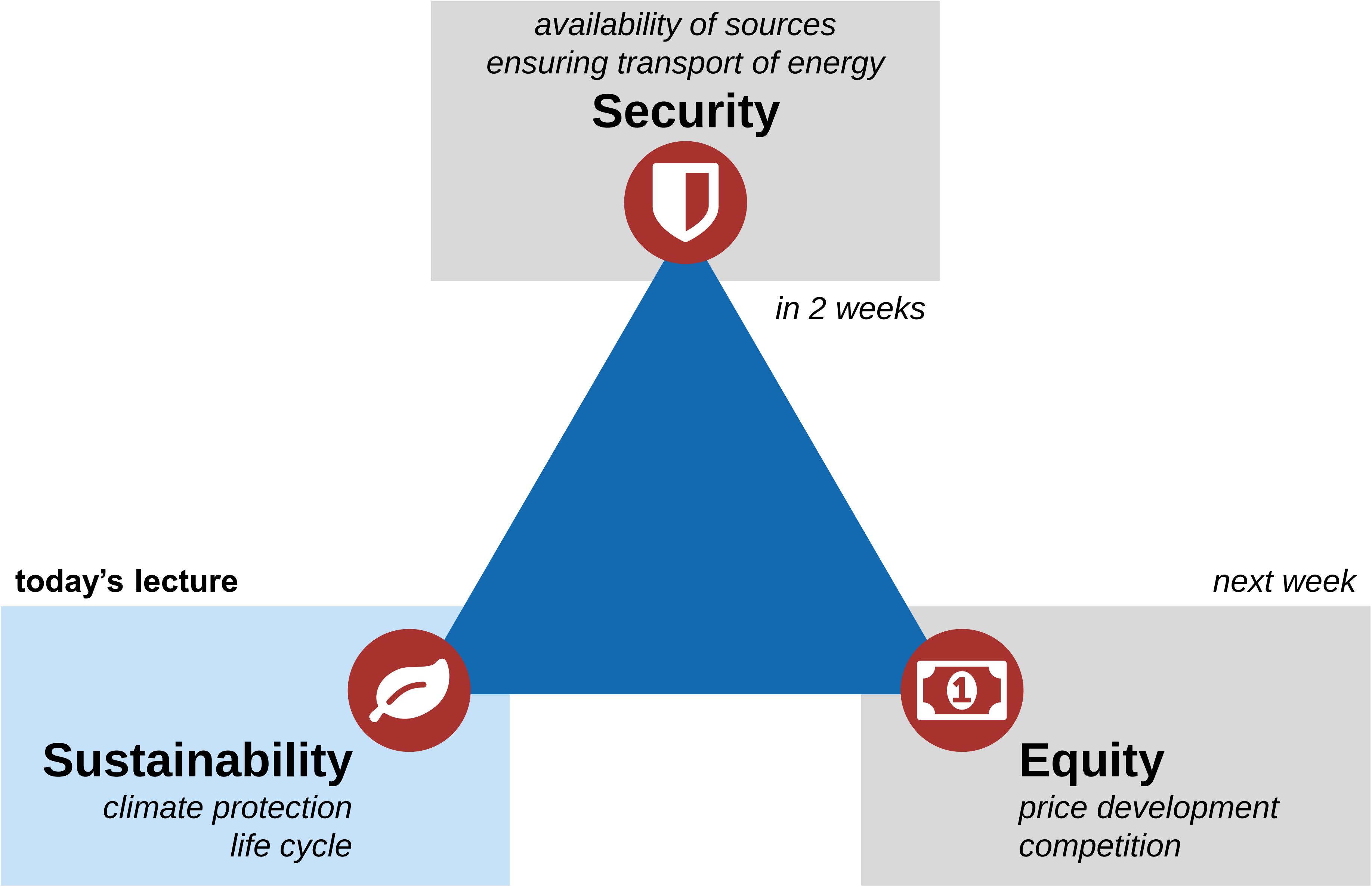
$$\text{s.t.} \quad g_j(x) \leq 0, \qquad j = 1, \ldots, n$$

$$h_i(x) = 0, \qquad i = 1, \ldots, o$$



e.g. linear problem (Lecture 2)

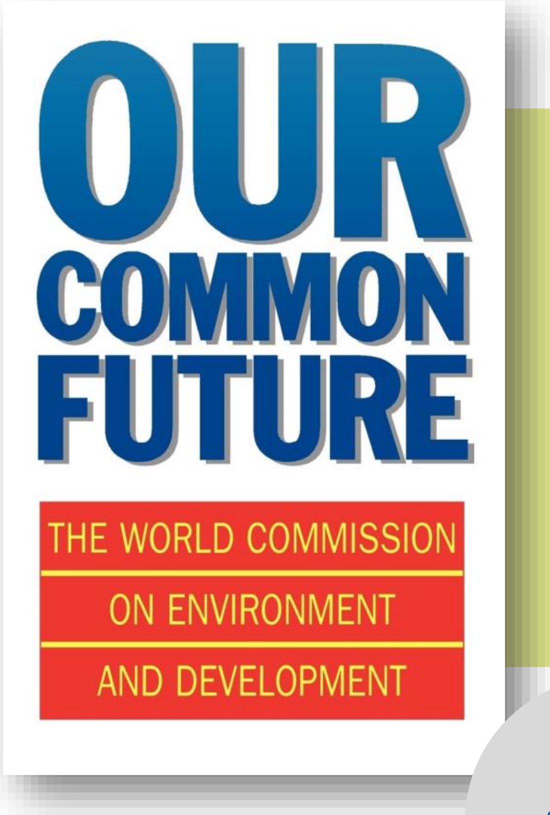
Sustainability of energy systems



What is sustainability?

ti amo
alla follia
amore mio

How to measure sustainability?



Sustainable development

meets the <u>needs of the present</u>
without compromising the <u>ability of future generations</u>
to meet their own needs.

Brundtland Commission (1987)

- efficiency?
- primary energy?
- cumulative energy demand?
- ecological risk assessment?
- emissions?
- Life cycle assessment?

Brundtland, G. H., Khalid, M., Agnelli, S., Al-Athel, S., & Chidzero, B. J. N. Y. (1987). Our common future. *New York*, *8*.

After this lecture, you are able to…

- **conduct a life cycle assessment:**
  - draw process flow diagrams
  - calculate energy and mass balances along a product life cycle
  - solve allocation problems
  - assess environmental impacts

- Interpret **life cycle assessment results**

Life cycle assessment (LCA)
– A holistic approach to impact assessment

they define what a life cycle ass. is

raw materials come from?

recycle

what is the end of life?

February 2021

DIN EN ISO 14040

DIN

ICS 13.020.10; 13.020.60

Supersedes
DIN EN ISO 14040:2009-11

Method : not perfect

"LCA addresses the **environmental aspects and potential environmental impacts**
(e.g. use of **resources** and the environmental consequences of **releases**)
throughout a product's **life cycle**
from raw material acquisition
through production,
use,
end of-life treatment,
recycling and
final disposal
(i.e. cradle-to-grave)."

AIM : LC of a process

desulforization

all diff. potential environ. problems

CO_2

acid rain

Stages of life cycle assessment (DIN EN ISO 14040)

Life cycle assessment framework

First path of any study!

Goal & scope definition

Most important path

collecting data

Inventory analysis (LCI)

- all material flow

Impact assessment (LCIA)

go back and on on this steps

Interpretation

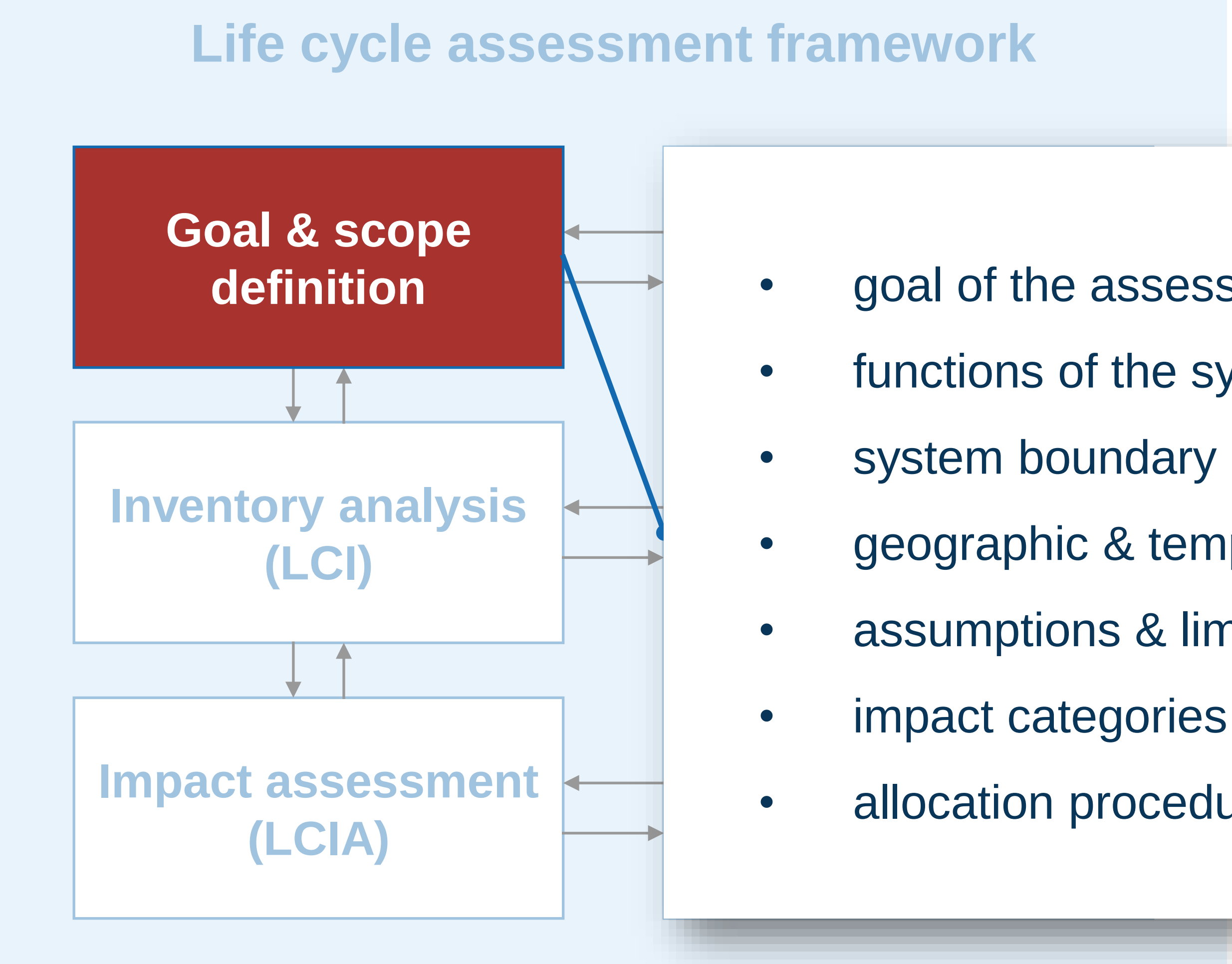
e.g. how to make a better bottle

Direct applications

- product development & improvement
- strategic planning
- public policy making
- marketing
- other

DIN EN ISO 14040:2021-02.

Stages of life cycle assessment (DIN EN ISO 14040)



- goal of the assessment including target group
- functions of the system, functional unit
- system boundary
- geographic & temporal reference
- assumptions & limitations
- impact categories
- allocation procedures

DIN EN ISO 14040:2021-02.

Functional unit – What do I need the system for?

"The **functional unit** defines
the quantification of the identified functions (performance characteristics) of the product.
The primary purpose […] is to provide a reference to which the inputs and outputs are related."[1]

	paper towels	air-dryer
functional unit	$1 \times$ dry hands	$1 \times$ dry hands
reference flow	x paper towels	x seconds of air
secondary functions	*faster, less noisy, drying other surfaces*	*avoid trash, contact-free*

Physical

Challenges

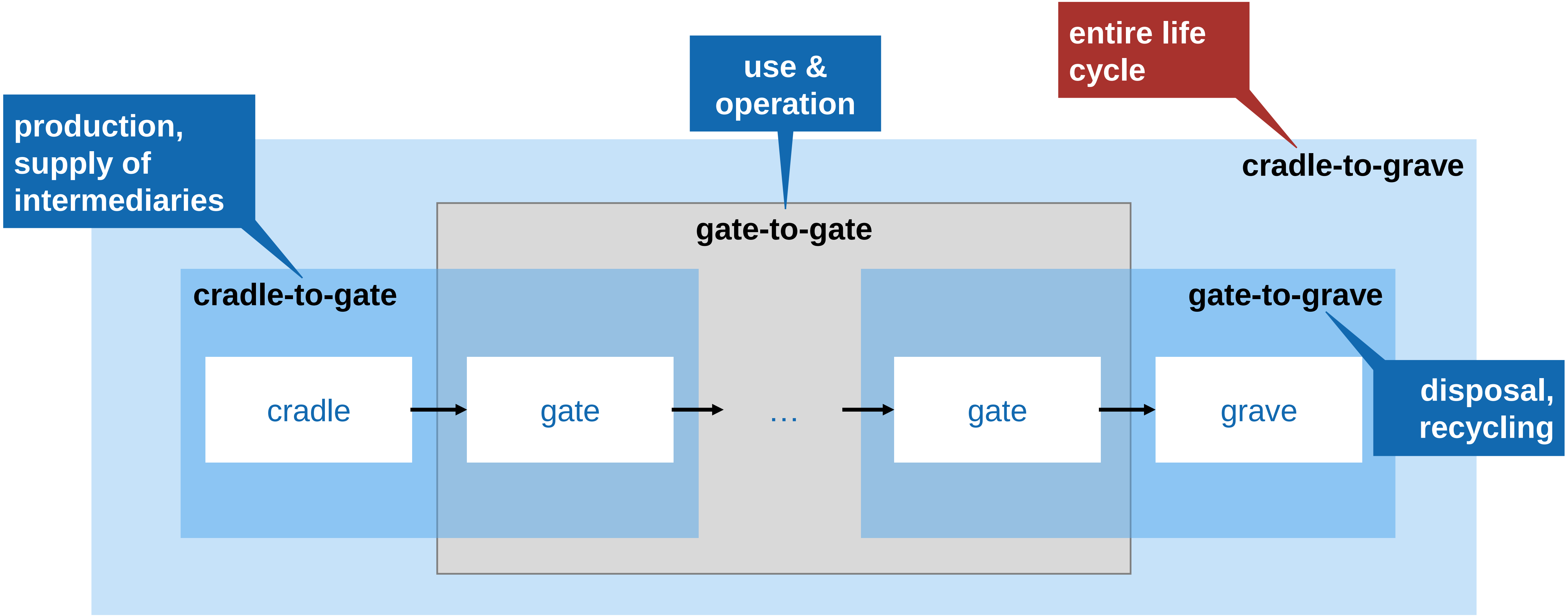
Basis

- **secondary functions**
  (e.g. fun/prestige for sports cars)
- **hard-to-quantify functions**
  (e.g. energy supply of an apartment building)

kilometer kilometer

DIN EN ISO 1

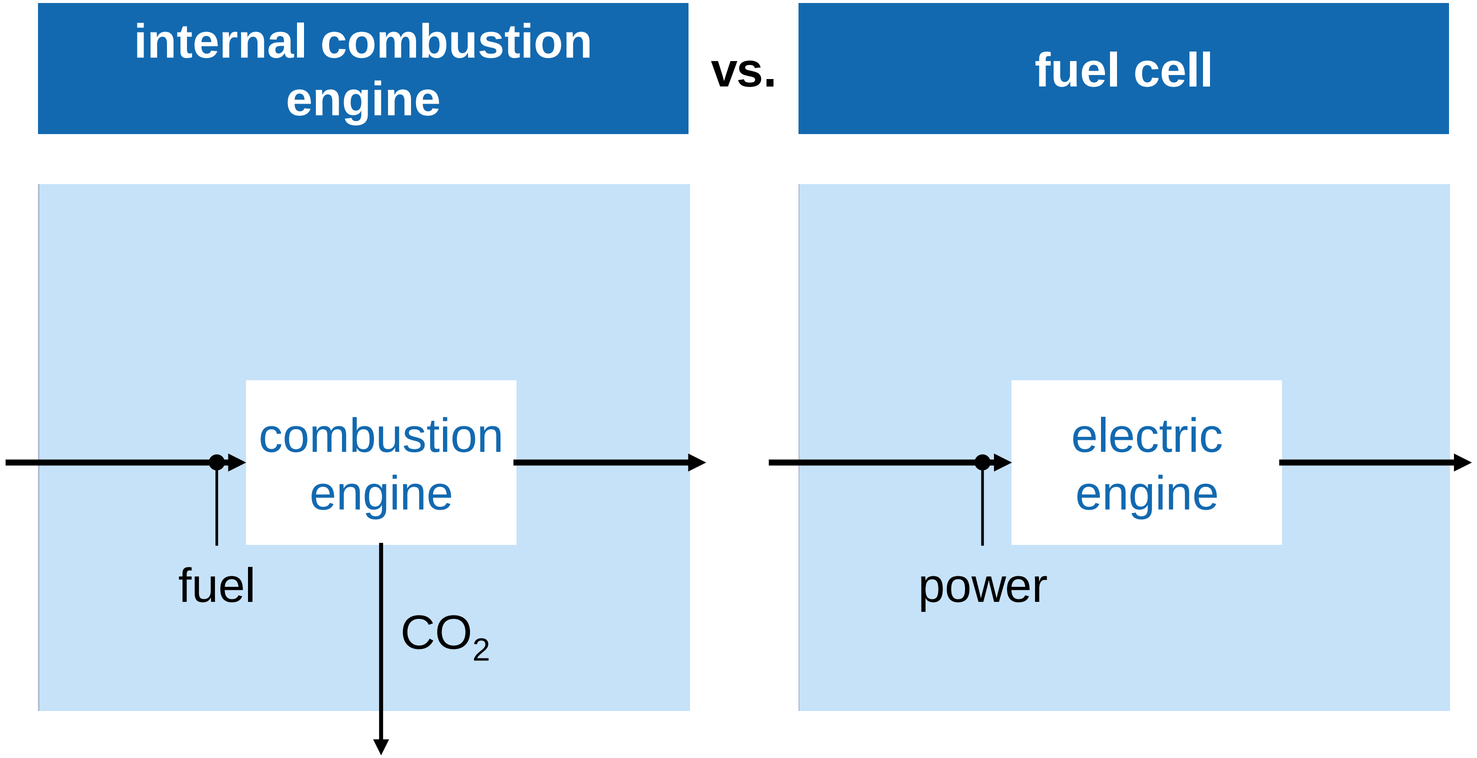
System boundaries



Only cradle-to-grave regards the full life cycle – but selected life stages are often sufficient for comparative analyses.

Example: System boundaries
Private transportation – internal combustion vs. fuel cell

1 functional unit: 1 pkm



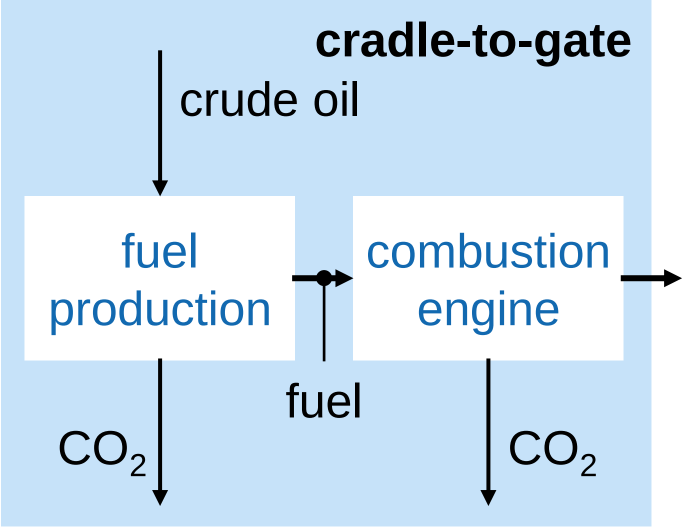
Example: System boundaries
Private transportation – internal combustion vs. fuel cell

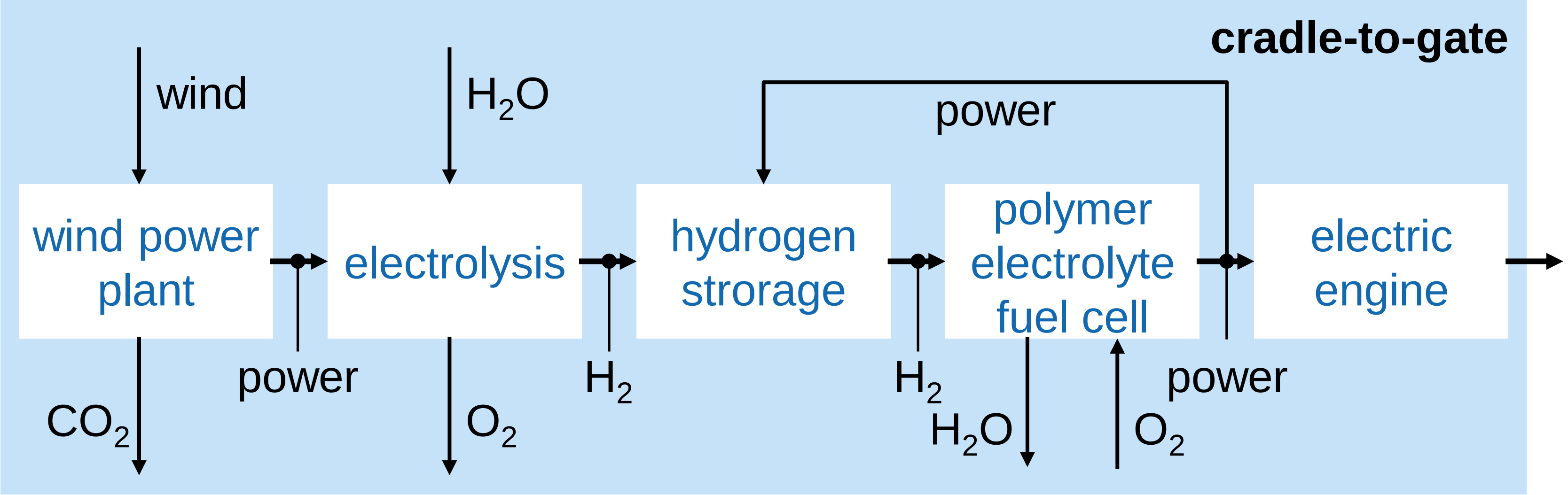
1 functional unit: 1 pkm

2 cradle-to-gate analysis

? recycling

internal combustion engine vs. **fuel cell**





Process flow diagrams

Elements

- processes
- material / energy flows
- functional unit (reference flow)
- system boundaries

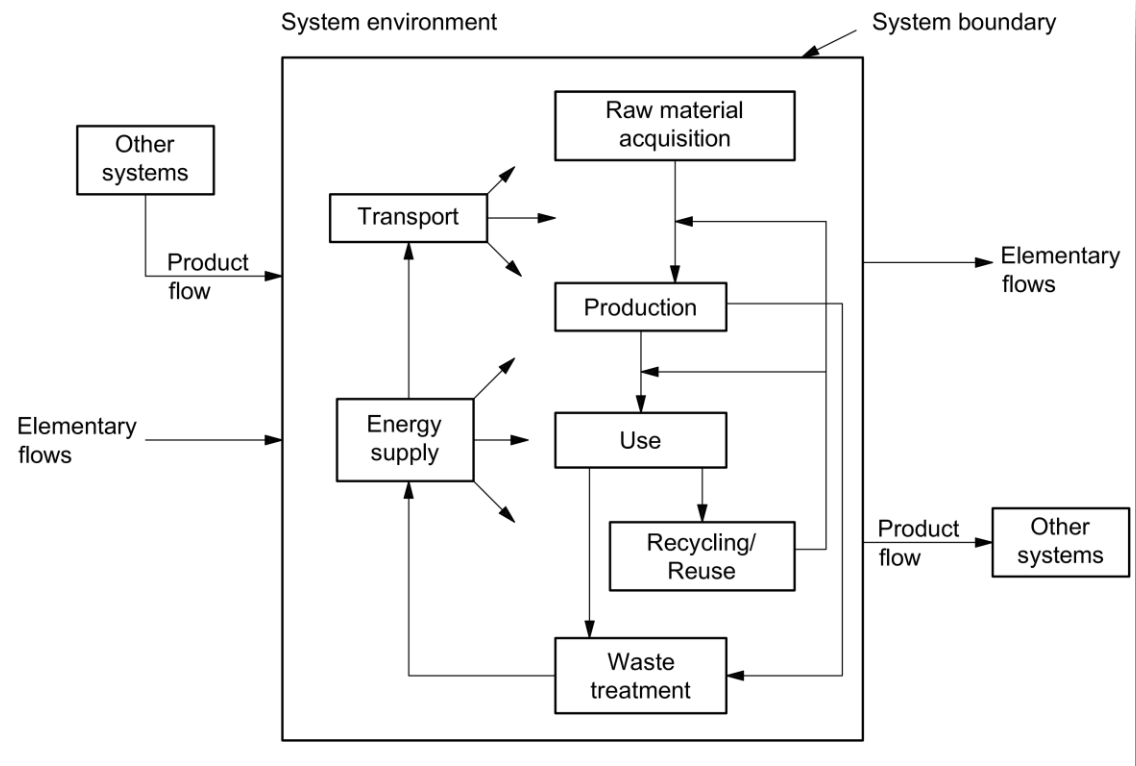


Figure 2 — Example of a product system for LCA

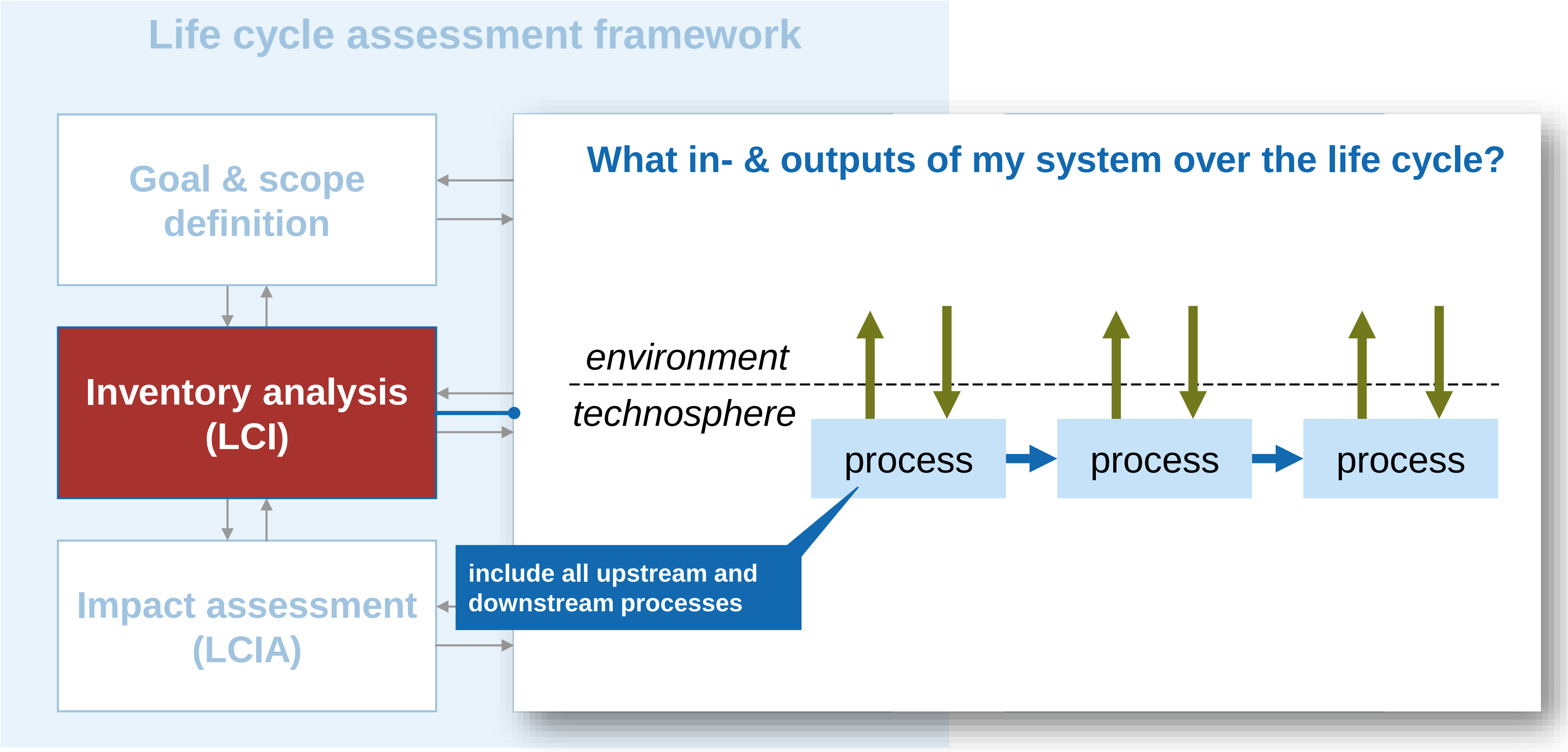
DIN EN ISO 14040:2021-02.

After this lecture, you are able to…

- conduct a life cycle assessment:
  - ✓ draw process flow diagrams
  - – calculate energy and mass balances along a product life cycle
  - – solve allocation problems
  - – assess environmental impacts

- critically interpret life cycle assessment results

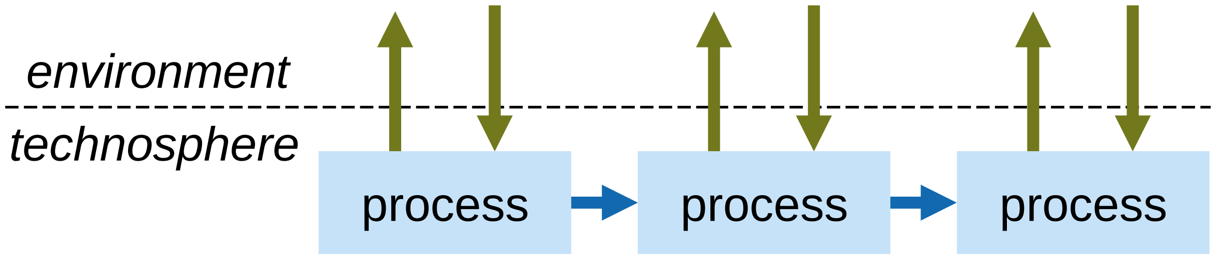
Stages of life cycle assessment (DIN EN ISO 14040)



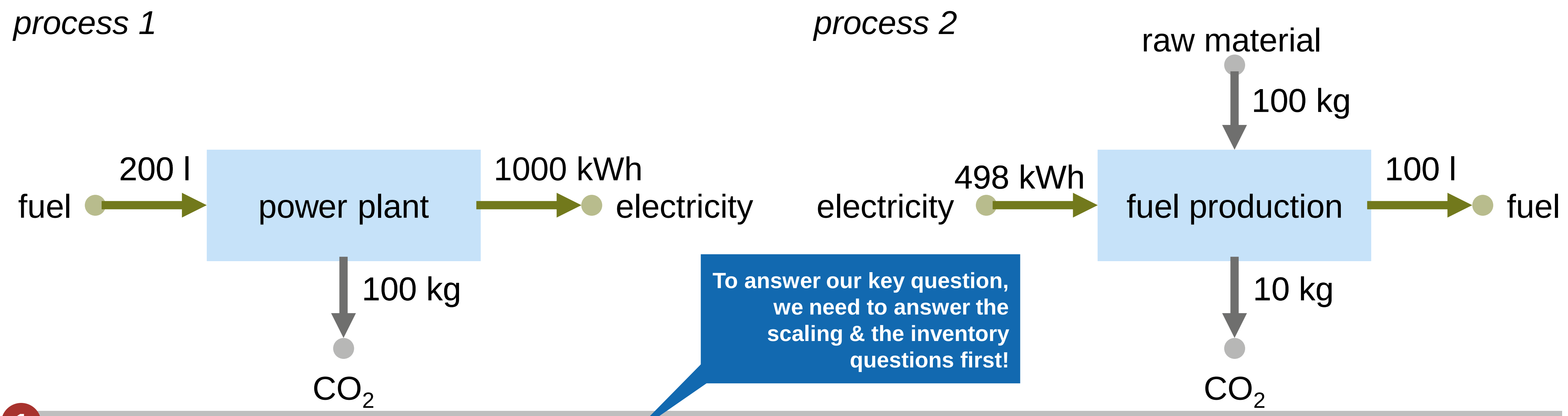
DIN EN ISO 14040:2021-02.

Capturing mass and energy flows of the system

elementary flows	(intermediate) product flows
flows entering/exiting the technosphere from/to the environment	flow between unit processes within the technosphere



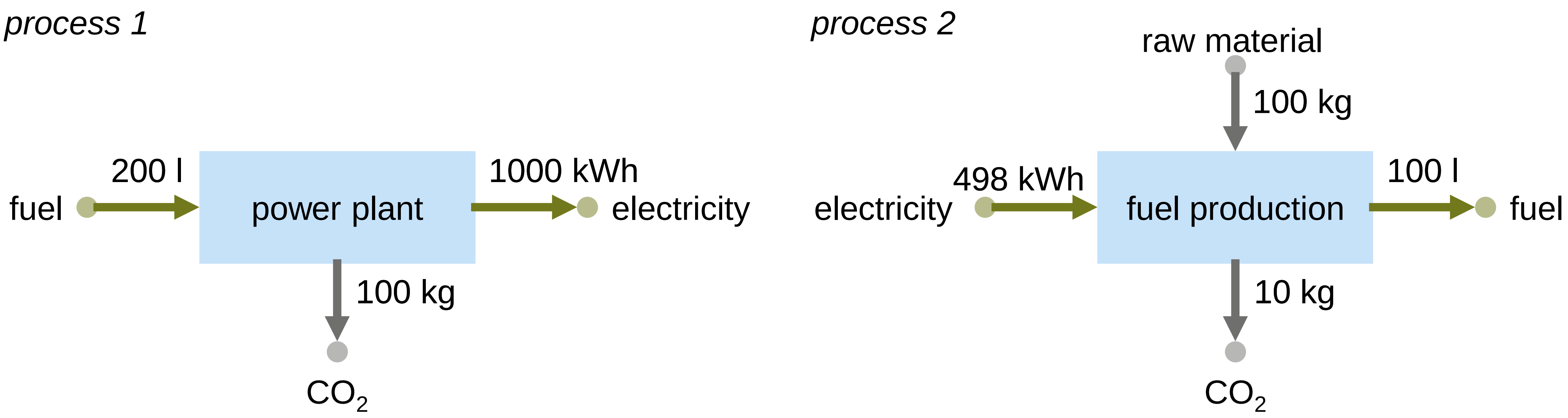
Inventory analysis as a linear system of equations
A hypothetical example



1. **How do we scale the two processes to achieve 1000 kWh net-generation of electricity?**
2. **How much CO_2 is emitted to produce 1000 kWh of electricity?**
3. **Key question: What is the global warming impact of producing 1000 kWh of electricity?**

adapted from: Heijungs, Reinout (2002) *The use of matrix perturbation theory for addressing sensitivity and uncertainty issues in LCA*. In *Proceedings of the Fifth International Conference on EcoBalance: practical tools and thoughtful principles for sustainability*, Nov. 6-Nov. 8, 2002 Tsukuba, Japan. Tokyo: Society of Non-Traditional Technology, pp. 77–81.

Inventory analysis as a linear system of equations
A hypothetical example



	power plant	fuel production	functional unit
electricity	1000 kWh	- 498 kWh	1000 kWh
fuel	- 200 l	100 l	-
CO_2	100 kg	10 kg	-
raw material	-	- 100 kg	-

adapted from: Heijungs, Reinout (2002) *The use of matrix perturbation theory for addressing sensitivity and uncertainty issues in LCA*. In *Proceedings of the Fifth International Conference on EcoBalance: practical tools and thoughtful principles for sustainability*, Nov. 6-Nov. 8, 2002 Tsukuba, Japan. Tokyo: Society of Non-Traditional Technology, pp. 77–81.

Inventory analysis as a linear system of equations
A hypothetical example

		power plant	fuel production	functional unit
product flows	electricity	1000 kWh	- 498 kWh	1000 kWh
	fuel	- 200 l	100 l	-
environmental flows	CO_2	100 kg	10 kg	-
	raw material	-	- 100 kg	-

technology matrix

$$\boldsymbol{A} = \begin{pmatrix} 1000 & -498 \\ -200 & 100 \end{pmatrix}$$

environmental intervention matrix

$$\boldsymbol{B} = \begin{pmatrix} 100 & 10 \\ 0 & -100 \end{pmatrix}$$

functional unit

$$\boldsymbol{f} = \begin{pmatrix} 1000 \\ 0 \end{pmatrix}$$

adapted from: Heijungs, Reinout (2002) *The use of matrix perturbation theory for addressing sensitivity and uncertainty issues in LCA*. In *Proceedings of the Fifth International Conference on EcoBalance: practical tools and thoughtful principles for sustainability*, Nov. 6-Nov. 8, 2002 Tsukuba, Japan. Tokyo: Society of Non-Traditional Technology, pp. 77–81.

Inventory analysis as a linear system of equations
A hypothetical example

		power plant	fuel production		functional unit
product flows	electricity	1000 kWh s_1	- 498 kWh s_2	=	1000 kWh
	fuel	- 200 l s_1	+ 100 l s_2	=	0
environmental flows	CO_2	100 kg	10 kg		-
	raw material	-	- 100 kg		-

technology matrix

$$\boldsymbol{A} = \begin{pmatrix} 1000 & -498 \\ -200 & 100 \end{pmatrix}$$

environmental intervention matrix

$$\boldsymbol{B} = \begin{pmatrix} 100 & 10 \\ 0 & -100 \end{pmatrix}$$

functional unit

$$\boldsymbol{f} = \begin{pmatrix} 1000 \\ 0 \end{pmatrix}$$

1

How do we scale the two processes to achieve 1000 kWh net-generation of electricity?

$$\boldsymbol{A} \cdot \boldsymbol{s} = \boldsymbol{f} \quad \Leftrightarrow \boldsymbol{s} = \boldsymbol{A}^{-1} \cdot \boldsymbol{f}$$

process scaling factors: how often is every process performed to obtain the functional unit?

adapted from: Heijungs, Reinout (2002) *The use of matrix perturbation theory for addressing sensitivity and uncertainty issues in LCA*. In *Proceedings of the Fifth Intern… al tools and thoughtful principles for sustainability*, Nov. 6-Nov. 8, 2002 Tsukuba, Japan. Tokyo: Society of Non-Traditional Techn…

Inventory analysis as a linear system of equations
A hypothetical example

technology matrix

$$\boldsymbol{A} = \begin{pmatrix} 1000 & -498 \\ -200 & 100 \end{pmatrix}$$

environmental intervention matrix

$$\boldsymbol{B} = \begin{pmatrix} 100 & 10 \\ 0 & -100 \end{pmatrix}$$

functional unit

$$\boldsymbol{f} = \begin{pmatrix} 1000 \\ 0 \end{pmatrix}$$

1

How do we scale the two processes to achieve 1000 kWh net-generation of electricity?

$$\boldsymbol{A} \cdot \boldsymbol{s} = \boldsymbol{f}$$

process scaling factors: how often is every process performed to obtain the functional unit?

$$\Leftrightarrow \boldsymbol{s} = \boldsymbol{A}^{-1} \cdot \boldsymbol{f}$$

$$\Leftrightarrow \boldsymbol{s} = \begin{pmatrix} 1000 & -498 \\ -200 & 100 \end{pmatrix}^{-1} \cdot \begin{pmatrix} 1000 \\ 0 \end{pmatrix}$$

$$\Leftrightarrow \boldsymbol{s} = \begin{pmatrix} 250 \\ 500 \end{pmatrix}$$

← power plant process

← fuel production process

adapted from: Heijungs, Reinout (2002) *The use of matrix perturbation theory for addressing sensitivity and uncertainty issues in LCA*. In *Proceedings of the Fifth International Conference on EcoBalance: practical tools and thoughtful principles for sustainability*, Nov. 6-Nov. 8, 2002 Tsukuba, Japan. Tokyo: Society of Non-Traditional Technology, pp. 77–81.

Inventory analysis as a linear system of equations
A hypothetical example

technology matrix	*environmental intervention matrix*	*functional unit*	*process scaling factors*
$\boldsymbol{A} = \begin{pmatrix} 1000 & -498 \\ -200 & 100 \end{pmatrix}$	$\boldsymbol{B} = \begin{pmatrix} 100 & 10 \\ 0 & -100 \end{pmatrix}$	$\boldsymbol{f} = \begin{pmatrix} 1000 \\ 0 \end{pmatrix}$	$\boldsymbol{s} = \begin{pmatrix} 250 \\ 500 \end{pmatrix}$

2

How much CO_2 is emitted to produce 1000 kWh of electricity?

Intervention totals

$$\boldsymbol{g} = \boldsymbol{B} \cdot \boldsymbol{s}$$

The interventional matrix can include many more rows for CH_4, N_2O, …

$$\Leftrightarrow \boldsymbol{g} = \begin{pmatrix} 100 & 10 \\ 0 & -100 \end{pmatrix} \cdot \begin{pmatrix} 250 \\ 500 \end{pmatrix}$$

$$\Leftrightarrow \boldsymbol{g} = \begin{pmatrix} 30000 \\ -50000 \end{pmatrix} \begin{array}{l} \leftarrow \text{kg of } CO_2 \text{ emissions} \\ \leftarrow \text{raw material consumption} \end{array}$$

elementary flows!

adapted from: Heijungs, Reinout (2002) *The use of matrix perturbation theory for addressing sensitivity and uncertainty issues in LCA*. In *Proceedings of the Fifth International Conference on EcoBalance: practical tools and thoughtful principles for sustainability*, Nov. 6-Nov. 8, 2002 Tsukuba, Japan. Tokyo: Society of Non-Traditional Technology, pp. 77–81.

After this lecture, you are able to…

- conduct a life cycle assessment:
  ✓ draw process flow diagrams
  ✓ calculate energy and mass balances along a product life cycle
  – solve allocation problems
  – assess environmental impacts

- critically interpret life cycle assessment results

Example: The allocation problem

What is the functional unit?

How are impacts allocated?

multi-functional process

solar irradiation → **concentrated solar power** → power
→ heat

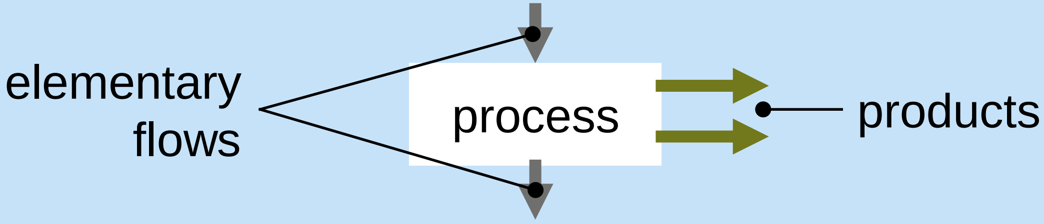
– 2 Functional units!

https://upload.wikimedia.org/wikipedia/commons/3/30/Parabolic_trough_solar_thermal_electric_power_plant_1.jpg

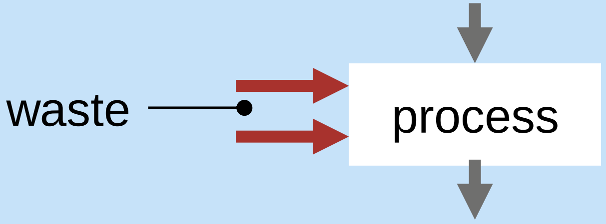
The allocation problem and multi-functionality

The allocation problem occurs in systems with multiple functions:

1 production of multiple products

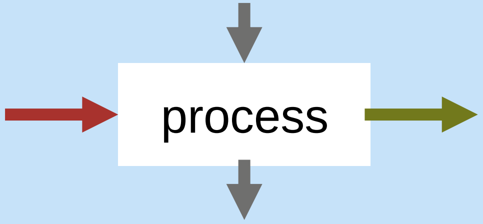


2 disposal of multiple waste streams

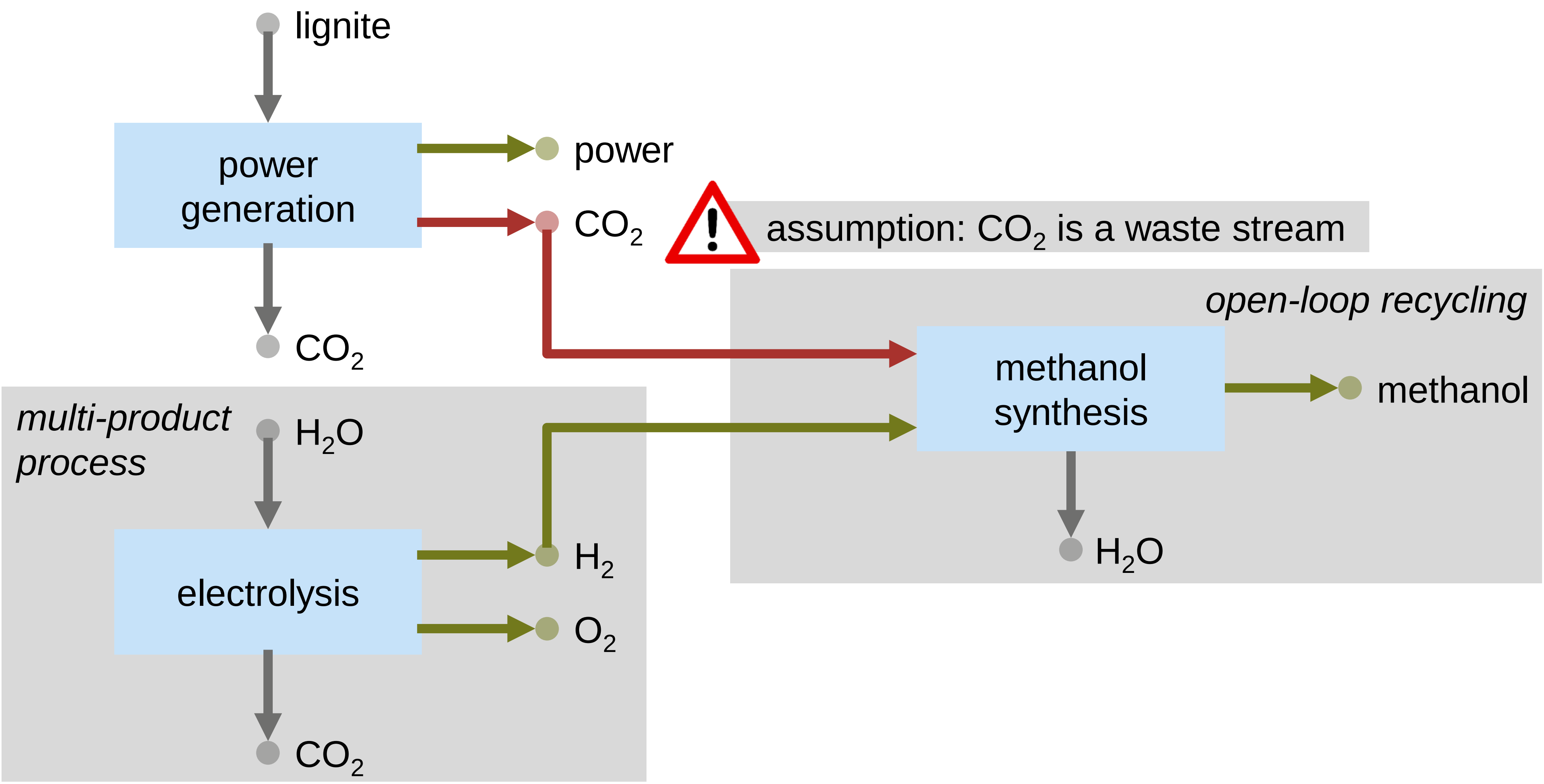


3 open loop recycling

production of products & disposal of waste



Example: Multi-functionality in Carbon Capture & Utilization



How to deal with multi-functionality
Solution approaches according to DIN EN ISO 14044

avoiding allocation

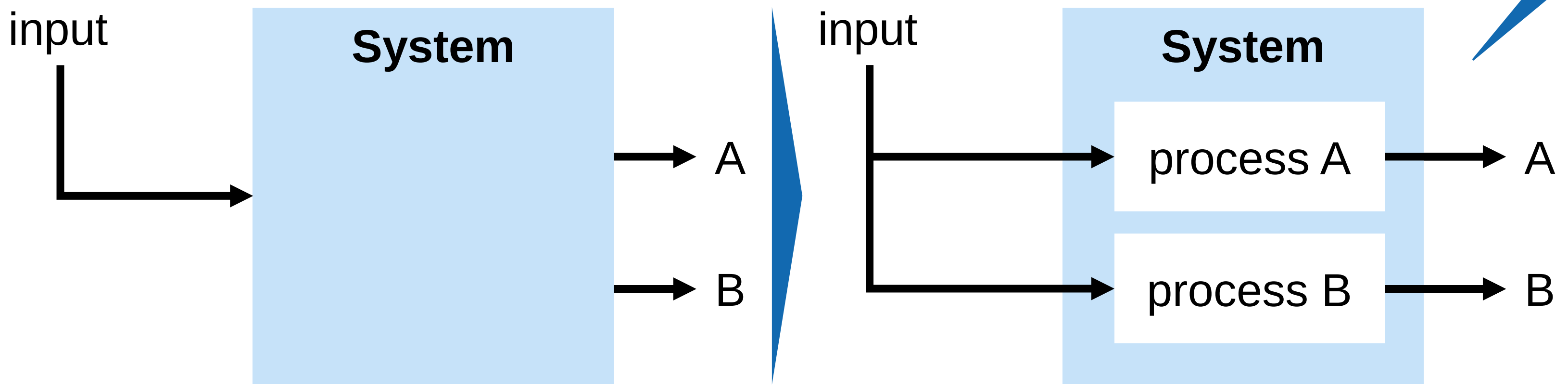
divide the system → expand the system → causation principle → proportionality

How to deal with multi-functionality
Solution approaches according to DIN EN ISO 14044

avoiding allocation

divide the system | expand the system | causation principle | proportionality

Divide, then assess separately.



! often impractical

How to deal with multi-functionality
Solution approaches according to DIN EN ISO 14044

avoiding allocation

divide the system | **expand the system** | causation principle | proportionality

1 basket of products

change the functional unit to include multiple functions

! unsatisfying set of bundled functions

2 avoided burden

impact credit for avoided processes

! an avoided process must exist
ambiguous choice of avoided process

How to deal with multi-functionality
Solution approaches according to DIN EN ISO 14044

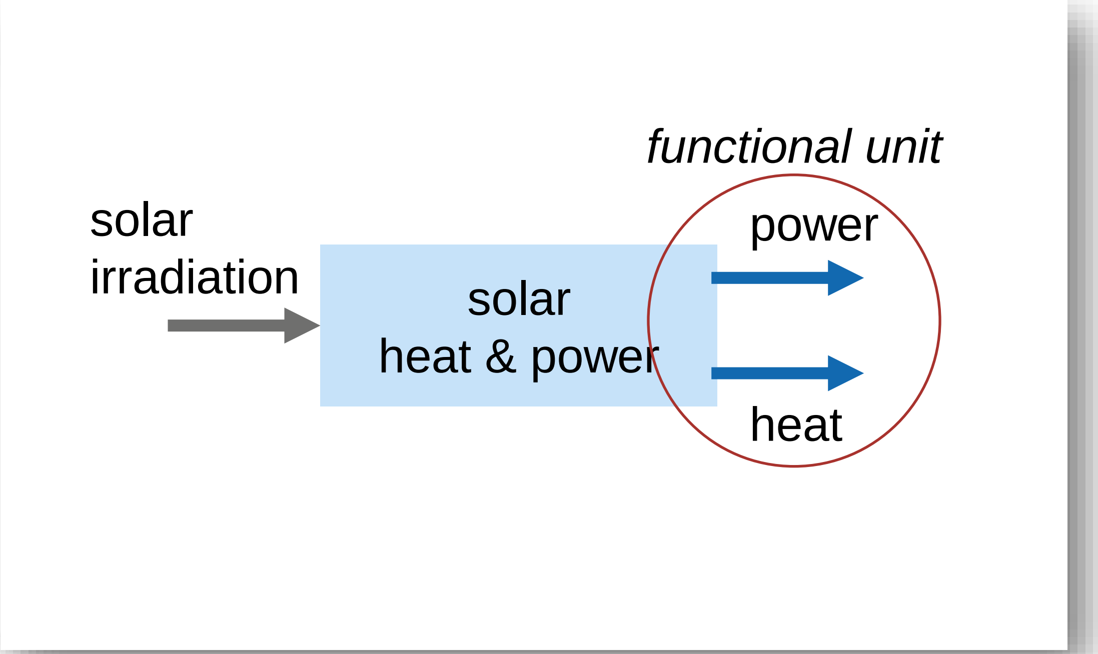
avoiding allocation

divide the system | **expand the system** | causation principle | proportionality

1 basket of products

change the functional unit to include multiple functions

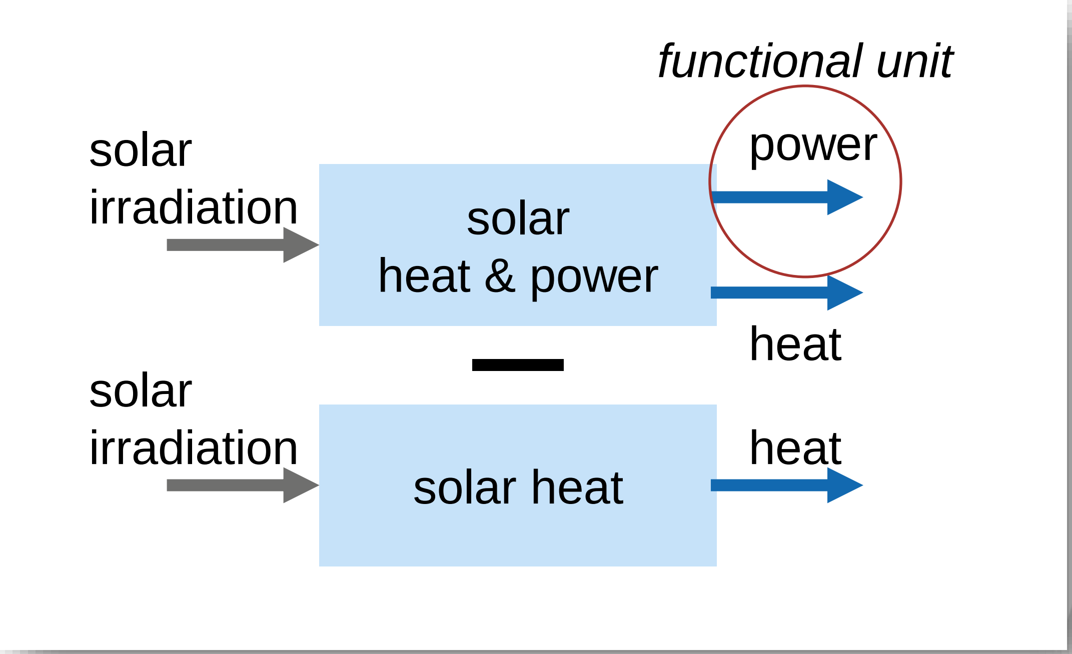
! unsatisfying set of bundled functions



How to deal with multi-functionality
Solution approaches according to DIN EN ISO 14044

avoiding allocation

divide the system | **expand the system** | causation principle | proportionality



2 avoided burden

impact credit for avoided processes

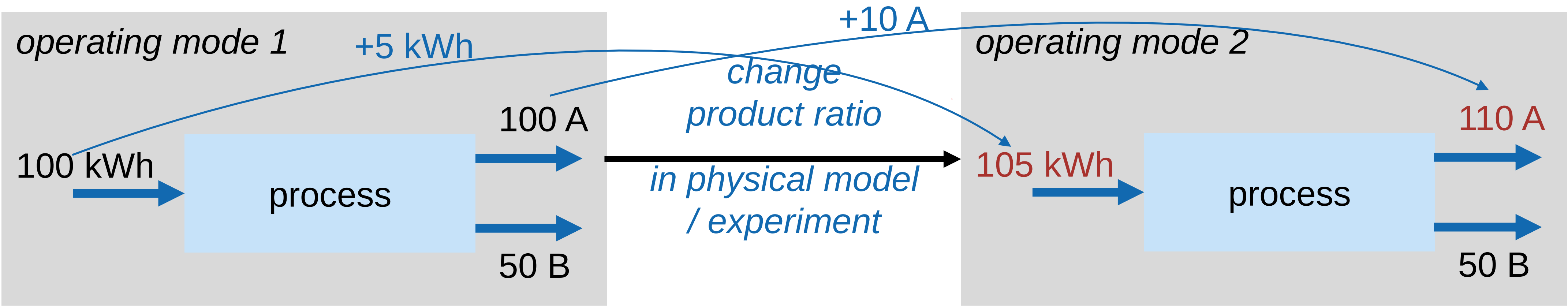
! an avoided process must exist
ambiguous choice of avoided process

How to deal with multi-functionality
Solution approaches according to DIN EN ISO 14044

avoiding allocation

divide the system → expand the system → **causation principle** → proportionality

Applicable to flexible co-production, i.e., processes with multiple products and flexible product ratios.



allocation

+5 kWh for +10 A → 50 kWh for 100 A → 50 kWh for 50 B

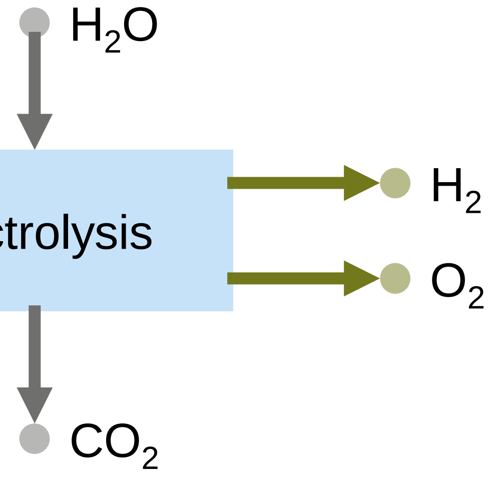
How to deal with multi-functionality
Solution approaches according to DIN EN ISO 14044

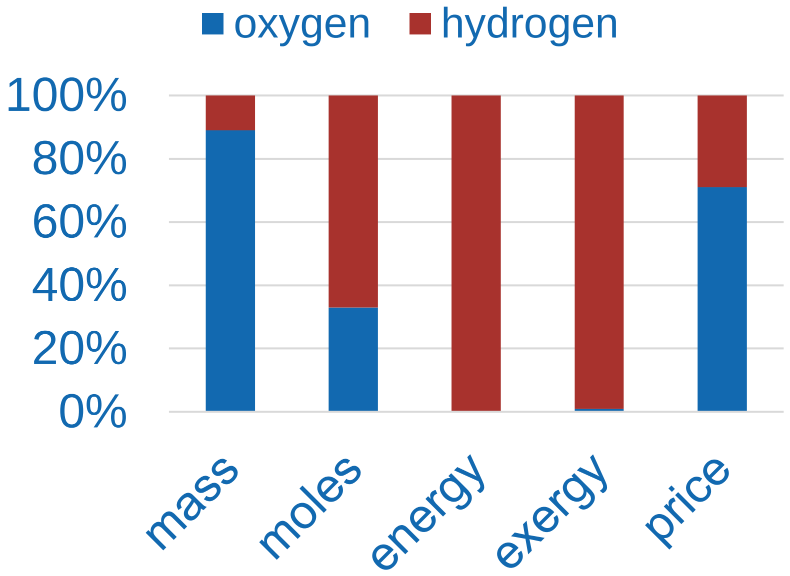
avoiding allocation

divide the system → expand the system → causation principle → **proportionality**

allocation based on

- mass
- amount of substance
- energy (lower heating value)
- exergy
- economic value





exergy: chemical exergy at standard conditions,
reference: average composition of atmosphere

Allocation: Summary

Causes	Remedies

Causes

1. production of **multiple products** — process
2. disposal of **multiple waste streams** — process
3. production of **products** & disposal of **waste** — process

Remedies

avoiding allocation

- divide the system
- expand the system
- causation principle
- proportionality

Allocation introduces subjectivity!

From allocation problem to optimization opportunity the perspective of matrix-based LCA

Allocation

$$\boldsymbol{A} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \begin{array}{l} \leftarrow \text{electricity} \\ \leftarrow \text{heat} \end{array}$$

$(n \times m)$ Technology matrix $\boldsymbol{A}$

with $n > m$

= „**more functions than processes**“

allocation problem due to overdetermined system of equations

Optimization

$$\boldsymbol{A} = \begin{array}{cc} \text{PV} & \text{wind} \\ \downarrow & \downarrow \\ (a_1 & a_2) \end{array} \leftarrow \text{electricity}$$

$(\mathrm{n} \times m)$ Technology matrix $\boldsymbol{A}$

with $n < m$

= „**more processes than functions**“

optimization opportunity due to underdetermined system of equations

Matrix-based life-cycle optimization: The technology choice model (TCM)

$(n \times m)$ Technology matrix $\boldsymbol{A}$
with $n < m$
= „**more processes than functions** “

Which processes to use to satisfy demand (functional unit)?

$$\min_{\boldsymbol{s}} \quad z = \boldsymbol{\kappa}^T \cdot \boldsymbol{F} \cdot \boldsymbol{s} \quad \leftarrow \text{cost for factor requirements}$$

s.t.

LCA constraints

$$\boldsymbol{A} \cdot \boldsymbol{s} = \boldsymbol{f} \quad \leftarrow \text{producing the functional unit } \boldsymbol{f}$$

$$\boldsymbol{h} = \boldsymbol{Q} \cdot \boldsymbol{B} \cdot \boldsymbol{s} \quad \leftarrow \text{resulting in category totals } \boldsymbol{h}$$

additional constraints

$$\boldsymbol{s} \geq \boldsymbol{0} \quad \leftarrow \text{processes have a defined direction}$$

$$\boldsymbol{F} \cdot \boldsymbol{s} \leq \boldsymbol{c} \quad \leftarrow \text{factor requirement matrix } \boldsymbol{F}:$$

inputs to processes (e.g., labor, taxes, resources)
limited by maximum available amount $\boldsymbol{c}$

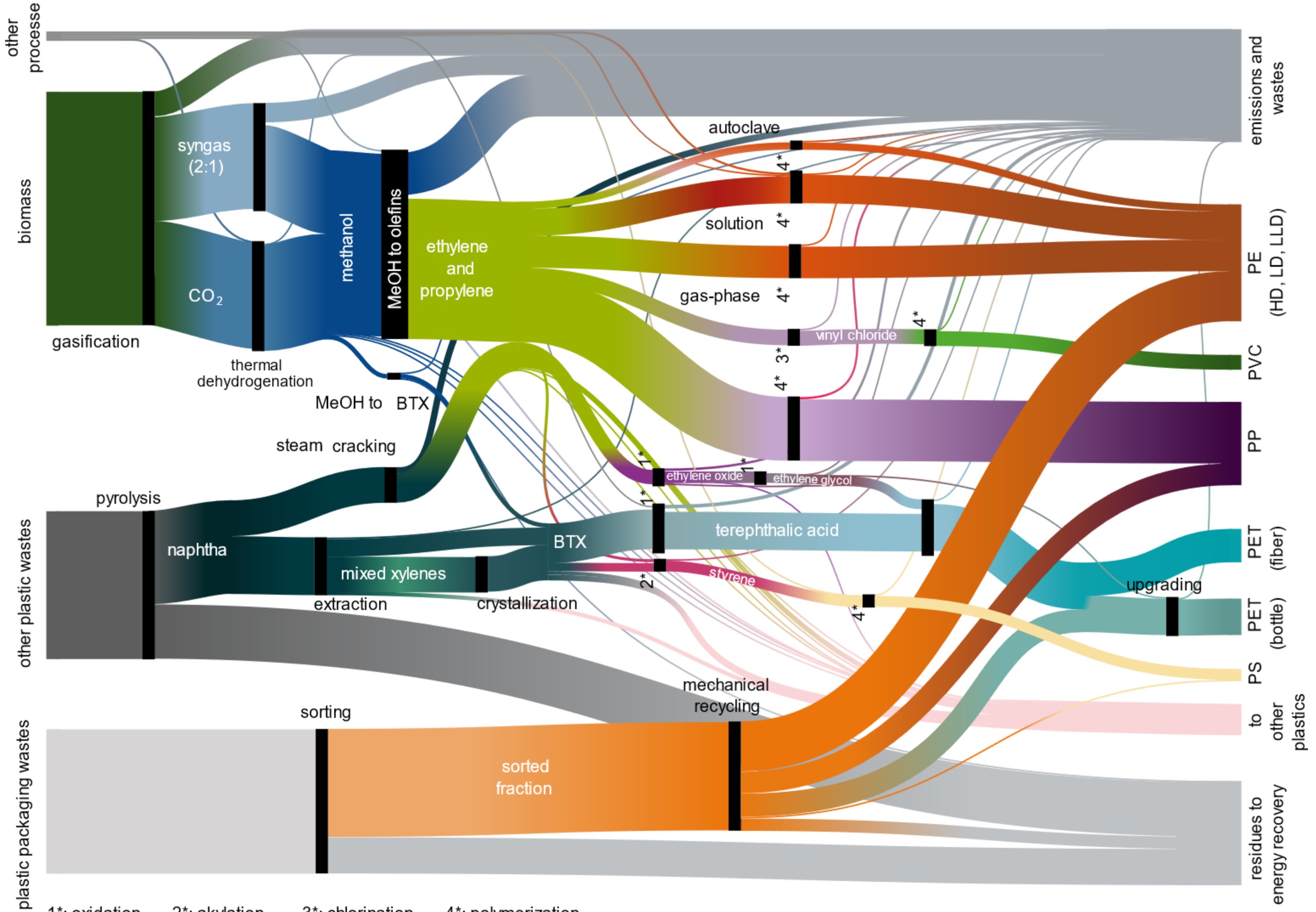
…

category totals (see slides on *Impact assessment*) can be considered in objective function or additional constraints as factor requirements!

$$\boldsymbol{\kappa} \in \mathbb{R}^o, \quad \boldsymbol{F} \in \mathbb{R}^{o \times m}, \quad \boldsymbol{s} \in \mathbb{R}^m_{\geq 0}, \quad \boldsymbol{A} \in \mathbb{R}^{n \times m}, \quad \boldsymbol{f} \in \mathbb{R}^n, \quad \boldsymbol{c} \in \mathbb{R}^o$$

Kätelhön A, Bardow A, Suh S. Stochastic Technology Choice Model for Consequential Life Cycle Assessment. Environ Sci Technol 2016;50(23):12575–83.

Mass flows of a net-zero circular plastics industry



1*: oxidation 2*: akylation 3*: chlorination 4*: polymerization
PS: polystyrene PET: polyethylene terephthalate PP: polypropylene PVC: polyvinylchloride
PE: polyethylene HD: high-density LD: low-density LLD: low linear-density

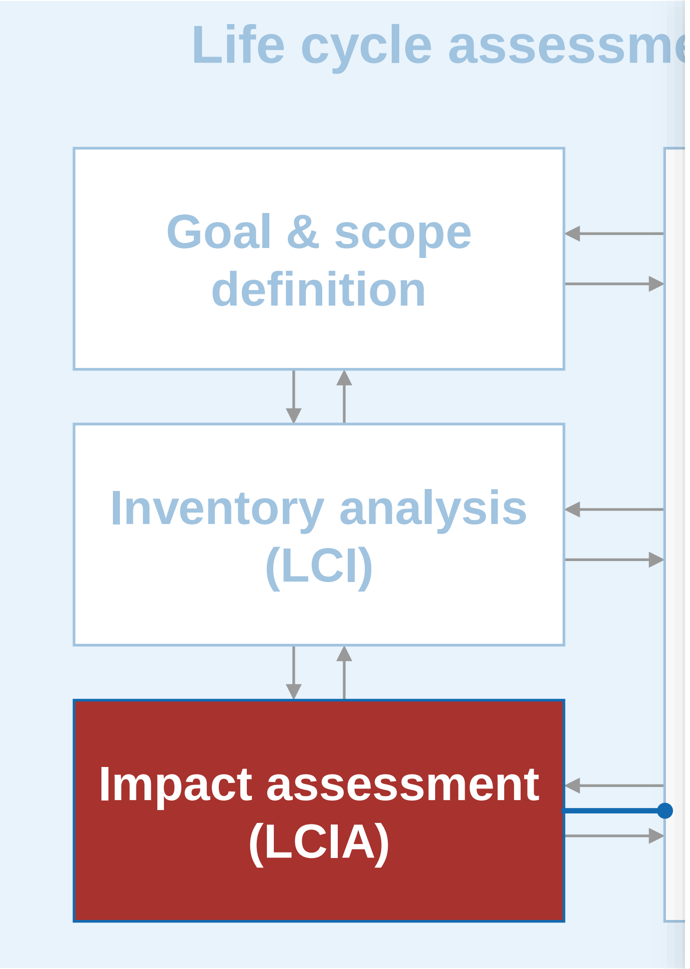
Meys R, Kätelhön A, Bachmann M, Winter B, Zibunas C, Suh S, Bardow A. Achieving net-zero greenhouse gas emission plastics by a circular carbon economy. Science 2021;374(6563):71–6.

After this lecture, you are able to…

- conduct a life cycle assessment:
  ✓ draw process flow diagrams
  ✓ calculate energy and mass balances along a product life cycle
  ✓ solve allocation problems
  – assess environmental impacts

- critically interpret life cycle assessment results

Stages of life cycle assessment (DIN EN ISO 14040)



What are potential environmental impacts?

must haves

- select **impact categories**, indicators & characterization models
- **classification**: Which environmental flow contributes to which impact category?
- **characterization**: How much environmental impact?

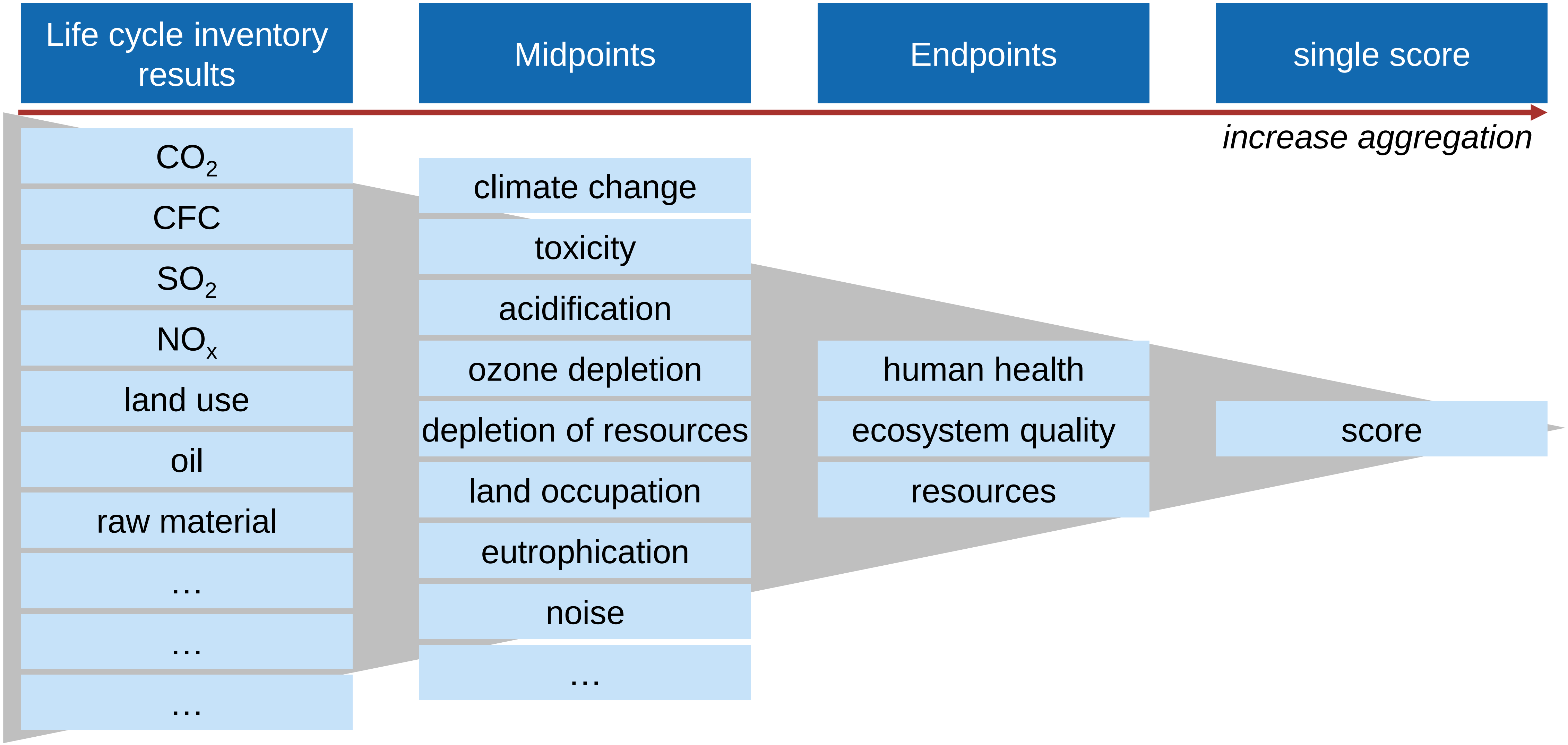
optional

- **normalization** with reference value
- **ordering/grouping** of impact categories
- **weighting**, e.g., single score indicators

subjective!

DIN EN ISO 14040:2021-02.

Impact assessment – Aggregation using impact categories



Impact assessment – Impact categories for energy systems

weighting Problem!

Life cycle inventory results	Midpoints	Endpoints	single score
CO_2	climate change		
CFC	toxicity		
SO_2	acidification		
NO_x	ozone depletion	human health	
land use	depletion of resources	ecosystem quality	score
oil	land occupation	resources	
raw material	eutrophication		
…	noise		
…	…		
…			

increase aggregation

traditional

increasingly important

smell, landscape…

-w1

-w2

Status of impact categories

Table 2 Impact categories recommended by European Commission's Joint Research Centre in the European context. For the corresponding LCIA models, please refer to ref. 34 and references therein. Quality levels: I: recommended and satisfactory, II: recommended but in need of some improvement, III: recommended but to use with caution

Quality level I ★★★★	Quality level II ★★★☆	Quality level III ★★☆☆
– Global warming[a] – Ozone depletion – Particulate matter/respiratory inorganics (I/II)	– Ionizing radiation, human health – Photochemical ozone formation – Acidification – Eutrophication, terrestrial and aquatic – Resource depletion, mineral and fossil – Human toxicity, cancer and non-cancer effects (II/III) – Ecotoxicity, freshwater (II/III)	– Land use – Resource depletion, water

[a] In LCA, the impact category 'global warming' is often called 'climate change'.[8]

Assen, Niklas von der; Voll, Philip; Peters, Martina; Bardow, André (2014): *Life cycle assessment of CO2 capture and utilization: a tutorial review*. In *Chemical Society reviews* 43 (23), pp. 7982–7994.

Impact assessment as a linear system of equations
A hypothetical example

technology matrix

$$A = \begin{pmatrix} 1000 & -498 \\ -200 & 100 \end{pmatrix}$$

environmental intervention matrix

$$B = \begin{pmatrix} 100 & 10 \\ 0 & -100 \end{pmatrix}$$

functional unit

$$f = \begin{pmatrix} 1000 \\ 0 \end{pmatrix}$$

process scaling factors

$$s = \begin{pmatrix} 250 \\ 500 \end{pmatrix}$$

3

Key question: What is the global warming impact of producing 1000 kWh of electricity?

Intervention totals

$$g = B \cdot s$$

$$\begin{array}{cccl} & CO_2 & \text{raw material} & \\ & \downarrow & \downarrow & \\ Q = & (1 & 0) & \leftarrow \text{global warming} \end{array}$$

rows: impact categories, columns: elementary flows

Characterization matrix: How much do elementary flows contribute to impact categories?

$$h = Q \cdot g$$

Category totals

e.g.

$$\begin{array}{cccccl} & CO_2 & CH_4 & N_2O & & \\ & \downarrow & \downarrow & \downarrow & & \\ Q = & \Big(1 & 25 & 298 & \ldots \Big) & \leftarrow \text{global warming} \\ & \ldots & \ldots & \ldots & \ldots & \leftarrow \text{acidification,}\ldots \end{array}$$

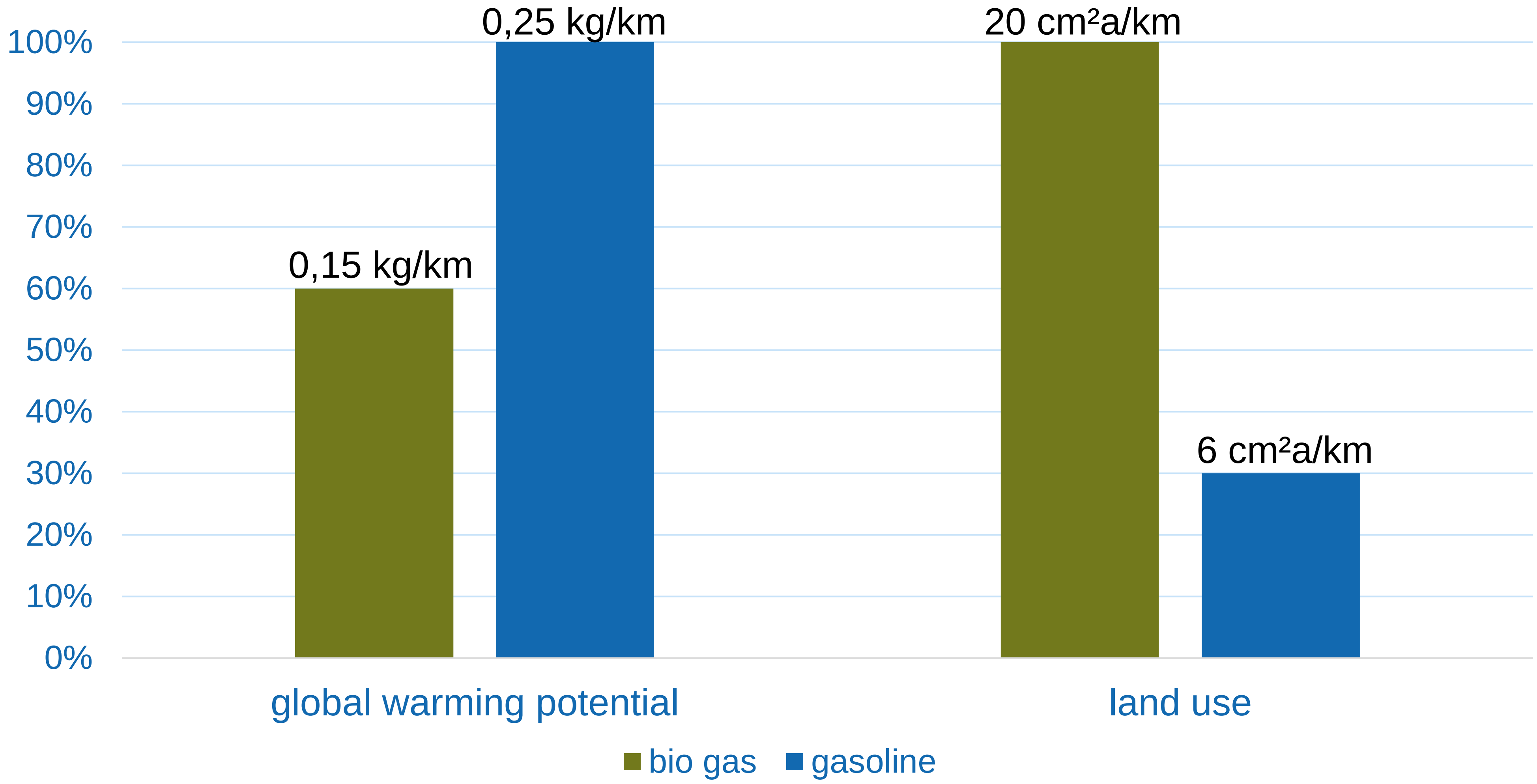
adapted from: Heijun… *…turbation theory for addr… …ncertai… International Conference on EcoBalance: practical tools and thoughtful principles for s…* …v. 8, 20… Technology, pp. 77–81.

Summary: Matrix-based LCA

symbol	name	dimensions (rows x columns)	formula
$\boldsymbol{f}$	functional unit	product flows $\times$ 1	-
$\boldsymbol{A}$	technology matrix	product flows $\times$ processes	-
$\boldsymbol{s}$	process scaling matrix	processes $\times$ 1	$\boldsymbol{s} = \boldsymbol{A}^{-1} \cdot \boldsymbol{f}$
$\boldsymbol{B}$	intervention matrix	environmental flows $\times$ processes	-
$\boldsymbol{g}$	intervention totals	environmental flows $\times$ 1	$\boldsymbol{g} = \boldsymbol{B} \cdot \boldsymbol{s}$
$\boldsymbol{Q}$	characterization matrix	categories $\times$ environmental flows	-
$\boldsymbol{h}$	category totals	categories $\times$ 1	$\boldsymbol{h} = \boldsymbol{Q} \cdot \boldsymbol{g}$

adapted from: Heijungs, Reinout (2002) *The use of matrix perturbation theory for addressing sensitivity and uncertainty issues in LCA*. In *Proceedings of the Fifth International Conference on EcoBalance: practical tools and thoughtful principles for sustainability*, Nov. 6-Nov. 8, 2002 Tsukuba, Japan. Tokyo: Society of Non-Traditional Technology, pp. 77–81.

Example: Biogas vs. gasoline

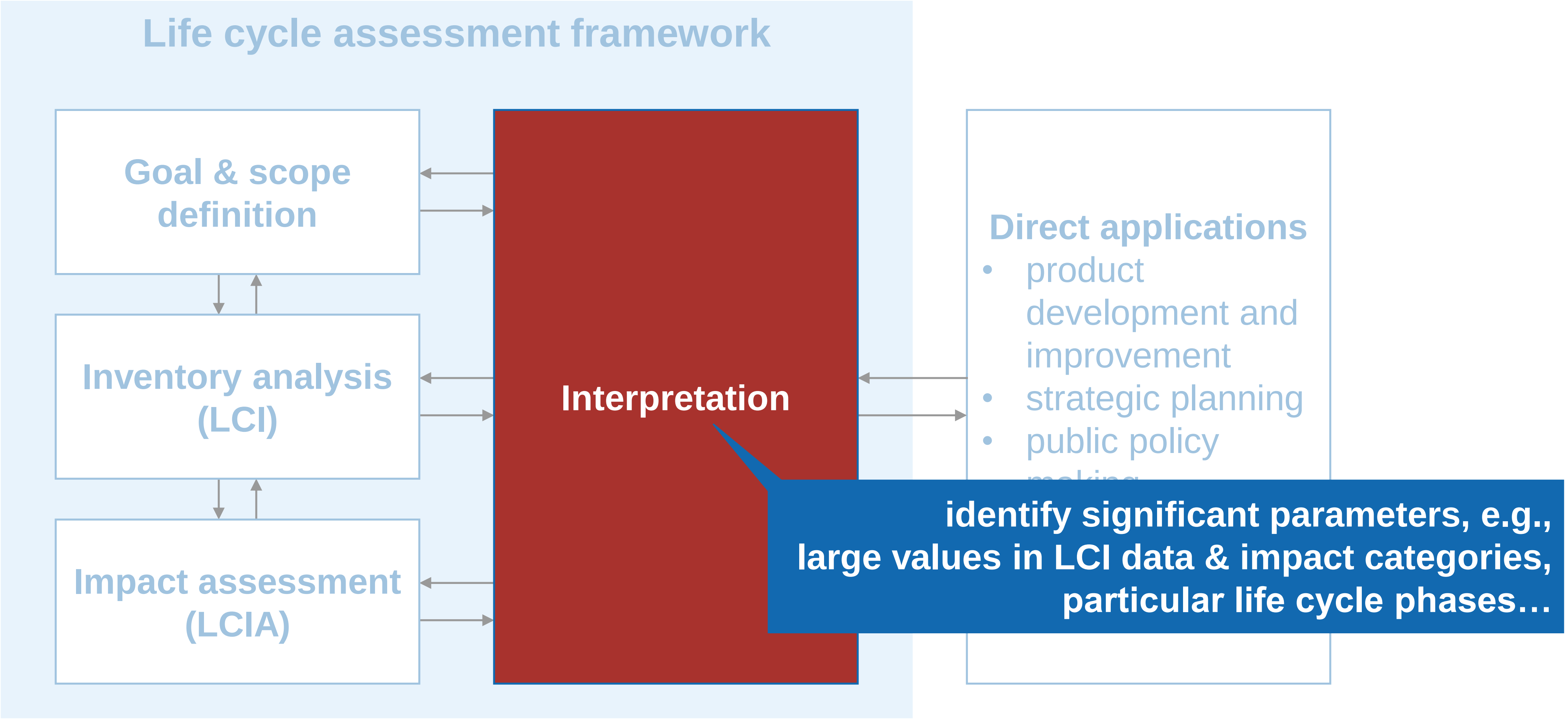


After this lecture, you are able to…

- ✓ conduct a life cycle assessment:
  - ✓ draw process flow diagrams
  - ✓ calculate energy and mass balances along a product life cycle
  - ✓ solve allocation problems
  - ✓ assess environmental impacts

- critically interpret life cycle assessment results

Stages of life cycle assessment (DIN EN ISO 14040)

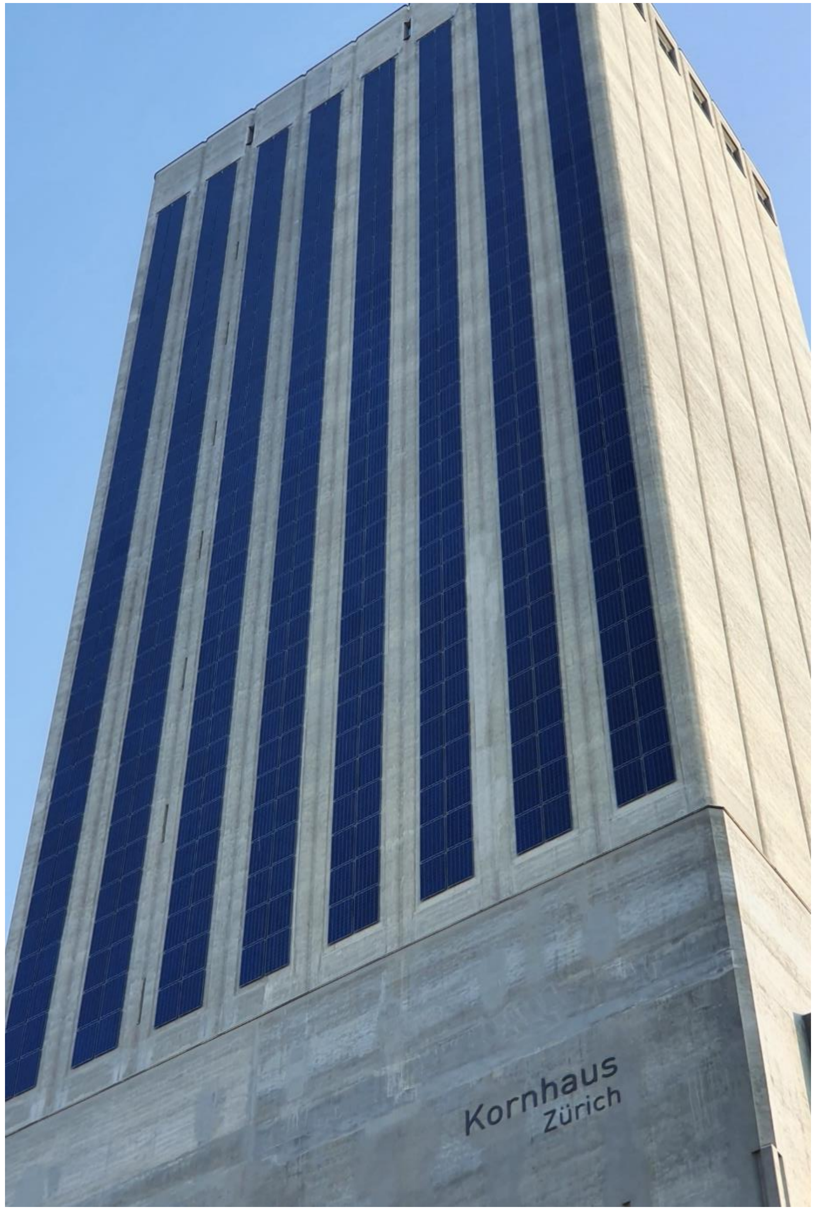


DIN EN ISO 14040:2021-02.

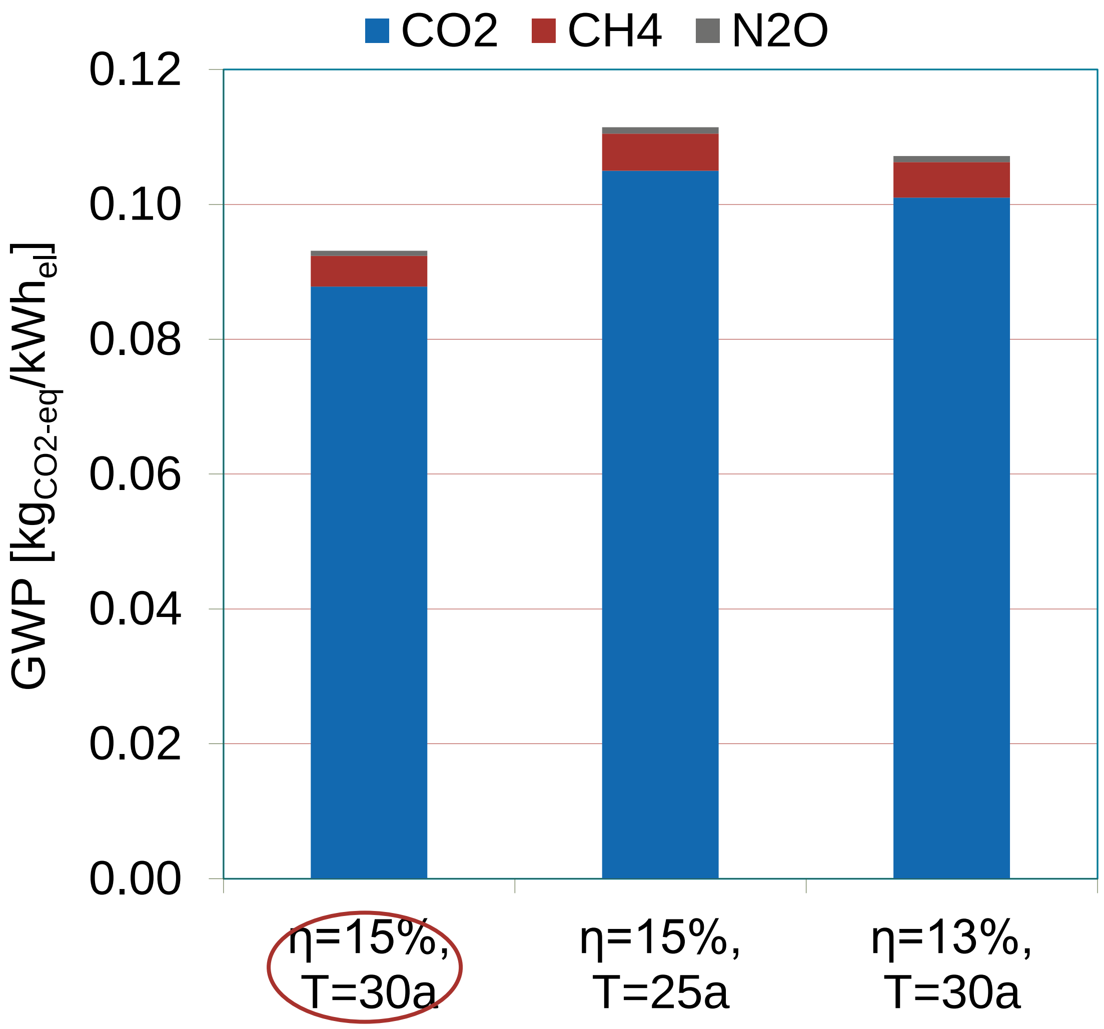
Example: Photovoltaic power generation

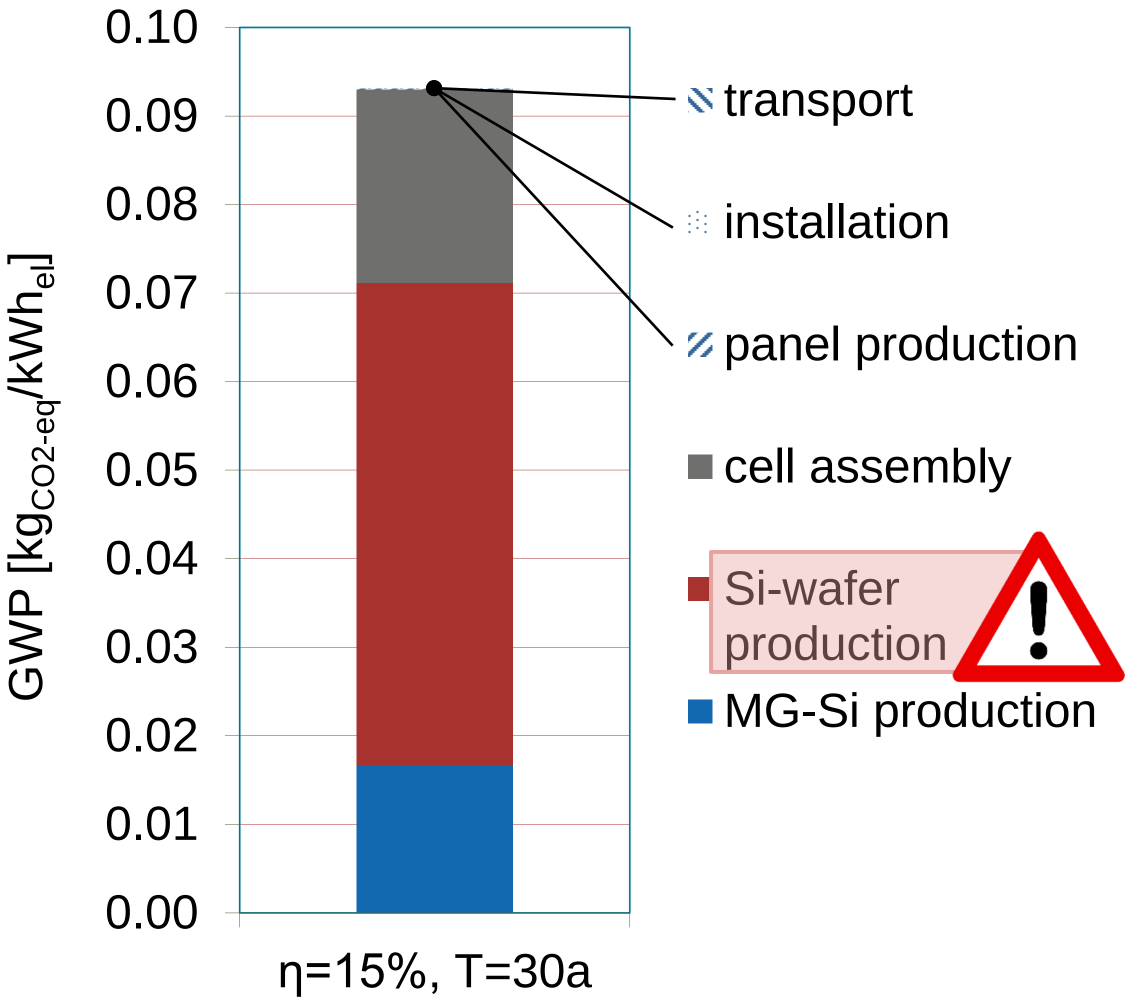
Objective:
Determine the Global Warming Potential (GWP) of PV in Zurich.

Assumptions:
- full life cycle of polycrystalline PV unit
- 30 year lifespan
- $\eta = 15\ \%$
- Solar irradiation $1100\ \mathrm{kWh/m^2a}$
- performance ration: $75\ \%$



Impact assessment – Greenhouse gas emissions





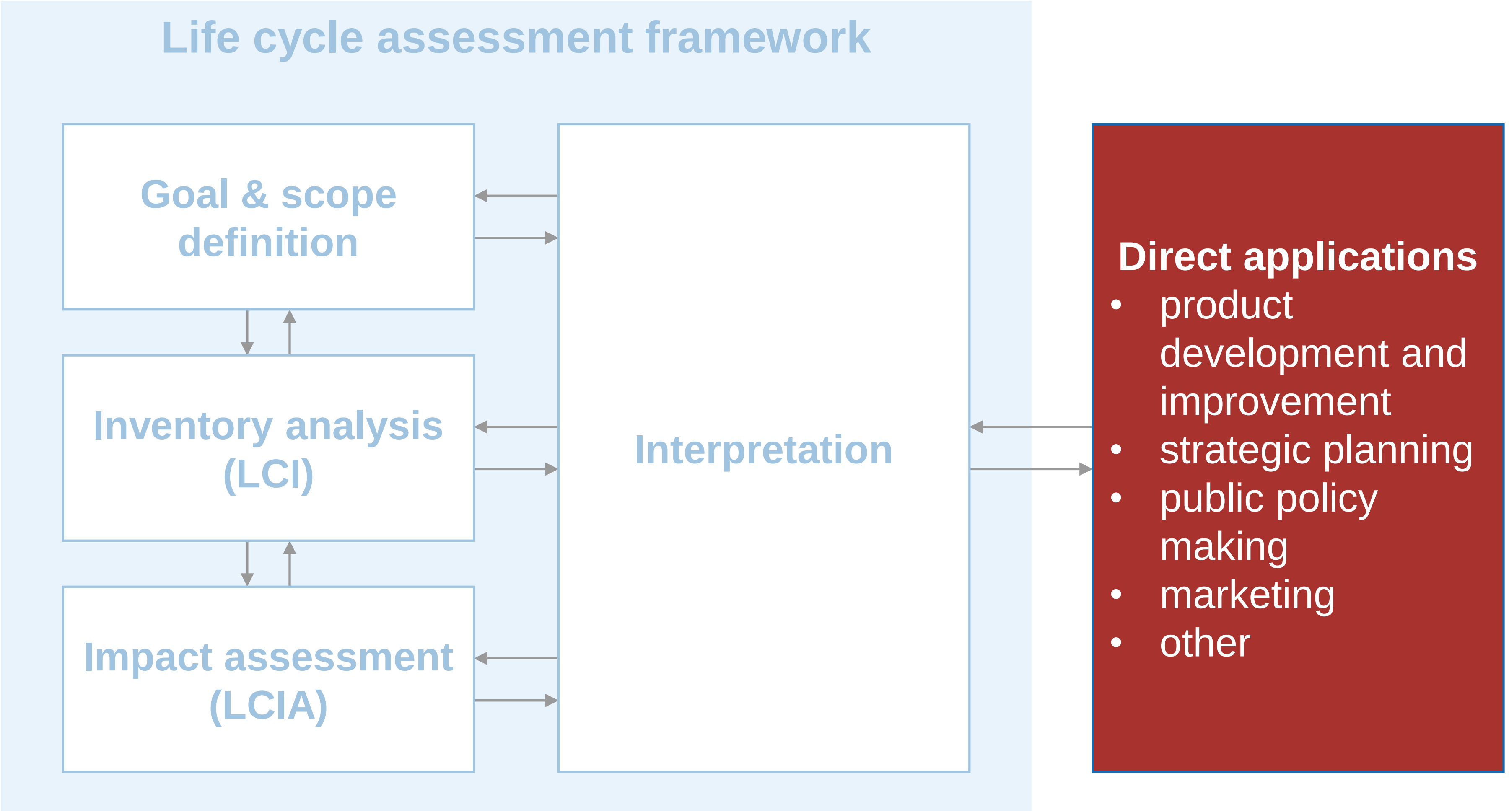
Interpretation

Consider LCI & LCIA results to **answer the research question** of the goal & scope definition.

Present a **complete** and **consistent** presentation of the results, including **sensitivity analyses**.

The interpretation should include a critical **conclusion**, **limitations**, and **recommendations**.

Stages of life cycle assessment (DIN EN ISO 14040)



DIN EN ISO 14040:2021-02.

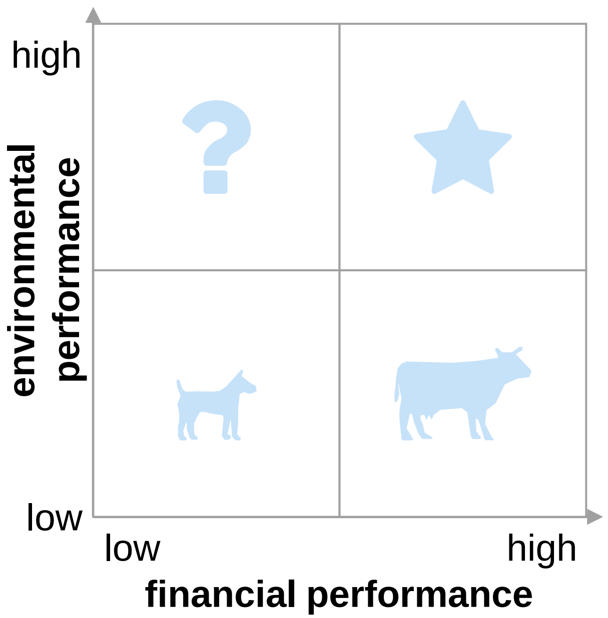
What is LCA good for?

- comparing environmental impacts of technologies with the same function
- identifying critical phases in the life cycle
- marketing, eco-labels, taxes

- considering the effects of failures
- research questions requiring spatial resolution
- social implications are missing

Applications

Marketing & Eco-controlling

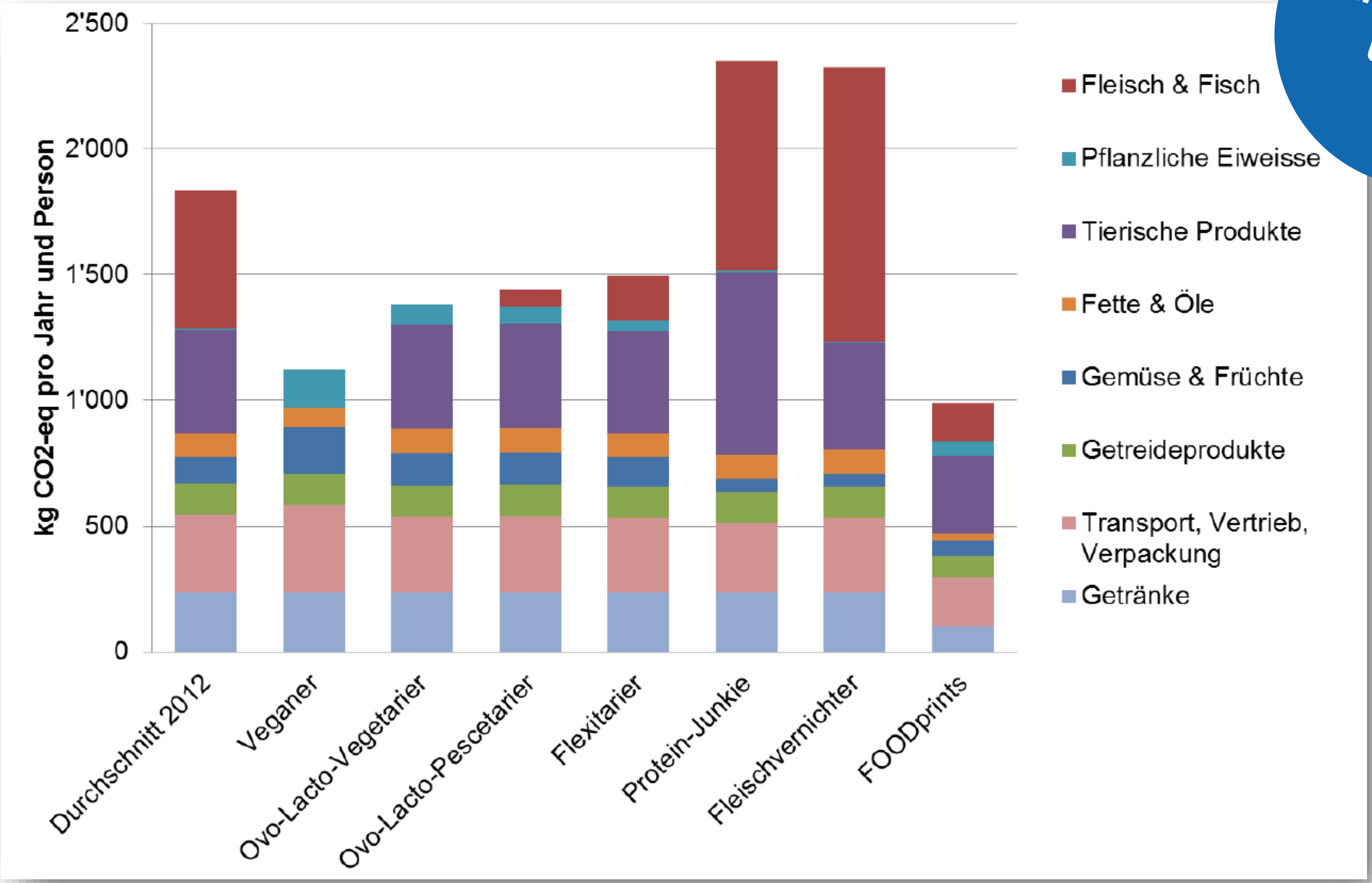


eco-labels

policy

- taxation?
- emission allowances?
- bio fuels EU:
  -35% / -60% life cycle CO_2-reductions compared to fossil fuels

Comparative LCA diets

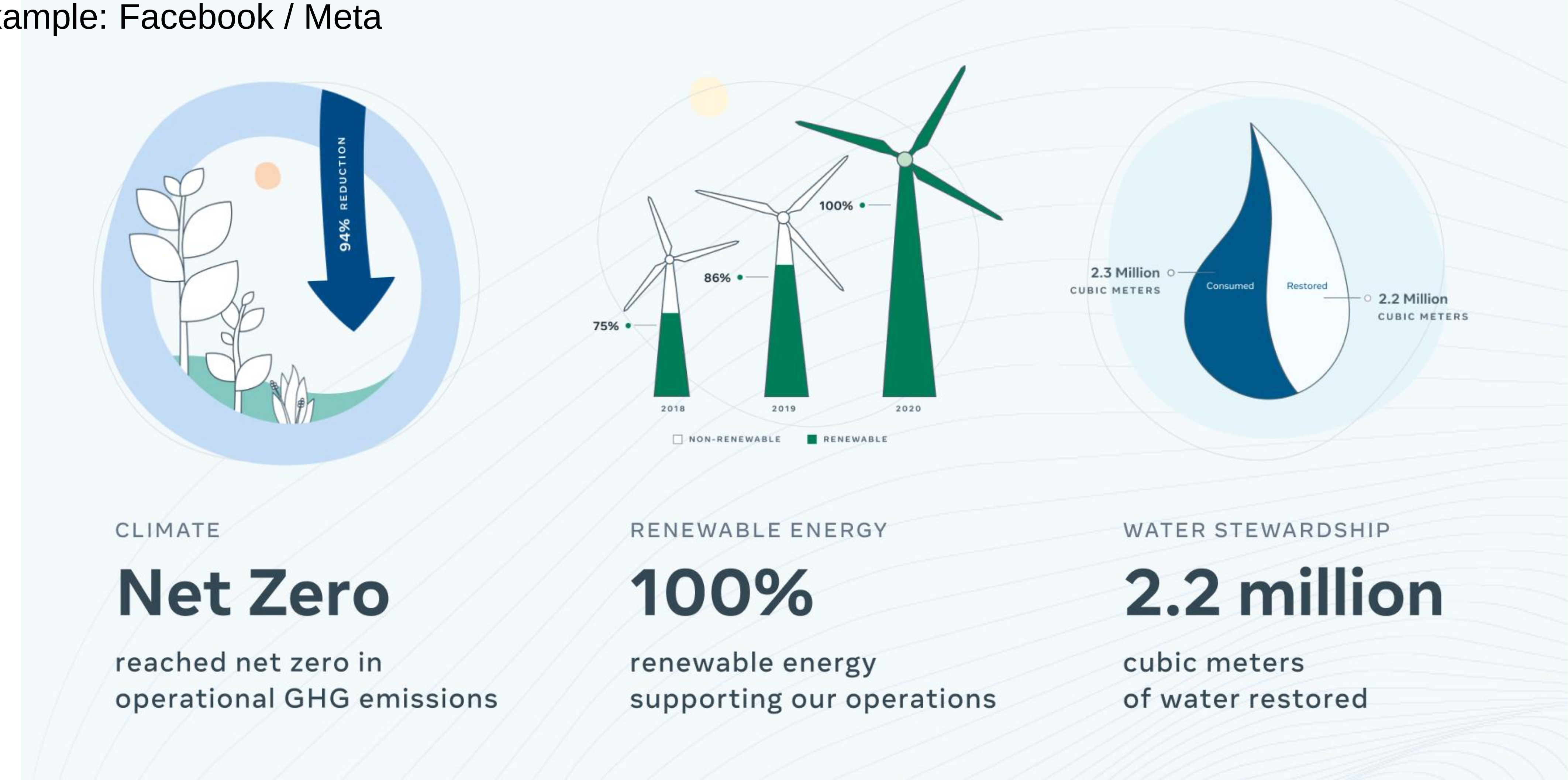


functional unit?

www.esu-services.ch/fileadmin/download/jungbluth-2015-Ernaehrungsstile-WWF.pdf

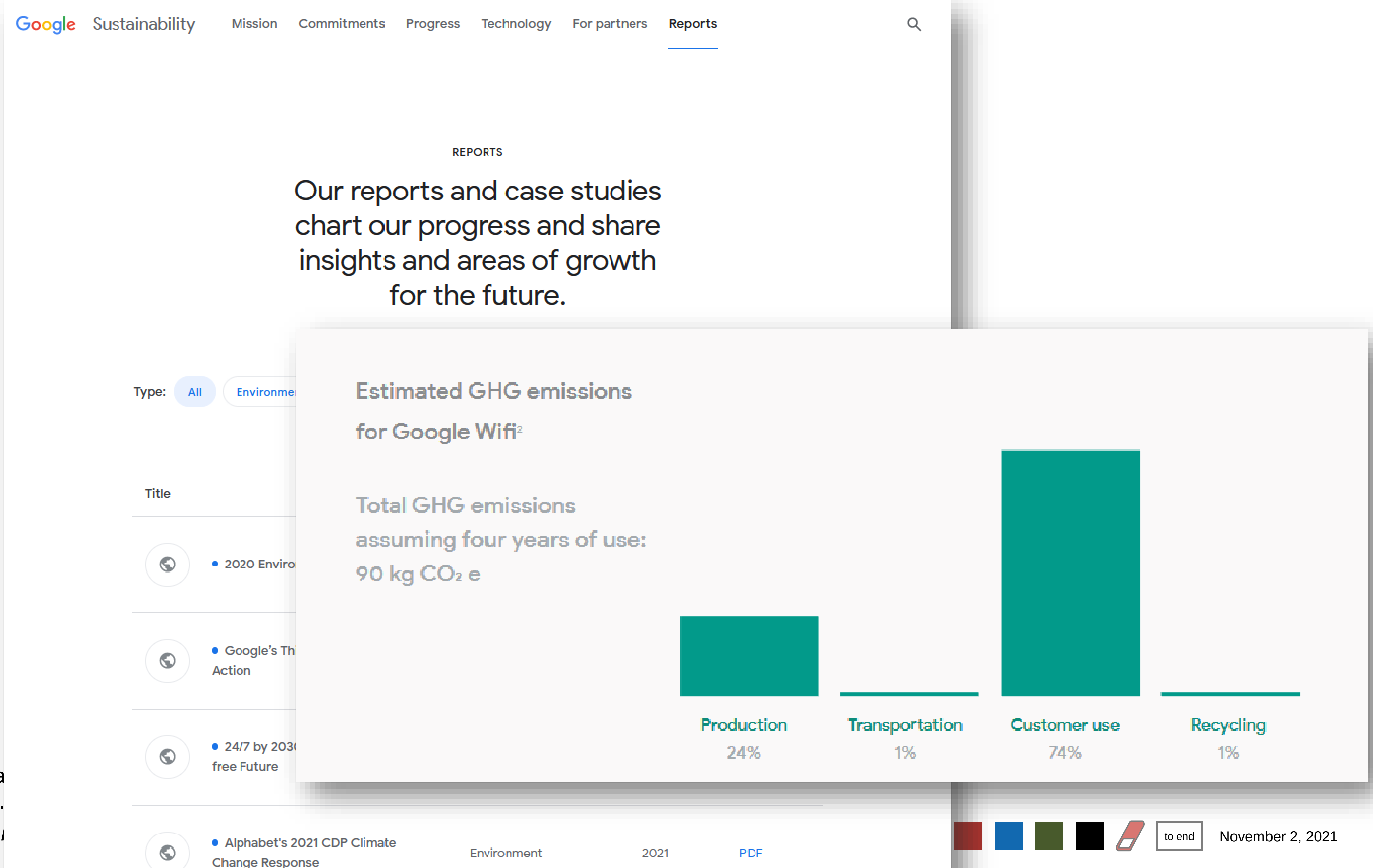
LCA & marketing

Example: Facebook / Meta



https://about.fb.com/wp-content/uploads/2021/06/NRP_2020Sustainability_Inline-1.jpg

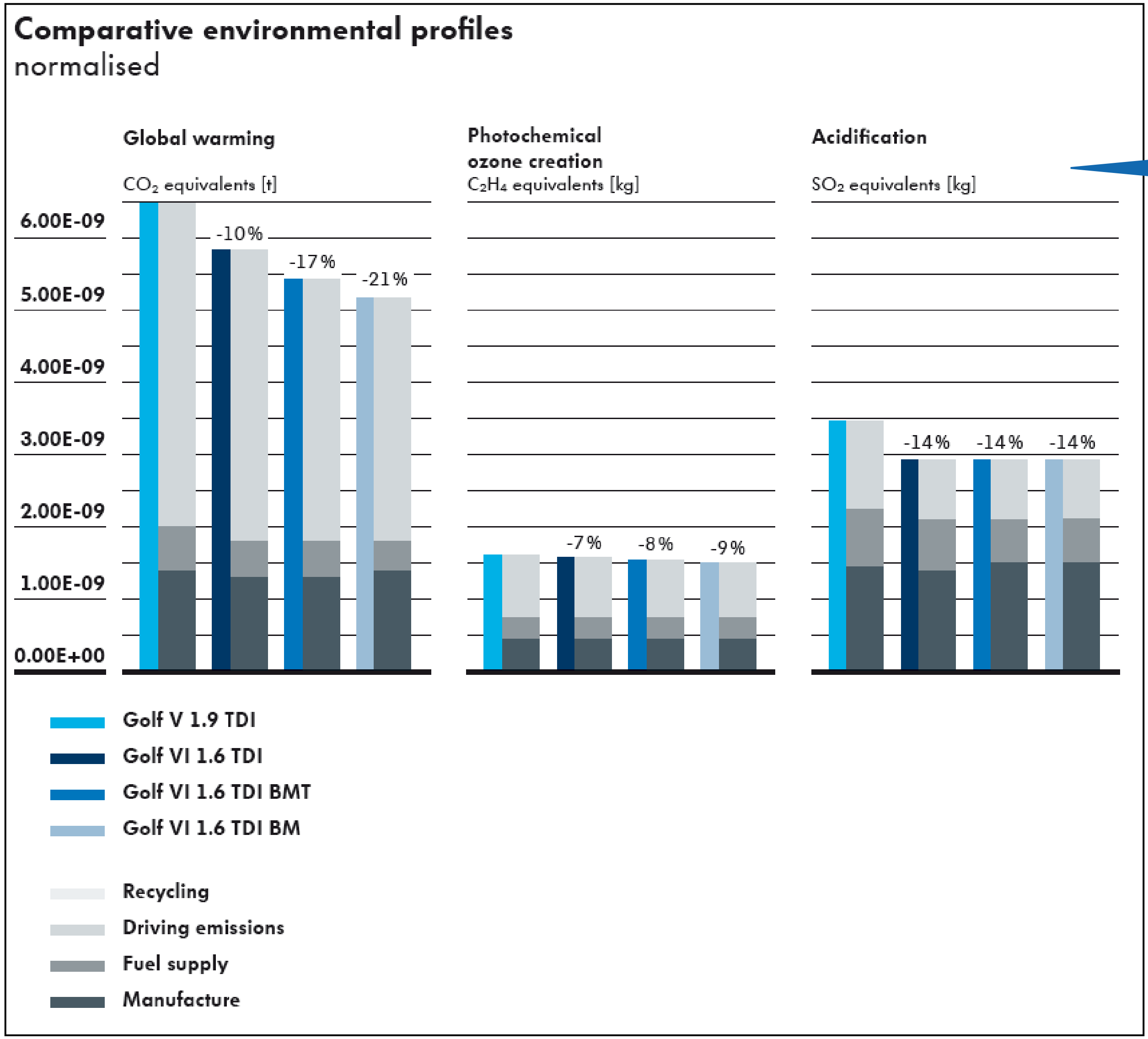
LCA, product reports & marketing



https://susta
https://www.

LCA of VW Golf

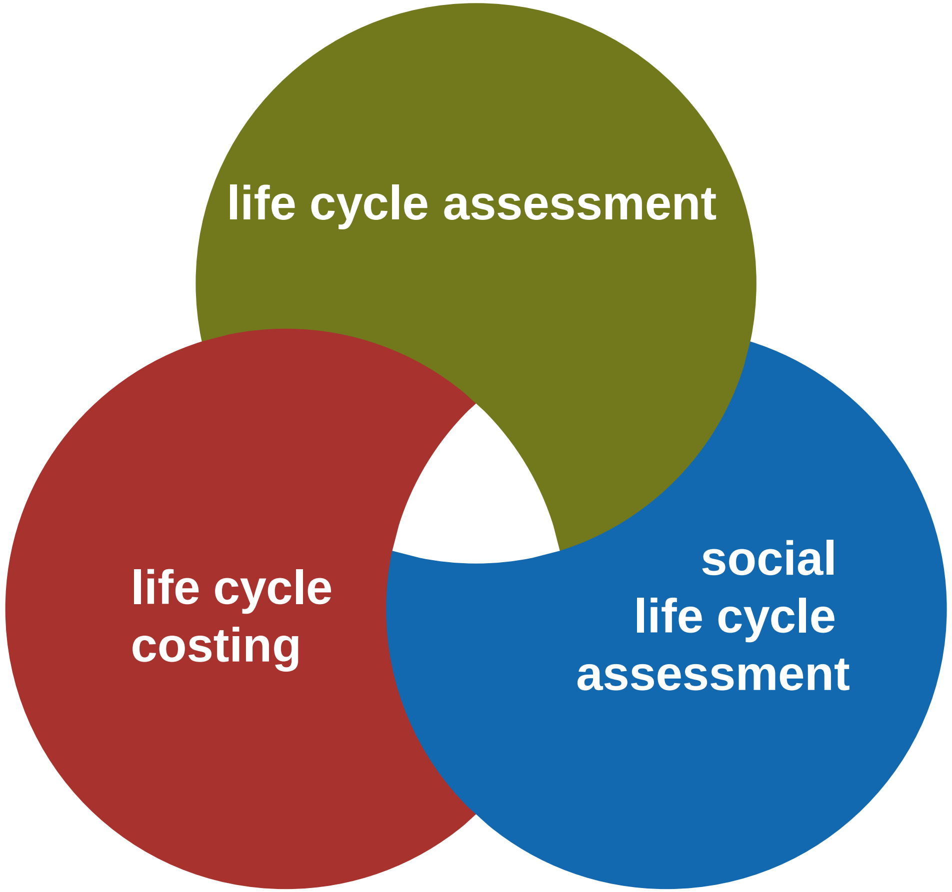
reference?



local vs. global?

http://www.volkswagenag.com/vwag/vwcorp/info_center/en/publications/2010/12/Golf_HB.-bin.acq/qual-BinaryStorageItem.Single.File/101129_VW_HB_Golf_GB.pdf

Quo vadis – LCA?



Life cycle sustainability assessment, a broader understanding of sustainability?

After this lecture, you are able to…

- ✓ conduct a life cycle assessment:
  - ✓ draw process flow diagrams
  - ✓ calculate energy and mass balances along a product life cycle
  - ✓ solve allocation problems
  - ✓ assess environmental impacts

- ✓ critically interpret life cycle assessment results