

Advancing Sustainability of Process Industries through Digital and Circular Water Use Innovations

# Design and Assessment of Water Reuse Systems

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AquaSPICE Summer School 2024



The AquaSPICE project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 958396.



- Understand the different options for water reuse and regeneration in an industrial plant with multiple processes
- Size and design a maximum water reuse system using Water Integration
- Introduce the main concepts of Life Cycle Assessment
- Compare a static/conventional and a dynamic Life Cycle Assessment
- Assess a water reuse system using Life Cycle Assessment



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# Design and Assessment of Water Reuse Systems

Part 1. Water Integration



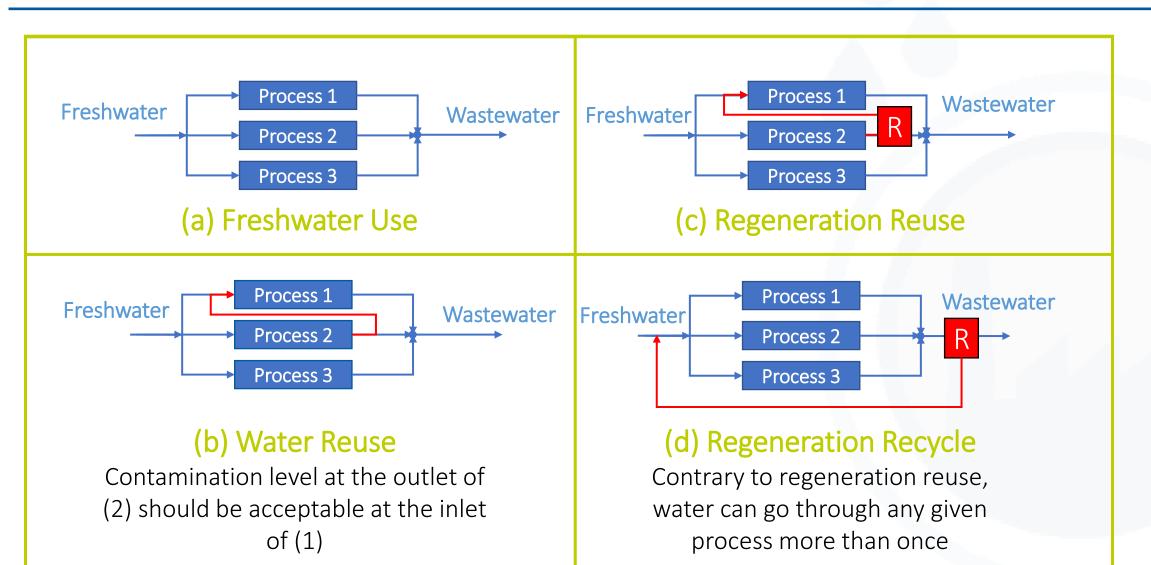
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- Water was assumed to be an infinite low-cost resource
- Nowadays, there is an increasing pressure on water resources
- Water scarcity is increasing as demand for water intensifies with population and economic growth
  - Restrictions in water use
  - Stricter discharge regulations
  - Recycle, Reuse & Regenerate



#### **Alternative Water Reuse Schemes**

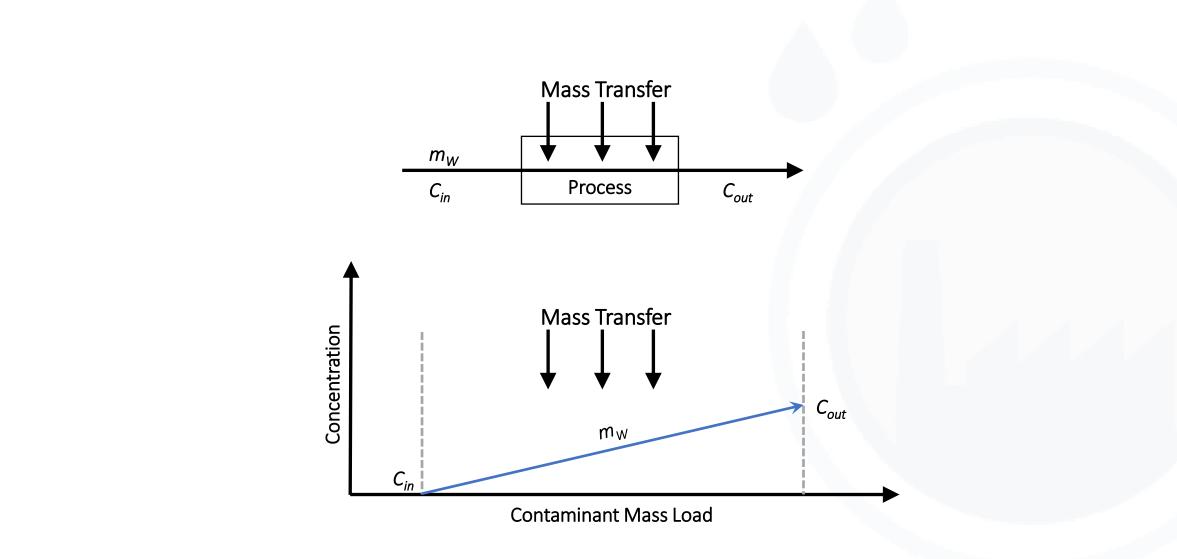




- All water use processes have one thing in common.
- Water comes into contact with process materials and becomes contaminated
- $\blacksquare$  For a given process, with a specific contaminant load ( $\Delta m_{c})$ , then:  $\Delta m_{C}=m_{W}\times\Delta C$ 
  - where  $m_W$  is the water flowrate and  $\Delta C = C_{out} C_{in}$  the concentration change of the water
- Note: Concentration is defined on the basis of the mass flowrate of the water and not of the mixture, since the difference between the two quantities is very small

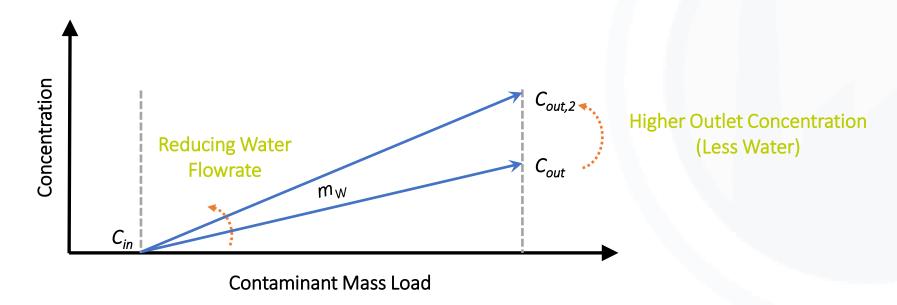


#### **Representing Water Use**





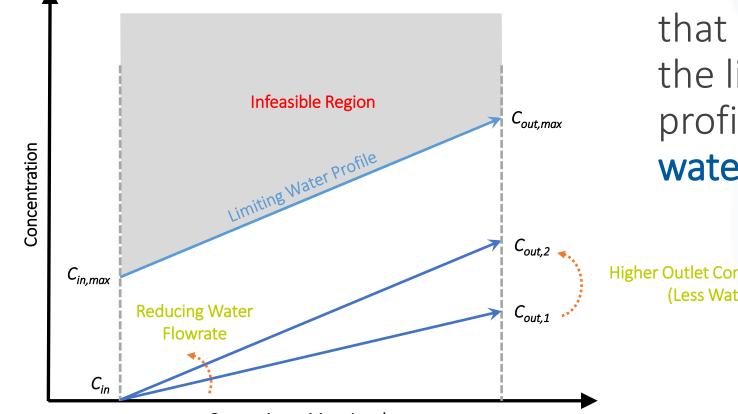
- If water flowrate is reduced for the same mass load of contaminant the result will be:
  - Higher outlet concentration
  - Steeper line





- The objective is to reduce water use as much as possible
- Limitations:
  - Minimum flowrate required by the operation
  - Maximum value for outlet concentration (discharge limitations)
- Moreover, in order to allow for reuse, some level of inlet contamination should be allowed





**Contaminant Mass Load** 

The water flowrate that corresponds to the limiting water profile is called **limiting** water flowrate

**Higher Outlet Concentration** (Less Water)

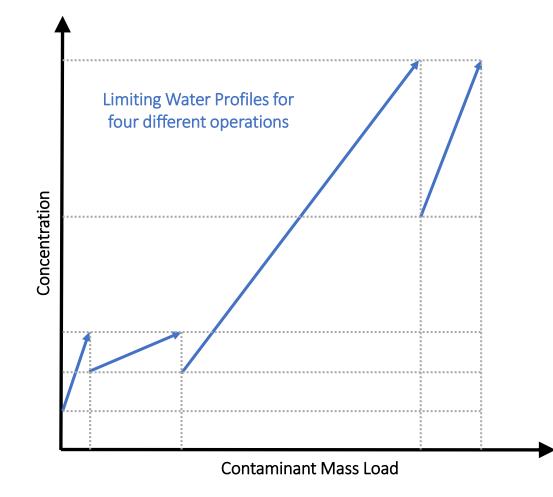


- Operations with different characteristics can be compared
- Mass transfer does not need to be modeled in detail
- The flow pattern does not affect the results
- Can be applied in all different types of water use operations (co-current, countercurrent)



## **Limiting Composite Curve**

The case of one contaminant

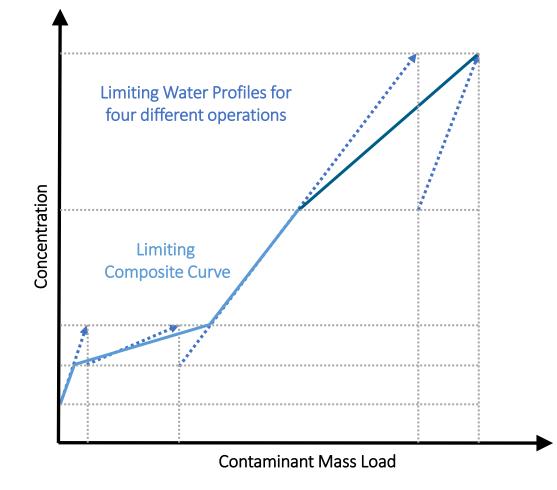


 When combining limiting water profiles for various operations in the same chart, the output will be the limiting composite curve of the water streams



## **Limiting Composite Curve**

The case of one contaminant

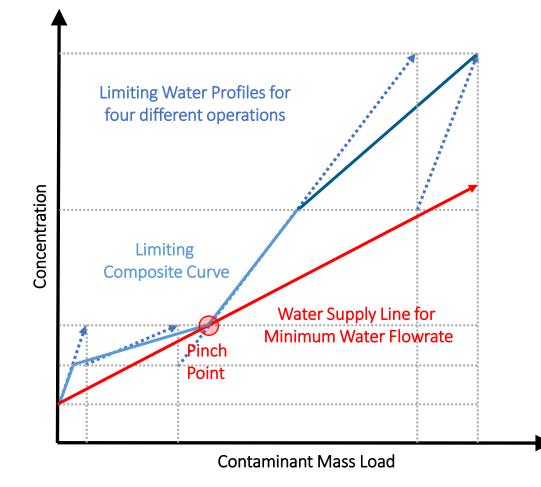


For the drawing of the limiting composite curve, the y-axis is divided into the corresponding concentration intervals and the contaminant loads in each interval are combined to create the composite curve.



## **Limiting Composite Curve**

The case of one contaminant



The minimum water flowrate for a given process can be specified by drawing the water profile curve which begins from the minimum acceptable inlet concentration and passes from the pinch point



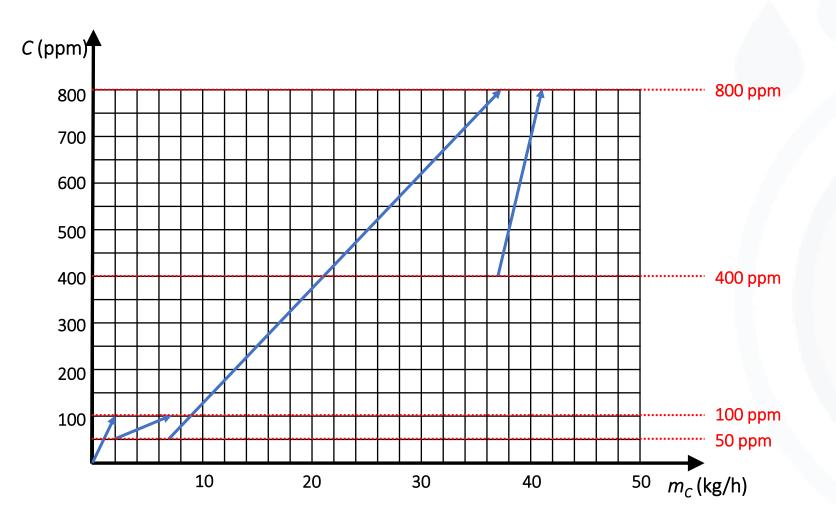
- An industrial unit has 4 operations which use water, and their specifications are presented in the following table. If the maximum inlet and outlet concentrations refer to a single contaminant:
  - Calculate the limiting water flowrate, which would maximize the water reuse in the system and draw the corresponding water supply line
  - Estimate the water savings compared to the case where all processes use freshwater

No	Contaminant Mass (g/h)	Maximum Inlet Concentration (ppm)	Maximum Outlet Concentration (ppm)	Limiting Water Flowrate (t/h)
1	2000	0	100	20
2	5000	50	100	100
3	30000	50	800	40
4	4000	400	800	10



# **Step 1. Limiting Water Profiles**

Draw the Limiting Water Profiles for the four different operations





# **Step 2. Concentration Intervals**

Calculate the concentration intervals and the corresponding contaminant loads in each interval

No	Maximum Inlet Concentration (ppm)	Maximum Outlet Concentration (ppm)	Limiting Water Flowrate (t/h)	Contaminant Load
C1	0	50	20	1000
C2	50	100	100 + 40 + 20	8000
C3	100	400	40	12000
C4	400	800	40 + 10	20000

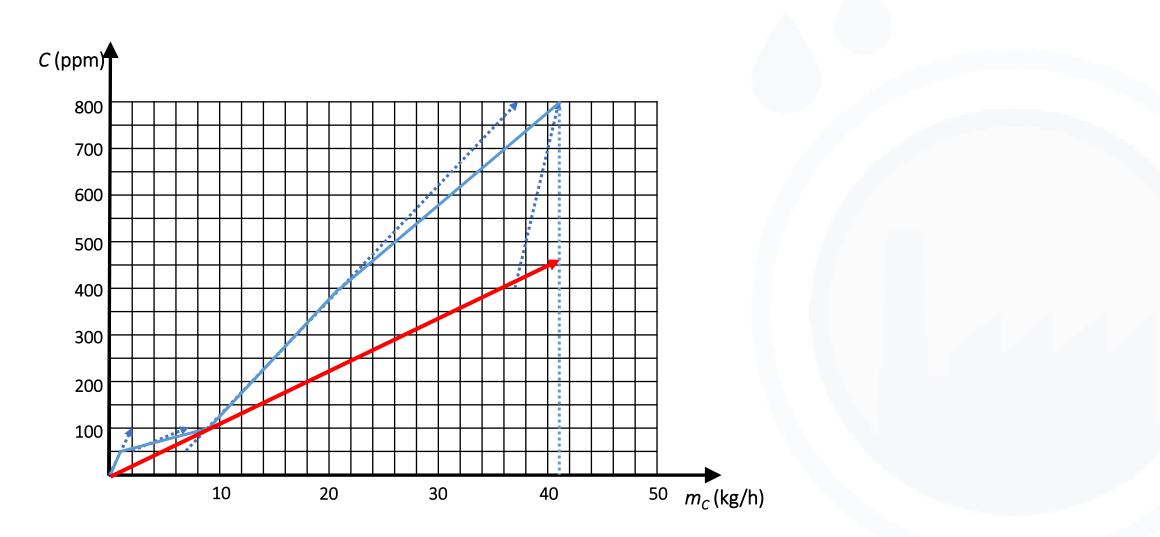
$$\Delta m_{C1} \ _{} m_{W1} \times \Delta C_1 = 20 \times (50 - 0) = 1000$$

 $\Delta m_{C2} = m_{W2} \times \Delta C_2 = 160 \times (100 - 50) = 8000$ 



## **Step 3. Composite Curve**

Draw the composite curve and the minimum flowrate water supply line





# **Step 4. Minimum Flowrate**

Calculate the minimum flowrate and water savings

• From the pinch point  $m_{w,min} = \frac{\Delta m_{C,pinch}}{\Delta C_{pinch}} = \frac{9000}{100} = 90 \text{ t/h}$ 

If all processes used freshwater:

No	Contaminant Mass (g/h)	Inlet Concentration (ppm)	Maximum Outlet Concentration (ppm)	Limiting Water Flowrate (t/h)
1	2000	0	100	2000/100 = 20
2	5000	0	100	5000/100 = 50
3	30000	0	800	30000/800 = 37.5
4	4000	0	800	4000/800 = 5

Savings = 112.5 - 90 = 22.5 t/h



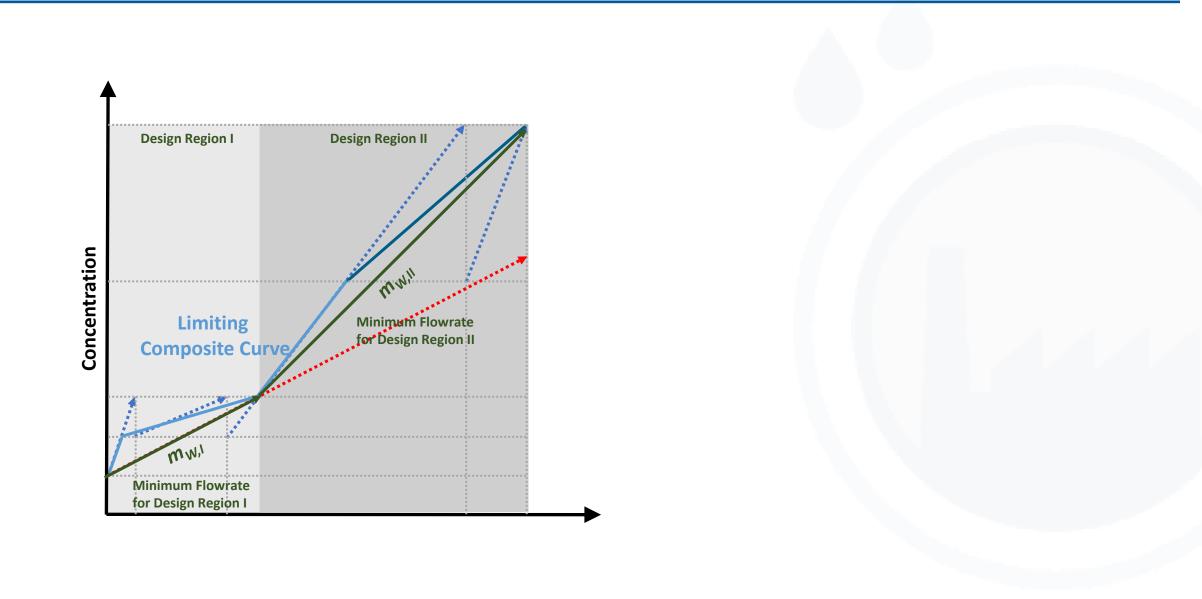
## **Designing a maximum reuse system**

In the case of a single contaminant

- After having calculated the minimum water flowrate required for the system, the next step is to actually design the system
  - Specify how exactly the water will flow among the different processes.
- Two (or more) different design regions can be identified in any scheme
  - **Below the pinch**, with limiting flowrate equal to the target minimum water flowrate of the system
  - Above the pinch, where the flowrate can be lower than the target minimum water flowrate



#### **Separate Design Regions**





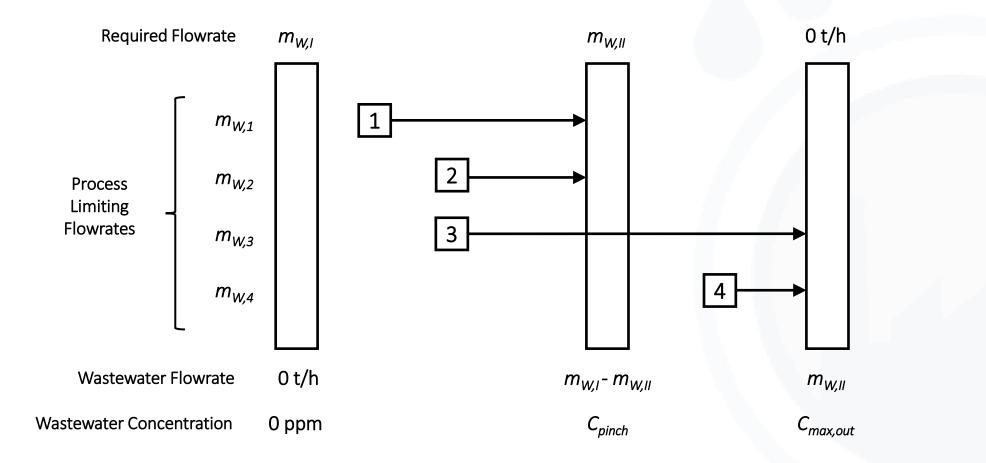
# Designing a maximum water reuse system

In the case of a single contaminant

- Objective of the design
  - Use the target flowrate below the pinch and only the required flowrate in the other regions
- Four step procedure
  - Set up the design grid and include all the necessary water mains
    - Freshwater stream
    - Stream(s) with pinch concentration
    - Stream with maximum acceptable concentration;
  - Connect all the processes with water mains;
  - Amend the individual processes where the flowrate changes among water mains; and
  - Remove all the unnecessary water mains and connect all the processes directly, where possible.



# A typical design grid





#### Designing a network for the target water consumption, as calculated earlier.

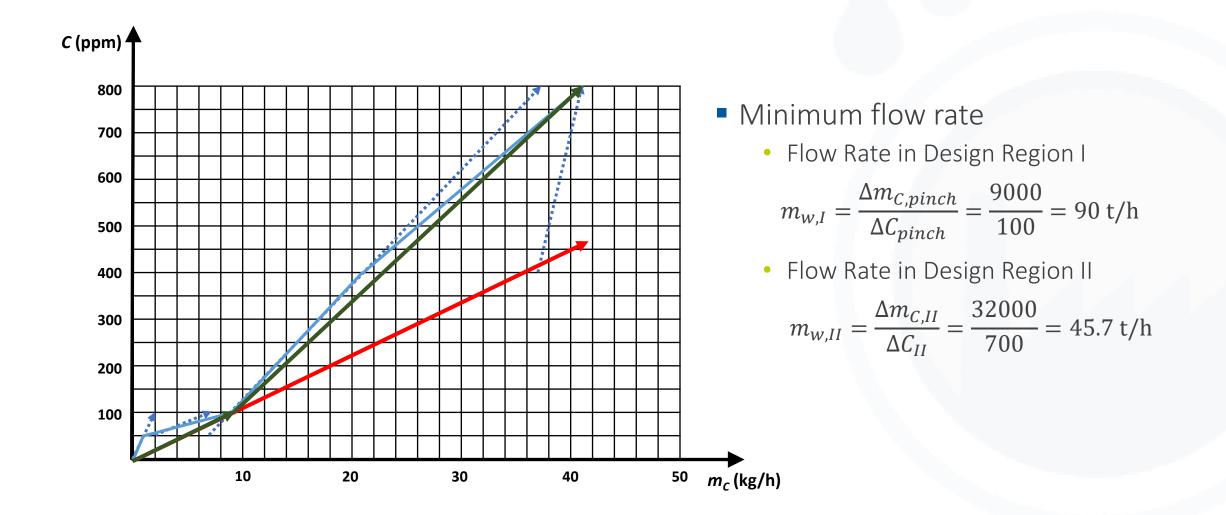
No	Contaminant Mass (g/h)	Maximum Inlet Concentration (ppm)	Maximum Outlet Concentration (ppm)	Limiting Water Flowrate (t/h)
1	2000	0	100	20
2	5000	50	100	100
3	30000	50	800	40
4	4000	400	800	10

Two processes operating below pinch (1 & 2), one process operating above pinch (4) and one process operating in both regions.



## **Step 5. Minimum water use per region**

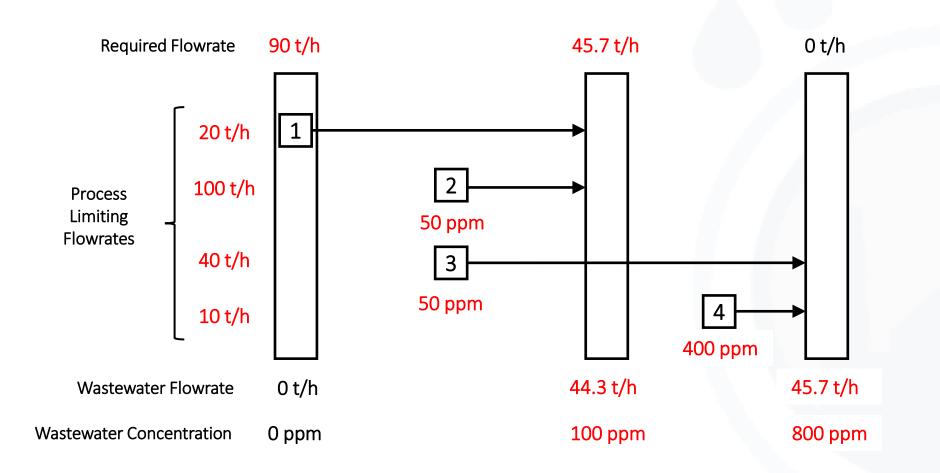
Calculate minimum flow rate for each design region



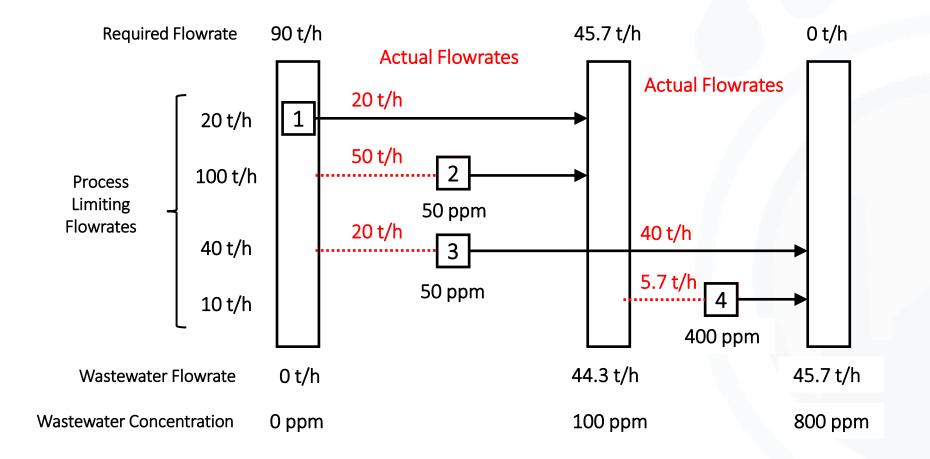


# **Step 6. Design Grip Setup**

Set up the design grid and include all the necessary water mains



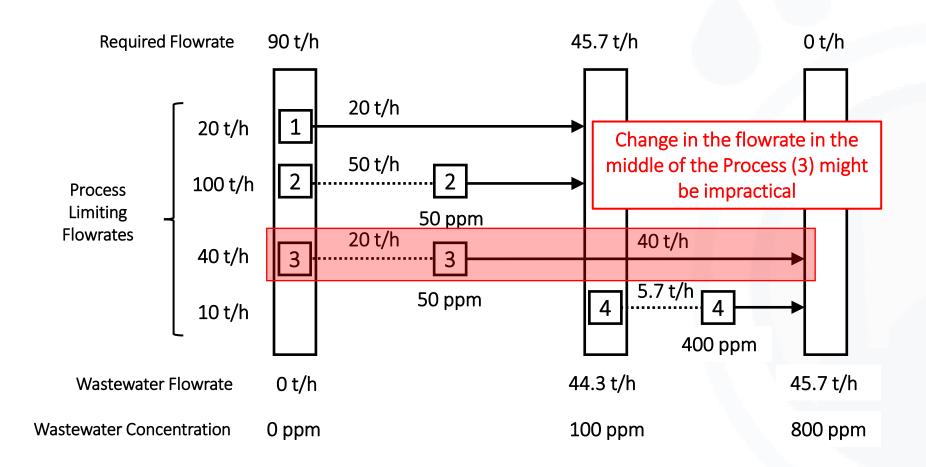






## **Step 8. Amend flowrate where necessary**

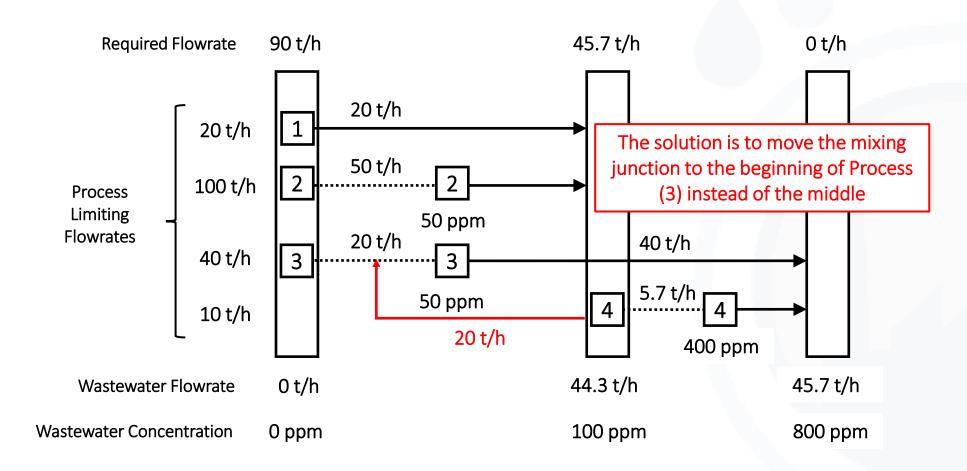
Amend the processes where the flowrate changes among water mains





## **Step 8. Amend flowrate where necessary**

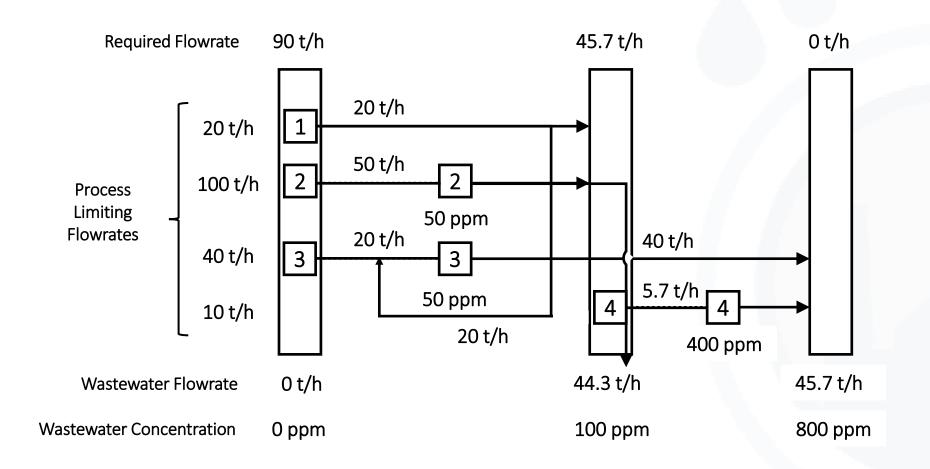
Amend the processes where the flowrate changes among water mains



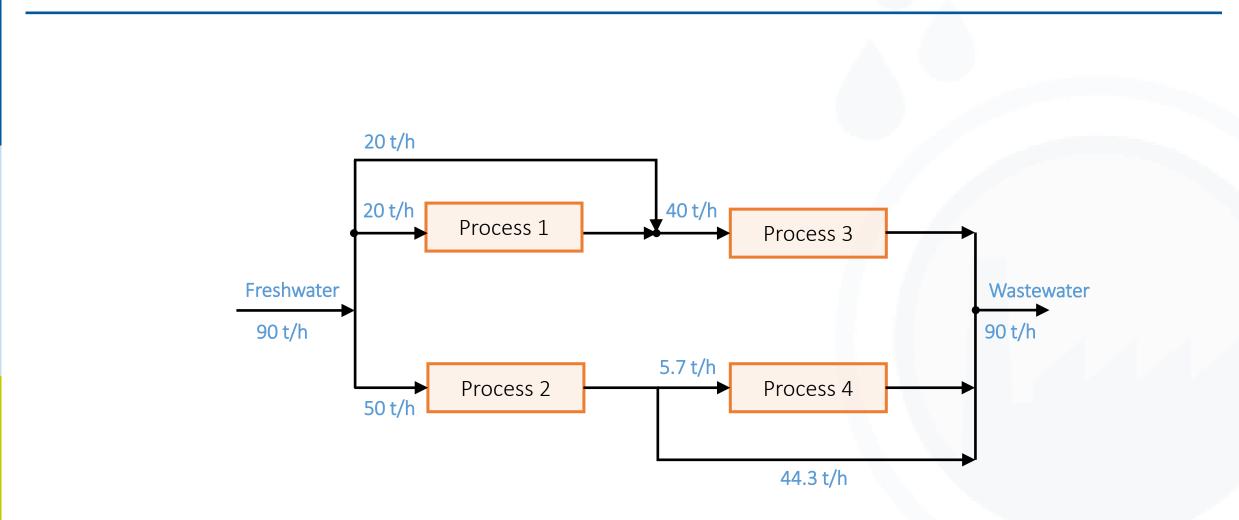


# **Step 9. Finalise the network**

Remove the unnecessary water mains and connect all processes directly





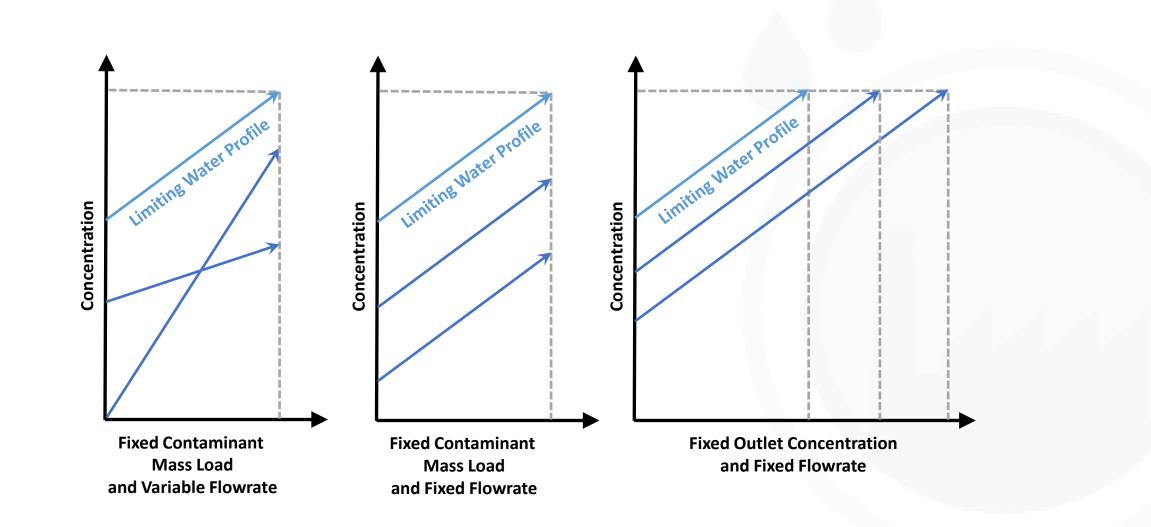




- Water losses in the systems
- More than one sources in the system (e.g. river, lake, potable, demineralized)
- More than one contaminants
- Different mass transfer models



#### **Different Mass Transfer Models**





- Alwi, S, Varbanov, P.S., Manan, Z.A. & Klemes, J.J. (2014). Process integration and intensification: saving energy and resources, De Gruyter.
- Smith, R. (2016), Chemical process design and integration, 2nd Ed. Wiley Blackwell, Chichester, West Sussex.



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# Design and Assessment of Water Reuse Systems

Part 2. Life Cycle Assessment



The AquaSPICE project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 958396.



#### **Life Cycle Assessment**

A Brief Definition

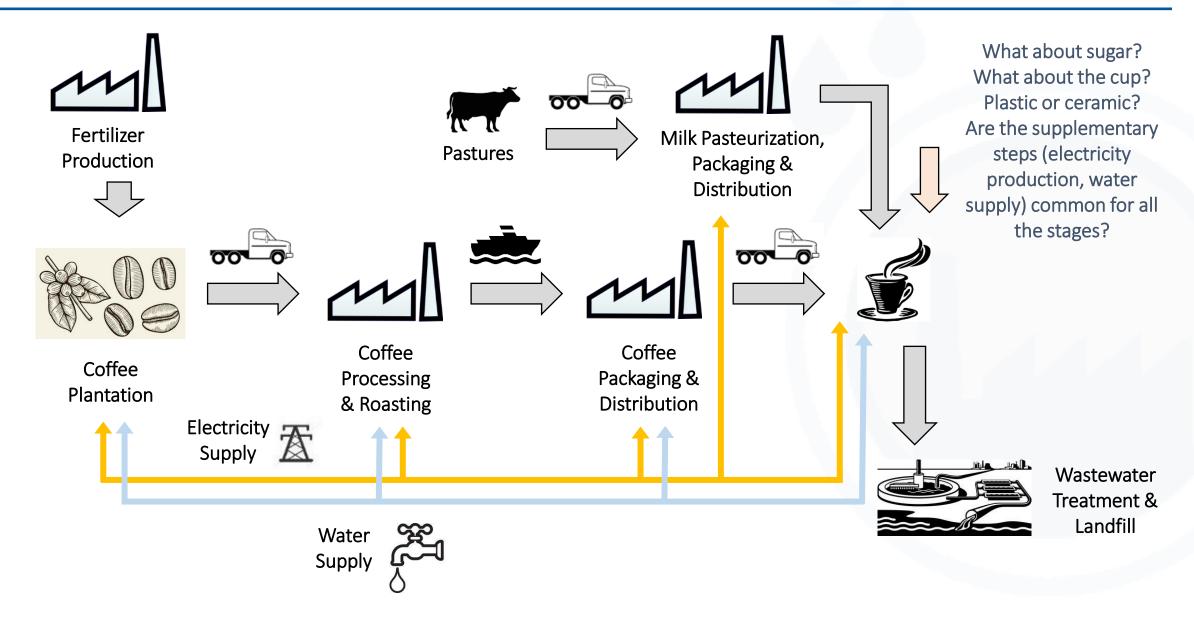
- Systematic monitoring and accounting of the flows and stocks of materials and energy in physical units within a system defined in space and time throughout its entire life cycle, and assessment of the associated environmental impact.
- From raw material extraction through production, distribution, use, end-of-life treatment, recycling to final disposal





## Life Cycle Assessment of a cup of coffee

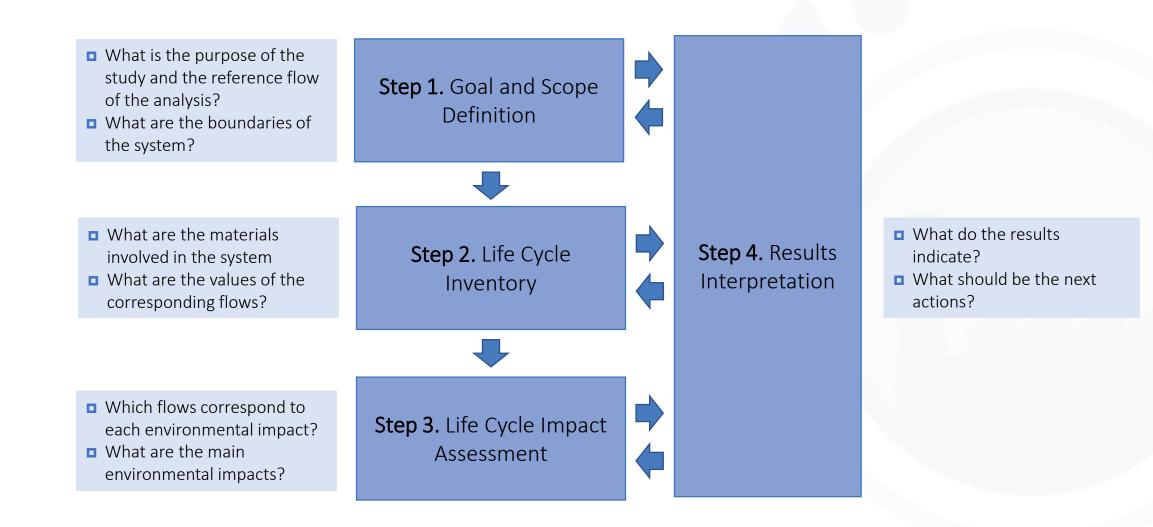
Where do we set the boundaries?





## **Steps of a Life Cycle Assessment**

According to ISO 14040:2006 - Environmental management





## What is the purpose of the study?

- Who will use the results?
- Identification of hot spots? Comparison of alternative products? Comparison of alternative procedures? Assess the consequences?
- What are the boundaries of the system?
- What will be the reference flow of the analysis?
  - Reference Flow: The flow to which all other input and output flows quantitatively relate
  - Functional Unit: The numeric value of the reference flow, a reference to which results are normalized and compared



# **Life Cycle Boundaries**

Common variants that can be used

- Cradle-to-grave
  - From resource extraction ('cradle') to the disposal stage ('grave')
- Cradle-to-gate
  - From resource extraction (cradle) to the factory gate (i.e., before it is transported to the consumer). The use and disposal stages are not included
- Cradle-to-cradle or closed loop production
  - Specific type of cradle-to-grave assessment, where the disposal stage for the product is a recycling process.
- Gate-to-gate
  - Specific type of LCA focusing on one value-added process in the entire production chain
- Well-to-wheel
  - Specific LCA used for transport fuels and vehicles



- An important element in the life cycle approach is the distinction between "foreground" and "background" systems
  - Foreground System: The set of processes whose selection or mode of operation is affected directly by decisions based on the study
  - Background System: Includes all other activities, which deliver energy and materials to the foreground system, usually via a homogeneous market



- The functional unit provides a reference to which results are normalized and compared
- Appropriate definition of functional unit to allow comparisons
- For a beverage bottling company possible functional units can include:
  - 1 bottle of beverage
  - 1 litre of beverage
  - 1 day/year of operation
  - •
- What about multiple products?



- Life cycle inventory (LCI) analysis involves creating an inventory of flows entering and leaving every process in the foreground system, i.e. the system within the defined system boundaries
- In a typical LCA methodology, the inventory of flows must be related to the functional unit defined in the goal and scope definition



### **Step 3. Life Cycle Impact Assessment**

Three mandatory elements

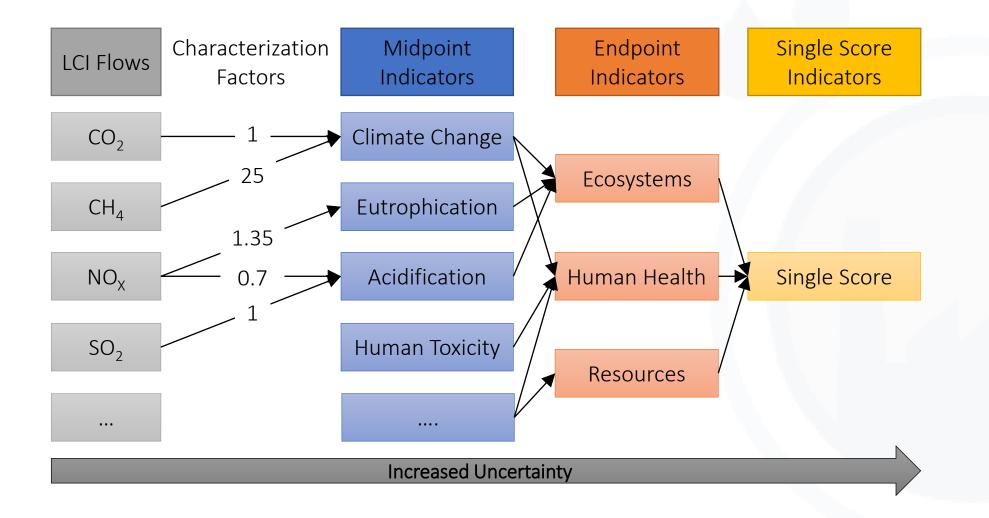
- Selection of relevant impact categories and the corresponding indicators
- Classification and characterization
  - Inventory flows are assigned to specific impact categories and are characterized into common equivalence units
- Impact calculation
  - Inventory flows are used to provide an overall environmental impact score per category



- An impact category represents a certain environmental issue of concern, to which the life-cycle inventory flow can contribute and thus a value may be assigned
- The selection of the most appropriate ones is case specific and is directly related to the information required to make concrete proposals for specific policies
- Distinction between midpoint and endpoint categories
  - Midpoint impact categories refer to specific environmental issues (such as climate change, acidification, eutrophication, human toxicity, etc.)
  - Endpoint categories refer to the three generally recognized issues of concerns (degradation of ecosystems, negative impact in human health and depletion of natural resources)



#### **Midpoint vs Endpoint**





- Quantify the impact of the elementary flows by aggregating the inventory flows into a limited number of midpoint or endpoint indicators
  - **Classification**: Organize and, if possible, combine the life cycle inventory flows into impact categories
  - Characterization: Quantify the extent to which each resource/emission contributes to different environmental impact categories
- The environmental impact for a given category (c) is expressed as a score (ESc) in the common unit for all contributions within the category



# Factors for Foreground Systems

- Retrieved from LCA databases
  - A widely used one (CML-IA) can be retrieved from the University of Leiden Department of Industrial Ecology webpage
- Vary based on the method used
- Factors for Foreground Systems
  - More difficult to retrieve
  - The background system is usually considered as a homogeneous market, so that individual plants and operations normally cannot be identified
  - Environmental impact factors are usually retrieved from databases, mainly provided with commercial and publicly available LCA software
  - Selection of which ones to include



- Many numbers/tables/charts!
- Identify the most significant issues based on the results of the environmental assessment
- Identify the stages/processes/flows that mainly contribute to the environmental impact
- Formulate conclusions and recommendations, according to the goal and scope of the study
- Explain the limitations of the analysis
- Provide recommendations for progressively improving the performance of the system



- In general, the term "dynamic" is used to express a system which is characterized by constant change.
- The changes that characterize a dynamic system can be:
  - directly linked to the operation of the system itself, affecting its performance in the short term
  - linked to the environment, which will affect the system and its performance indirectly, and probably in the longer term.
- However, usually these changes are not considered when assessing the system's environmental impact through a traditional static LCA.



- Static LCA, based on data from historical time series, enables the stakeholders to better understand the environmental impacts caused by the product system under consideration.
- At the same time though the digital transformation of the industry is one of the biggest shifts we see moving forward.
- Production processes are in the throes of Industry 4.0 transformation, towards a more agile, resilient, and flexible way of operation which increases their capacity to response rapidly to challenges



- New tools based on real-time modelling as well as robust datadriven approaches, enable the formation of Cyber-Physical Systems (CPS) and allow to better monitor processes and to operate systems much more efficiently.
- Thus, in the context of Industry 4.0 and the CPSs, static LCA is inflexible, providing only a single static snapshot in the time of the complex interactions of a product system.
- That means, it cannot be used to identify hotspots and trade-offs in real-time and support operational actions. The developed concept of Dynamic LCA could overcome these barriers.



 Dynamic Life Cycle Assessment can be defined as the LCA that incorporates elements of temporally induced changes that affect the results and the interpretation of the modeled system

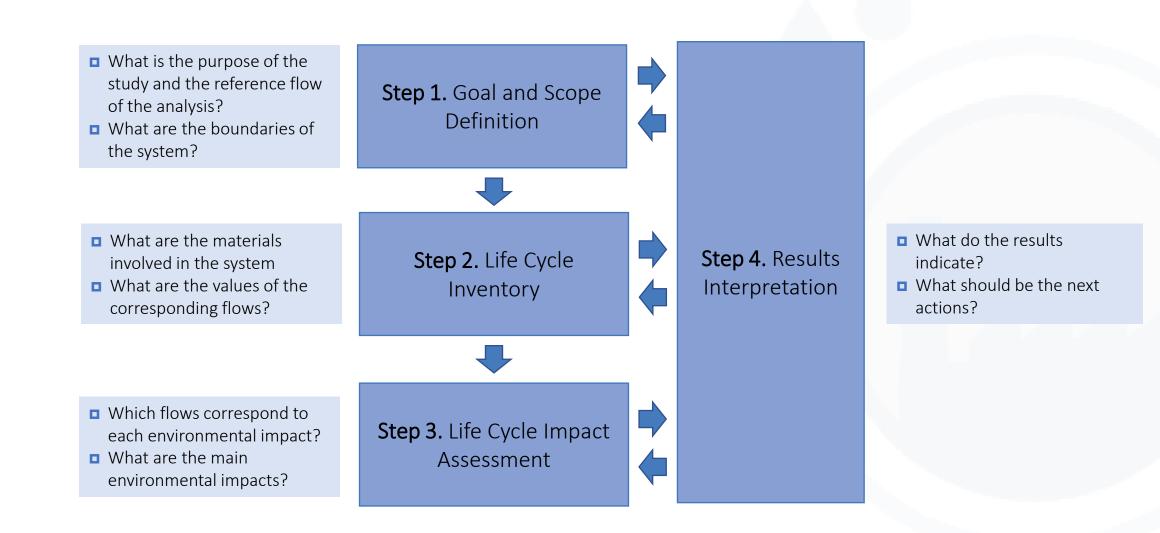
However:

- Can we use the same framework for Dynamic LCA?
- Which part of LCA will be dynamic?
- Are there any differences regarding indicators/data requirements?



### **Steps of a Static Life Cycle Assessment**

According to ISO 14040:2006 - Environmental management



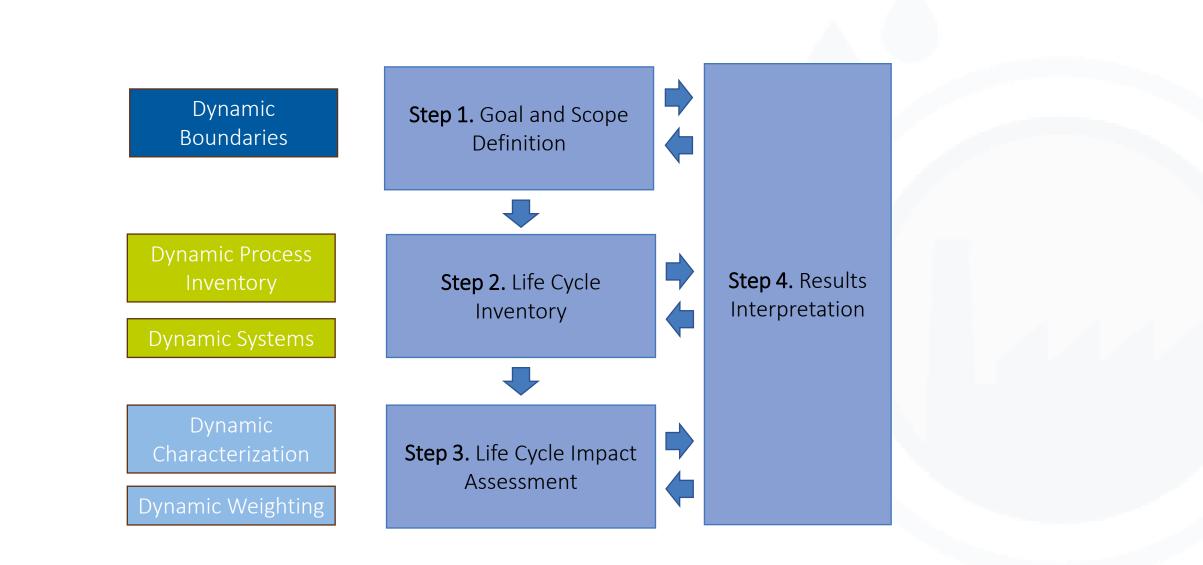


## **From LCA to Dynamic LCA**

- Sohn et al (2020) suggested an adapted methodological approach where, the first and last steps remain unchanged but the other can be converted into dynamic.
- Three different types of dynamism are described:
  - **Dynamic Process Inventory (DPI)**, which is the most frequently applied type of dynamism, implements temporal changes in input and/or output flows.
  - **Dynamic Systems (DSys)**, where changes are implemented in unit processes within the modelled systems.
  - **Dynamic Characterization (DChar)**, where the characterization factors change temporally.
- DPI and DSys are the dynamic variations of the LCI, whereas DChar is the dynamic implementation of LCIA.



#### **Steps of a Dynamic Life Cycle Assessment**





- Characterization factors change temporally
- Dynamic characterization based on the expected global temperature changes and time-adjusted cumulative radiative forcing (CRF), as defined by the IPCC to express the global warming potential
- Time-horizon-dependent ecotoxicity characterization factors, developed based on the USEtox fate model
- Time horizon-adjusted CFs for acidification, ozone depletion
- Long term consideration: 100-500 years' time horizon



# **Dynamic Inventory**

Long Term Scenarios vs Real Time Monitoring

## Using Scenarios

- The most frequently applied type of dynamism, implementing temporal changes in input and/or output flows
- Most common application is based on the development of future scenarios

### Real Time

- In conjunction with real time monitoring systems
- Real time data collection to continuously update the inventory
- Why would you need to do that? Which sectors?



- Dynamic Process Modelling, where changes are implemented in unit processes within the modelled systems
- Used in conjunction with/incorporated into existing process modelling tools
- Common application in the building sector with the Building Information Model (BIM), a tool developed for monitoring the building over its entire life cycle, by collecting an interoperable data set



#### **Dynamic Life Cycle Assessment**

- From the four steps of LCA, three have been incorporated in the Dynamic Life Cycle Assessment AquaSPICE framework:
  - Dynamic Goal and Scope (via link to Process Simulation and Modelling tool)
  - Dynamic Life Cycle Inventory (via link to Real Time Monitoring platform and Process Simulation and Modelling tool)
  - Dynamic Interpretation (via link to a Cyber Physical System)
- Dynamic Characterisation is not suitable for short-term (near real time) life cycle assessment
  - Characterisation Factors will only change in the long term (50 or 100 years), and definitely not in a very short time horizon



- A slaughterhouse in Romania wants to assess the environmental impact of alternative options for their wastewater treatment facilities.
- A volume-based unit is the most common functional unit in the LCA of wastewater treatment and, for this study, 1 m<sup>3</sup> of wastewater effluent prior to entering the wastewater treatment system is chosen.
- The focus of the study was the operational Life Cycle Assessment on the water line, which implies that the design, building and maintenance of different process equipment have not been included.

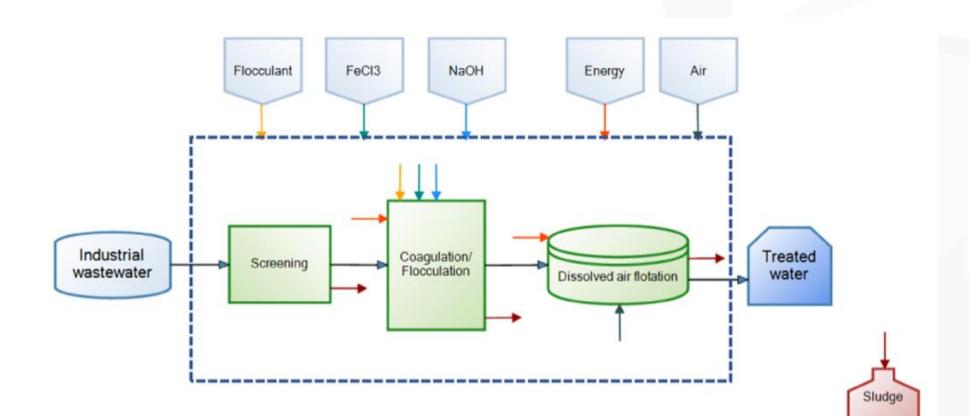


- The Environmental Footprint (EF) impact assessment method has been selected for the impact assessment of the alternative scenarios.
- The EF is an LCA methodology, adopted by the European Commission in the Environmental Footprint transition phase of the commission to incentivise industries manufacturing products with improved environmental performance, based on reliable, verifiable, and comparable information.
- Version 3.7.1 of the ecoinvent database was used for the assessment.



#### **Option 1 for Wastewater Treatment**

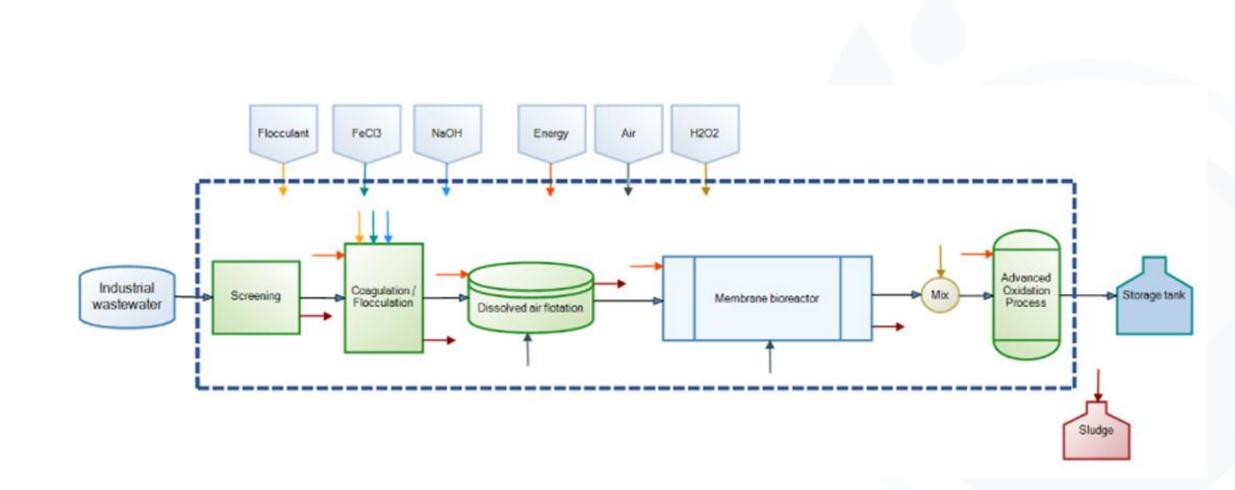
As modelled and illustrated using the PSM tool developed by TUC





#### **Option 2 for Wastewater Treatment**

As modelled and illustrated using the PSM tool developed by TUC





#### **Life Cycle Inventory**

The Life Cycle Inventory has been populated using: (a) real-time data from online sensors and (b) outputs from a process simulation and modelling tool (digital twin of the process)

Life Cycle Inventory – Input with the functional unit as  $1 \text{ m}^3$  of wastewater prior to entering the wastewater treatment system.

Resource	Scenario 1	Scenario 2	Scenario 3
Ferric (III) Chloride	-	462 g/m <sup>3</sup>	462 g/m <sup>3</sup>
Sodium Hydroxide	-	270 g/m <sup>3</sup>	277 g/m <sup>3</sup>
Flocculant	-	5.05 g/m <sup>3</sup>	5.05 g/m <sup>3</sup>
Hydrogen peroxide	-	-	50.0 g/m <sup>3</sup>
Electricity (for coagulation)	-	0.276 kWh/m <sup>3</sup>	0.276 kWh/m <sup>3</sup>
Electricity (for DAF)	-	0.170 kWh/m <sup>3</sup>	0.170 kWh/m <sup>3</sup>
Electricity (for MBR)	-		2.95 kWh/m <sup>3</sup>
Electricity (for AOP)	-		$0.420 \text{ kWh/m}^3$

Life Cycle Inventory – Output with the functional unit as  $1 \text{ m}^3$  of wastewater prior to entering the wastewater treatment system.

Resource	Scenario 1 *	Scenario 2	Scenario 3
Alkalinity	85.0 g/m <sup>3</sup>	54.2 g/m <sup>3</sup>	57.1 g/m <sup>3</sup>
pH	7.10	7.51	7.62
Chemical Oxygen Demand	1288 g/m <sup>3</sup>	146 g/m <sup>3</sup>	0.010 g/m <sup>3</sup>
Biological Oxygen Demand	525 g/m <sup>3</sup>	363 g/m <sup>3</sup>	24.3 g/m <sup>3</sup>
Total Organic Carbon	1570 g/m <sup>3</sup>	160 g/m <sup>3</sup>	$0.160 \text{ g/m}^3$
Total Suspended Solids	686 g/m <sup>3</sup>	103 g/m <sup>3</sup>	1.03 g/m <sup>3</sup>
FGO	183 g/m <sup>3</sup>	4.80 g/m <sup>3</sup>	4.80 g/m <sup>3</sup>
Total Nitrogen	215 g/m <sup>3</sup>	215 g/m <sup>3</sup>	157 g/m <sup>3</sup>
Total Phosphorus	33.5 g/m <sup>3</sup>	33.5 g/m <sup>3</sup>	0.000 g/m <sup>3</sup>
Sulphate	622 g/m <sup>3</sup>	622 g/m <sup>3</sup>	617 g/m <sup>3</sup>
Nickel	3.28 g/m <sup>3</sup>	3.28 g/m <sup>3</sup>	3.28 g/m <sup>3</sup>
Lead	1.36 g/m <sup>3</sup>	1.36 g/m <sup>3</sup>	0.0300 g/m <sup>3</sup>
Zinc	1.88 g/m <sup>3</sup>	1.88 g/m <sup>3</sup>	0.430 g/m <sup>3</sup>
Copper	10.6 g/m <sup>3</sup>	10.6 g/m <sup>3</sup>	0.530 g/m <sup>3</sup>
Cadmium	0.750 g/ m <sup>3</sup>	0.740 g/m <sup>3</sup>	0.240 g/m <sup>3</sup>
Sludge	-	0.510 m <sup>3</sup> <sub>aludge</sub> /h	1.37 m <sup>3</sup> <sub>sludge</sub> /h
Sludge (normalised per functional unit)	-	0.0124 m <sup>3</sup> <sub>aludge</sub> /h/ m <sup>3</sup>	0.0333 m <sup>3</sup> <sub>aludge</sub> /h/ m <sup>3</sup>
Wastewater	41.1 m³/h	40.6 m <sup>3</sup> /h	39.3 m³/h

\*Indicates experimental data, provided by an industrial unit



#### Life Cycle Impact Assessment

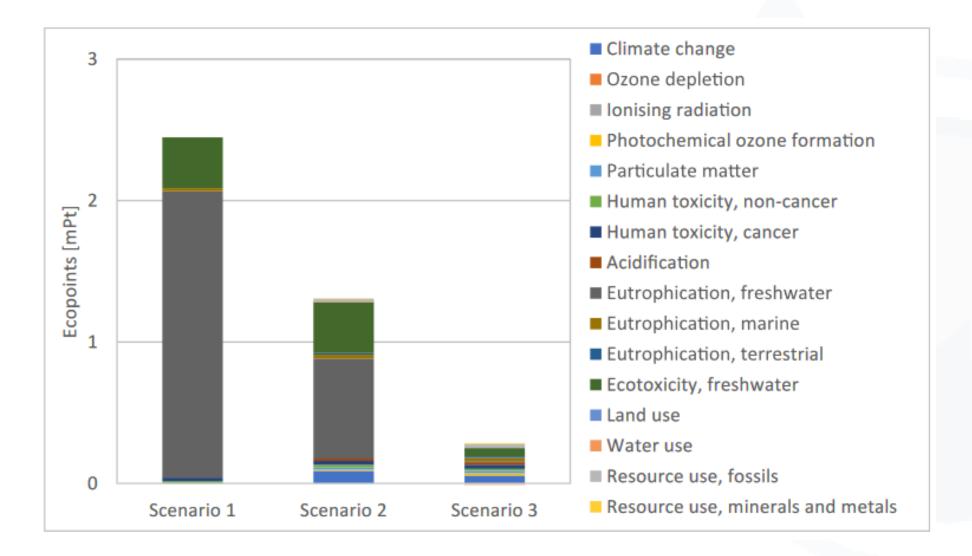
Retrieval of Characterisation Factors

Resource	Ecoinvent Entry		
Citric Acid	1 kg Citric acid {GLO}  market for   APOS, U (of project Ecoinvent 3 - allocation		
	at point of substitution - unit)		
Sodium	1 kg Sodium hypochlorite, without water, in 15% solution state {RER}  market		
Hypochlorite	for sodium hypochlorite, without water, in 15% solution state   APOS, U (of		
	project Ecoinvent 3 - allocation at point of substitution - unit)		
Electricity	1 MJ Electricity, medium voltage {RO}  market for   APOS, U (of project		
	Ecoinvent 3 - allocation at point of substitution - unit)		
Water	1 m <sup>3</sup> Water, deionised {Europe without Switzerland}   market for water,		
	deionised   APOS, U		
Sludge	1kg Digester sludge {GLO}  treatment of digester sludge, municipal		
Treatment	incineration   APOS, U		



#### Life Cycle Impact Assessment

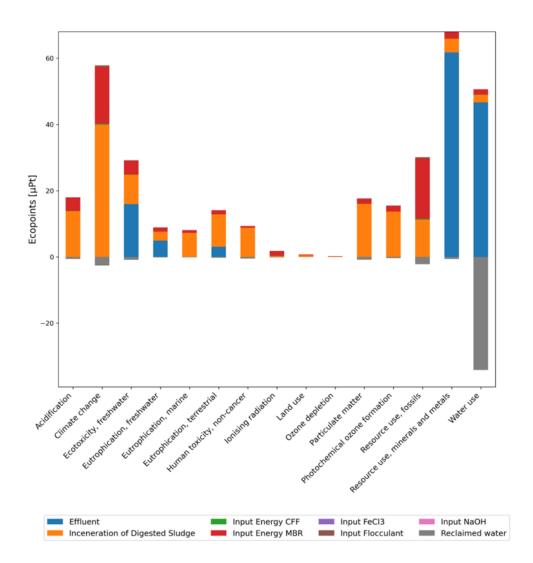
**Environmental Footprint Calculation** 





#### Life Cycle Impact Assessment

Interpretation of Results



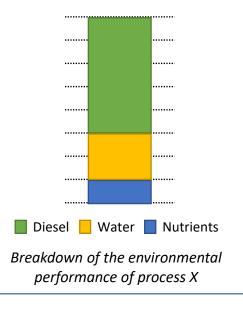
Finding the environmental hotspots, i.e. the processes/flows/stages with the highest contribution to the environmental impacts

Identifying further potential improvements to reduce the environmental impact



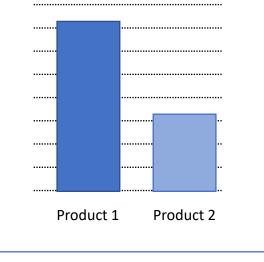
#### **Identify Hot Spots**

Identify the stage or the flow that is responsible for the higher share of environmental impact



#### Compare Alternative Processes/Products

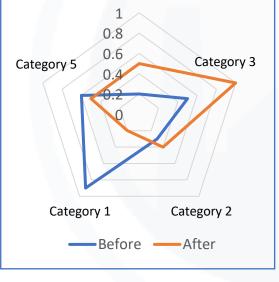
Compare the environmental performance of two similar products, with different production methods



# Estimate the Consequences

Assess the environmental performance of a process before and after certain interventions

Category 4



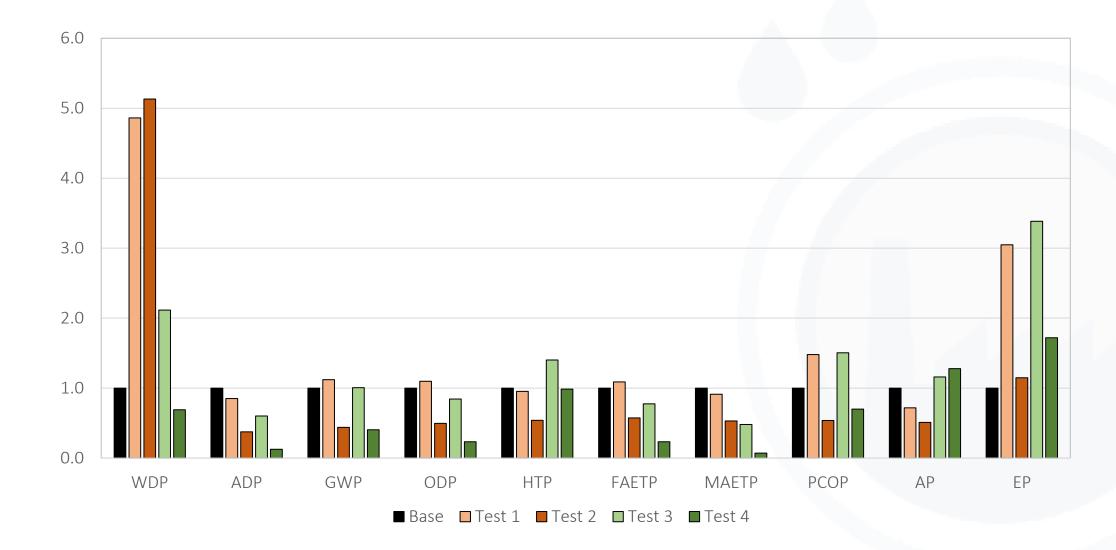


# The entire lifecycle of **one pair** of Levi's<sup>®</sup> 501<sup>®</sup> jeans equates to:



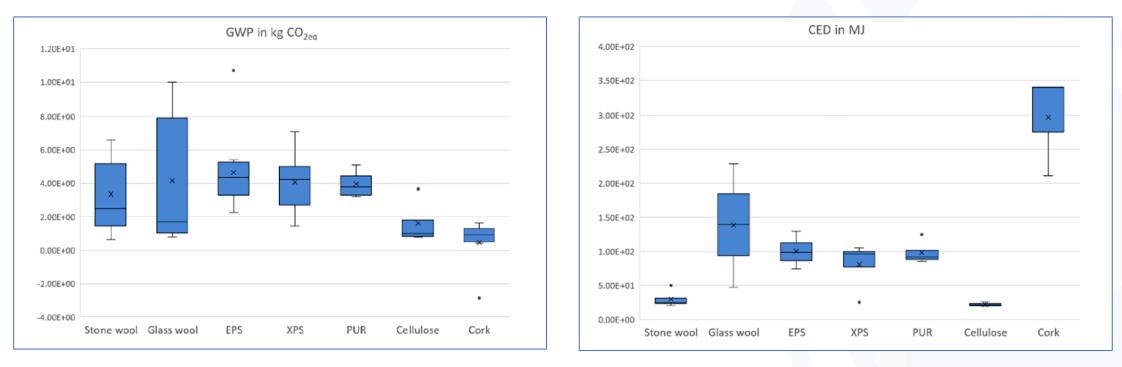


#### **Product Development**





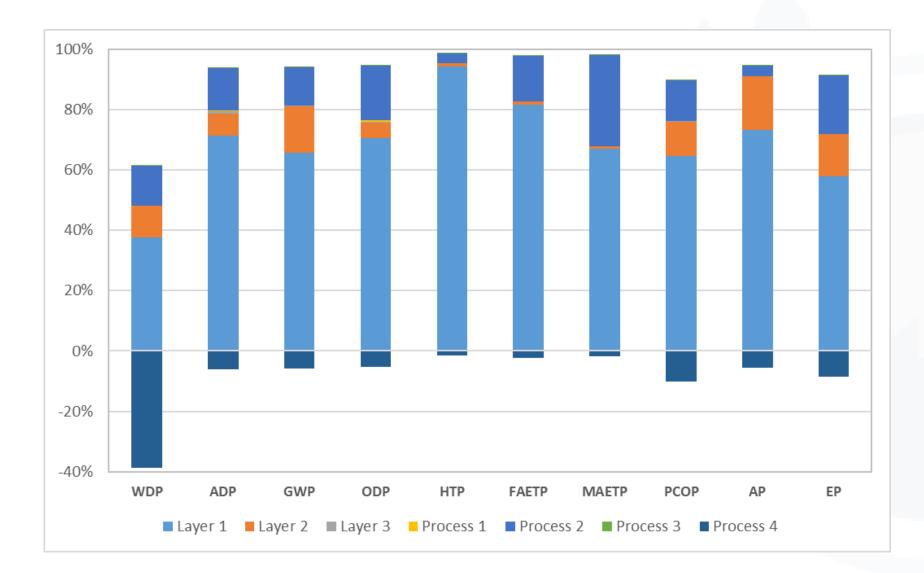
#### **Benchmarking Products**



Source: Füchs, S., Rheude, F., Roder, H. Life cycle assessment (LCA) of thermal insulation materials: A critical review, Cleaner Materials, 5 (2022) 100119



#### **Identify the hot spots**



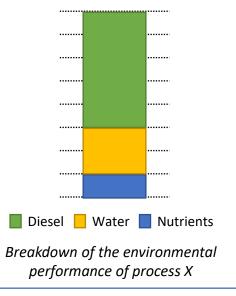


	Product with Recycled Raw Material	Product with Virgin Raw Material	
Carbon Footprint	8.2 kgCO <sub>2, eq</sub> /kg	10.5 kgCO <sub>2, eq</sub> /kg	-21.9%
Water Footprint	0.67 m³/kg	0.71 m³/kg	-4.5%
Eutrophication Potential	0.014 kgPO <sub>4</sub> /kg	0.014 kgPO <sub>4</sub> /kg	-0.8%
Resource Depletion	102.4 MJ/kg	162.7 MJ/kg	-37.1%



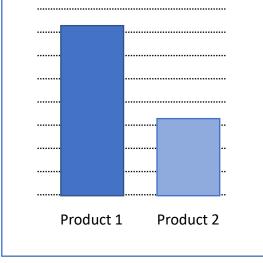
#### Identify Hot Spots

Identify the stage or the flow that is responsible for the higher share of environmental impact



#### Compare Alternative Processes/Products

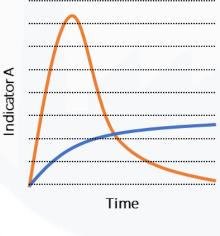
Compare the environmental performance of two similar products, with different production methods



#### Estimate the Consequences Assess the environmental performance of a process before and after certain interventions Category 4 0.8 0.6 Category 3 Category 5 Category 1 Category 2 -Before -After

#### Assess Impact Over Time

Monitor or estimate the environmental impact variation over time, under different assumptions





Advancing Sustainability of Process Industries through Digital and Circular Water Use Innovations

# Design and Assessment of Water Reuse Systems

Dr Athanasios Angelis-Dimakis, University of Huddersfield

AquaSPICE Summer School 2024



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