Environmental Life Cycle Assessment and risk analysis of NextGen demo case solutions

Deliverable D2.1.

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Technical References

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[1] PU = Public
PP = Restricted to other programme participants (including the Commission Services)
RE = Restricted to a group specified by the consortium (including the Commission Services)
CO = Confidential, only for members of the consortium (including the Commission Services)

Document history

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1	30.09.2022	KWB	Christian Remy, Fabian Kraus, Lea Conzelmann, Wolfgang Seis, Malte Zamzow
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Tracking of updates in revision

Comments of reviewer (22.12.2022)	Reply and relevant updates of the document
It is not clear why the LCA was only conducted for selected case studies (6 out of 10) and not for all (see also comment in the previous review).	LCA case studies were selected during the first reporting period “depending on data availability, complexity and system maturity” as referred in DoA. Decision matrix and selection criteria added in the introductory section.
The application of QRMA and QCRA was also limited to 4 demos each, despite of the feedback after the first and second project review that it should address all 10 demos.	QMRA was done for case studies with water reuse and resulting potential risk for humans (5x). QCRA was done for case studies with nutrient recycling where analytical sampling data for pollutants was available (3x). For both QMRA and QCRA and related selection of case studies, a rationale was added in the introductory section.
the deliverable lacks an overall description of the LCA method applied, ensuring a coherent approach across the various demos.	Overall description of LCA method added in front of LCA section.
Even though the DoA foresees that depending on data availability also LCC and CEA will be performed, this is not addressed in the deliverable.	LCC and CEA are addressed separately in Deliverable D2.2 as foreseen in the DoA. Remark added in introductory section that links to D2.2.
The linkage to T1.1 (TEB) as stipulated in the DoA is not sufficiently described.	Links to assessment results are included in the TEB for relevant case studies. Link to TEB and D1.7 added in the introductory section.
to include a transparent overview (e.g. overview table) on the LCA results of the demos.	Overview table of all LCA results has been added in the conclusion of the LCA chapter

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Disclaimer

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Management Summary

Within the NEXTGEN project, different innovative approaches for circular economy (CE) in the wastewater sector were investigated and demonstrated in pilot and full-scale systems. This report presents the assessment of selected case studies and CE concepts in their environmental impacts, and regarding potential risks from the use of CE products. Life Cycle Assessment (LCA) is used to investigate potential environmental benefits of CE approaches, but also potential drawbacks that could be associated with CE implementation. The focus of risk assessment is on microbial risks for human health in the case of water reuse, and on chemical risks from recycling of nutrients from wastewater to agriculture. Both types of risk assessment are applied here with a scientific approach based on a probabilistic calculation with quantitative data.

The LCA results of six case studies have shown that CE concepts and technologies can lead to a lower environmental footprint of wastewater treatment, considering the value of recovered products and the substitution of conventional alternatives from the linear economy. However, it depends on the specific situation at the site of these potentials can actually be realized, or if CE leads to a higher environmental footprint at least in some areas of environmental concern. Water reuse can be a good alternative to other energy-intensive options for water supply such as seawater desalination or water import over long distance, which then leads to overall savings in energy demand and related GHG emissions for water supply. For energy recovery from wastewater or sludge, it is important to assess the holistic energy balance of the systems rather than focusing only on the additional biogas or heat recovered. In principle, anaerobic treatment of wastewater yields the potential for energy-neutral or even energy-positive wastewater schemes. Nutrient recovery from wastewater is affected by trade-offs between chemical and energy intensive “high-tech” processes and the need for pure and high-quality products. “Low tech” nutrient recovery with sludge or compost yields more benefits in energy and GHG balance, but product quality can be minor.

Quantitative microbial risk assessment (QMRA) of water reuse demonstrated the potential for safe implementation of water reuse applications using almost all tested treatment configurations. However, the results also identify the need for local validation monitoring: in the absence of additional local information, default values for treatment performance generally result in wide ranges of potential removal of pathogens, which are less informative. The results are consistent with the approach proposed by the new EU water reuse regulation. The QMRA tool used in NEXTGEN is freely available for use in an online version.

In quantitative chemical risk assessment (QCRA), it was shown that no unacceptable or critical risk for ecosystems or humans originate from the application of nutrient products recovered in CE concepts. Few substances have been identified which could pose a potential risk to ecosystems (PFOS, mercury), and more analytical data is required to assess these substances more precisely in the recovered products. In addition, analytical limits of detection and also available knowledge of toxicity and environmental behavior for PFOS have to be improved to make sure that risk from these substances to ecosystems is acceptable.

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Acronyms

AD	Anerobic digestion
AnMBR	Anaerobic membrane bioreactor
ASS	Ammonia sulphate solution
BCF	Bioconcentration factor
BOD	Biological oxygen demand
CE	Circular economy
CEA	Cost Effectiveness Analysis
CED	Cumulative energy demand
CFU	Colony Forming Units
CHP	Combined heat and power
COD	Chemical oxygen demand
COP	Coefficient of performance
DAF	Dissolved air flotation
DALY	Disability adjusted life years
DM	Dry matter
EBCT	Empty bed contact time
EDC	Endocrine disrupting compounds
EGSB	Enhanced granular sludge bed
FEP	Freshwater eutrophication potential
FOG	Fat, oil and grease
GAC	Granular activated carbon
GHG	Greenhouse gas
GWP	Global warming potential
HT	High temperature
IPCC	International panel for climate change
KPI	Key performance indicator
LCA	Life Cycle Assessment
LCC	Life Cycle Costing
LOD	Limit of detection
LOQ	Limit of quantification
LRV	Log reduction value
MBBR	Moving bed biofilm reactor
MBR	Membrane bioreactor
MBM	Meat and bone meal
MCS	Monte Carlo simulation
MEP	Marine eutrophication potential
MF	Microfiltration

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MNR	Metabolic network reactor
N	Nitrogen
NF	Nanofiltration
P	Phosphorous
PBR	Photobioreactor
PE	Population equivalent
PEC	Predicted environmental concentration
PI	Probability of infection
PFOA	Perfluorooctanoic acid
PFOS	Perfluorooctansulfonic acid
PNEC	Predicted no-effect concentration
PPPY	Per person per year
QCRA	Quantitative chemical risk assessment
QMRA	Quantitative microbial risk assessment
RO	Reverse osmosis
RQ	Risk quotient
SBR	Sequencing batch reactor
SD	Standard deviation
SMU	Sewer mining unit
TAP	Terrestrial acidification potential
TEB	Technology evidence base
TEQ	Toxicity equivalency factor
TGD	Technical guidance document
TOC	Total organic carbon
TPH	Thermal pressure hydrolysis
TrOCs	Trace organic compounds
TS	Total solids
UF	Ultrafiltration
UV	Ultraviolet
VS	Volatile solids
WFD	Water framework directive
WHO	World Health Organisation
WP	Work package
WWTP	Wastewater treatment plant

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Introduction

Within the NEXTGEN project, different innovative approaches for circular economy (CE) in the wastewater sector were investigated and demonstrated in pilot and full-scale systems. This included concepts for the recovery of water, energy, or nutrients and other materials from wastewater of municipal or industrial origin (Figure 1).

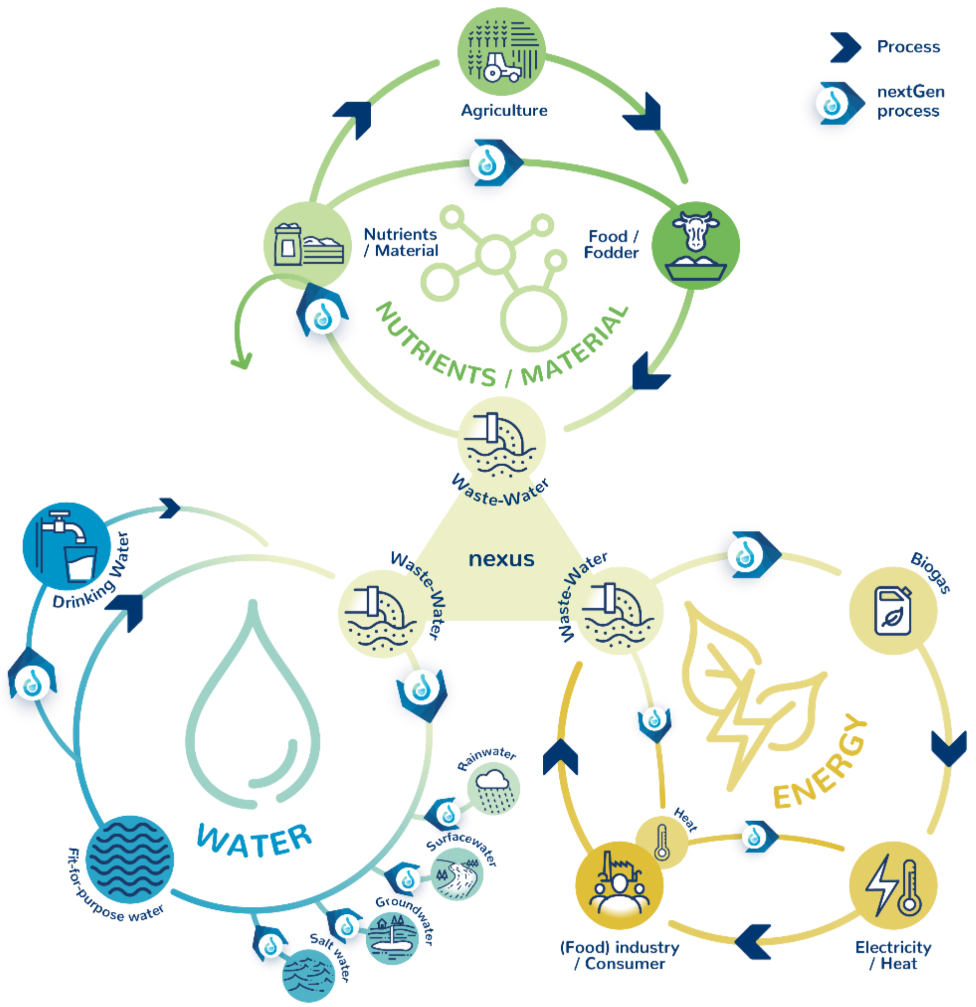

Figure 1: Concepts of circular economy in the wastewater sector for recycling of water, energy, and nutrients or materials in NEXTGEN

However, the recovery of resources from wastewater in CE is often connected to additional demand for energy, chemicals and infrastructure. Simultaneously, conventional products from the linear economy can be substituted with CE products, which generates savings in their production. Both effects have an impact on the environmental profile of CE approaches when compared to conventional water and wastewater treatment. Life Cycle Assessment (LCA) is a suitable tool to identify all relevant direct and indirect impacts of a system on the environment (ISO 14040, 2006). LCA quantifies these impacts related to a defined functional unit, which enables the direct comparison of alternatives in their environmental impacts. Within NEXTGEN, LCA is used to investigate potential environmental benefits of CE approaches, but also potential drawbacks that could be associated with CE implementation.

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Besides environmental impacts, an assessment of economic impacts of CE technologies and concepts is also part of NEXTGEN. The economic impacts are quantified with Life Cycle Costing (LCC) and also Cost Effectiveness Analysis (CEA). For these results and related KPIs, the reader is referred to deliverable D2.2 of the project (Nättorp and Misev, 2022).

Another important aspect of CE is the safety of use of the recovered products for human health or ecosystems. As wastewater is usually contaminated with a variety of chemical substances or microbial pathogens, related products from this feed could be contaminated as well. Hence, a sound and scientifically based risk assessment is required for all CE products to assess potential risks from their use for humans and ecosystems to ensure that no unacceptable risk is associated with their use. Within NEXTGEN, the focus of risk assessment is on microbial risks for human health in the case of water reuse, and on chemical risks from recycling of nutrients from wastewater to agriculture. Both types of risk assessment are applied with a scientific approach based on a probabilistic calculation with quantitative data.

Selection of case studies

As defined in the DoA (task 2.2), the selection of case studies for LCA, LCC and CEA was decided within the consortium during the first reporting period of the project based on defined criteria for maturity, system complexity and size, and data availability and quality (Table 1). Four case studies (Gotland, Westland, Filton and Timisoara) had either only conceptual work with low or no data availability (e.g. process data, technical layout) and quality, or high complexity due to more regional approaches. Finally, it was decided to assess environmental and economic aspects for those six case studies where suitable data was available or could be generated together with the partners during the project.

Table 1: Criteria for selection of case studies for LCA, LCC and CEA (Status at end of first reporting period)

Case study	CE sphere	Maturity	Complexity/ size	Data availability	Data quality	Selection for LCA/LCC/CEA
Altenrhein	N Mat	Full-scale Pilot	Medium	Okay	++ +	Yes
Braunschweig	N + E	Full-scale	Medium	Okay	++	Yes
Tossa de Mar	W	Pilot + regional	Low	Okay	++	Yes
LaTrappe	W N	Full-scale Pilot	Low Medium	Okay	++ +	Yes
Spernal	N + E	Large pilot	Medium	Okay	++	Yes
Athens	W + N + E	Pilot	Low-medium	Okay	+	Yes
Filton	W + E	Concept	High	Concept only	-	No
Timisoara	W N	Concept Pilot	High Low	Concept only Okay	- -	No
Gotland	W	Pilot	High	Unclear	?	No
Westland	W E N	Concept Pilot Concept	High Medium High	Concept only Unclear Concept only	- ? -	No

N: nutrients, E: energy, W: water, Mat: materials

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For quantitative microbial risk assessment (QMRA), the work in NEXTGEN focused on case studies where reused water could potentially lead to hazards for humans (irrigation, direct or indirect potable reuse, toilet flushing). This relates to the case studies Tossa de Mar, Athens, Filton, Timisoara, and Gotland. The project applied an online tool for QMRA from a previous project and expanded it to new technologies of NEXTGEN.

For quantitative chemical risk assessment (QCRA), 3 case studies with nutrient recycling were selected for assessment as stated in the DoA where potential hazards for humans and/or ecosystems could be expected. In addition, availability of analytical data for potential contaminants in recovered products was also crucial as a mandatory input for QCRA.

The final selection of case studies for LCA, QMRA and QCRA is presented below (Table 2). This report presents the detailed methods, definitions, input data and results for all assessments.

Table 2: Case studies for LCA and risk assessment presented in this report

Case study	CE technology	Products	LCA	QMRA	QCRA
Altenrhein	Membrane stripping Pyrolysis GAC from sludge	Ammonium sulphate PK fertilizer GAC	X X X		
Braunschweig	Thermal hydrolysis Struvite precipitation Ammonia stripping	Biogas Struvite Ammonium sulphate	X X X		 X X
Tossa de Mar	Regenerated membranes	Water for irrigation	X	X	
LaTrappe	Metabolic network reactor NF membrane	 Water for industry	X X		
Spernal	UASB + UF IEX IEX	Biogas CaP Ammonium sulphate	X X X		X
Athens	Sewer mining Rapid composting Heat exchanges	Water for irrigation Compost Heat	X X X	X	 X
Filton	Rainwater harvesting	Water for toilets		X	
Timisoara	Concept study	Water for irrigation		X	
Gotland	Membranes	Water for drinking		X	

LCA: Life Cycle Assessment; QMRA: quantitative microbial risk assessment, QCRA: quantitative chemical risk assessment, NF: nanofiltration, UASB: upflow anaerobic sludge blanket, UF: ultrafiltration, IEX: ion exchange

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Integration of results into Technology Evidence Base and transferability

As defined in the DoA, the results of LCA and risk assessment are integrated into the online technology evidence base (TEB), which is available at the NEXTGEN marketplace (mp.water-europe.eu). A link to the related deliverable is available at the TEB fact sheet of each relevant case study (Kleyböcker et al., 2022). This way, interested readers can view the full details of the various assessments and judge environmental impacts and potentials risks for humans and/or ecosystems based on the case-study specific results of NEXTGEN.

Furthermore, the transferability of results and the related potential for selected CE technologies in the EU has been elaborated in deliverable D7.5 (Frijns et al., 2022).

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Life Cycle Assessment

General method of LCA

In general, Life Cycle Assessment (LCA) in this study is closely aligned with the relevant ISO standards 14040 and 14044 (ISO 14040, 2006; ISO 14044, 2006), following the structure of goal and scope definition, life cycle inventory, life cycle impact assessment, and interpretation. For all case studies, an attributional LCA is conducted.

In particular, the following aspects are considered for each LCA of the individual case studies:

Goal and scope definition

- The function of systems and their functional unit is defined via their primary goal, which is the treatment of wastewater in most cases. CE services such as recovery of water, nutrients, materials or energy are reflected as secondary functions. Relevant input data is reported for all input flows to enable recalculation of LCA results to other functional units if needed for comparison.
- System boundaries are set to include all relevant processes upstream and downstream of the core system under study. This relates explicitly to the supply of energy, fuels, chemicals, or material for infrastructure, but also to the disposal of relevant waste. CE products are credited with substituting the production of an equivalent material in a conventional route ("avoided burden"), e.g. mineral N or P fertilizer, drinking water from other sources, or grid energy.
- Allocation is avoided by defining a suitable functional unit and associating all impacts to this function. This reflects the perspective of the operator.
- Scenarios are defined based on the specific situation and CE concept of the case study. For all case studies, a comparison with a baseline ("status quo") is done to illustrate the changes with implementing a CE approach in each case.
- All cases are assessed in a hypothetic or actual "full-scale" based on their individual situation.

Life Cycle Inventory (LCI)

- Relevant process data from pilot or full-scale plants is collected and validated in close cooperation with project partners.
- Up-scaling and extrapolation of available process data from pilot operation to projected full-scale is done based on expert knowledge, available literature and partner consultation. If needed, data gaps are filled also with process inventory data from previous projects.
- If possible, input data for LCA is reported in specific process-related units (e.g. kWh/m^3) to ease cross-comparison and validation by external readers.
- Background data is used from the LCA database ecoinvent (Ecoinvent, 2019).
- System models are built in the LCA software UMBERTO LCA+ (IFU, 2018).

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Life Cycle Impact Assessment

- Indicators for LCIA are selected to reflect most relevant environmental impacts of wastewater treatment. For all case studies, this includes LCIA midpoint indicators for process efforts (i.e. energy demand and related greenhouse gas emissions), water quality (i.e. eutrophication of marine and freshwater ecosystems) and relevant air emissions (terrestrial acidification). All case studies are evaluated with the same indicator models. If relevant for the case study goal, LCIA is extended with other indicators to elaborate specific aspects of the individual CE concept.
- Indicators are calculated and reported in total scores, and also in a differential approach showing the changes between baseline and CE scenario. Total scores are useful to show the contribution of CE concepts in relation to the total environmental footprint of the systems, whereas the differential approach better illustrates the detailed changes in the environmental footprint due to CE implementation.
- If meaningful, a sensitivity analysis is conducted for selected hotspots of environmental concern to show the impact of changes in LCI data or background processes towards the environmental profile of the individual CE concept or scenario.

Interpretation

- LCIA results are discussed and interpreted in relation to the individual CE concept of each scenario and its consequences for the overall environmental impact of the system.
- All LCA results and related conclusions are summarized in an overview table and bullet point list in the final part of each LCA study.

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Altenrhein (CH): nutrient recovery and renewable activated carbon

This case study investigates new approaches for the recovery of nitrogen and phosphorus from wastewater treatment and sewage sludge, and also for the production of activated carbon from renewable raw materials. These innovative processes are tested for the wastewater treatment plant (WWTP) Altenrhein, which is located close to Lake Constance in Eastern Switzerland (Figure 2).

The WWTP Altenrhein treats municipal and industrial wastewater from the surrounding municipalities, handling a capacity of around 105,000 population equivalents (pe). After primary settling, the wastewater is treated in an activated sludge process (70% of inflow) or a fixed bed biofiltration system (30% of inflow). After final clarification, the water is further treated with sand filtration, ozonation, and filtration using granular activated carbon (GAC) to remove residual phosphorus and organic micropollutants. Sludge is digested on-site, then dewatered and dried before disposal in a nearby cement kiln. Biogas is used in a CHP plant to generate electricity and heat for internal use. On top, a large heat pump is operated at Altenrhein which extracts heat from the WWTP effluent to be used for sludge drying. Surplus heat of the entire system can be fed to the local district heating network.

Figure 2: Aerial view of WWTP Altenrhein

Apart from the primary and excess sludge of wastewater treatment, WWTP Altenrhein also receives high amounts of external sludge (~ 200.000 pe) and co-substrates. Acting as a local “sludge center”, the WWTP processes raw sludge, digested sludge, and dewatered sludge from other WWTPs in the area. This leads to a high amount of centrate from dewatering, and consequently a high return load in nitrogen which is currently recycled to the WWTP inlet. The additional N load to the WWTP from centrate amounts to 22% of the total N load to the biological stage.

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In NEXTGEN, different options have been explored to recycle both nitrogen and phosphorus from wastewater and sludge, and also to produce renewable GAC for the final treatment step of the WWTP. In particular, the following processes have been tested:

- **Stripping of nitrogen from centrate with a membrane process**: After extensive pre-treatment to remove suspended solids, the centrate is heated and pH is increased by dosing of NaOH to shift the chemical equilibrium from NH_4-N to gaseous NH_3. Using a gas-permeable membrane, NH_3 can then be extracted from the centrate and collected in a solution of concentrated sulfuric acid. The product of diammonium sulfate (DAS) can be further concentrated and sold as a ready-to-use fertilizer to local farmers. The process is realized in full-scale at WWTP Altenrhein and was assessed and optimized during the NEXTGEN project.
- **Production of a PK fertilizer from dried sludge:** using a combination of pyrolysis and fluidized bed incinerator (Pyrophos® process), this process incinerates the organic matter in dried sludge together with a reductive additive (potassium hydroxide). The main product is an ash with high content of plant-available P and K. On top, the process generates electricity from off-gas heat and surplus heat, which can be exported to other processes. Off-gas is cleaned in a multi-stage off-gas treatment. The Pyrophos® process was tested in pilot-scale in NEXTGEN using samples of dried sludge from WWTP Altenrhein.
- **Production of renewable GAC from dried sludge:** to replace conventional GAC made from fossil resources (hard coal), FHNW investigated the production of renewable GAC using dried sludge as organic input. Performance of the renewable GAC for removal of organic micropollutants was assessed in pilot trials with column experiments to determine maximum standing time until regeneration compared to conventional GAC. Regeneration of renewable GAC was also tested to estimate material losses and regeneration efficiency of the innovative material.

The three concepts have been tested for the conditions present at WWTP Altenrhein. Based on the findings in full-scale and pilot trials, the concepts are evaluated in their environmental impacts compared to the status quo ("baseline") of WWTP operation in 2020. Therefore, the performance and scale of the pilot systems are extrapolated from the pilot trials to a suitable full-scale size for WWTP Altenrhein.

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Goal and scope definition

The goal of this LCA is to analyse potential environmental impacts of different innovative processes for WWTP Altenrhein. It will compare the impacts of the NEXTGEN innovations to a baseline which represents the status quo of WWTP operation at the site. In detail, the following aspects will be analysed in the LCA:

- Impacts of WWTP operation and sludge disposal
- Impacts of operation and infrastructure for membrane stripping of the centrate from dewatering
- Impacts of operation and infrastructure for PK fertilizer production from dried sludge in the Pyrophos® process
- Impacts of operation for production and regeneration of renewable GAC from dried sludge
- Credits for avoided production of electricity, heat, and mineral N/P/K fertilizers in relation to the products of each scenario

This LCA serves as an example for upgrading a large WWTP with innovative processes for nutrient removal or production of renewable GAC. The specific situation of WWTP Altenrhein as a local sludge centre with significant input of external sludge has to be considered when extrapolating the results to other sites. The target group of this study consists primarily of professionals dealing with planning and operation of WWTPs, such as plant operators, engineering companies, and researchers in this field.

Function/ Functional Unit

The function of the systems under study is the treatment of wastewater and sludge according to the quality required for its disposal. In detail, it comprises of a) the treatment of wastewater to reach local effluent standards and b) the treatment and disposal of sludge from internal and external sources, including co-substrates. The LCA includes all relevant processes related to these two functions. However, it is very difficult to identify a dedicated functional unit, as the system functions cover different input materials and services. Hence, it was decided to define an overarching functional unit as “the operation of the systems fulfilling these functions for a period of one year” (“per a”). The amount of raw wastewater and external sludge or co-substrate treated in the system is defined based on information of the WWTP (Table 3).

System boundaries

This LCA includes all relevant processes for wastewater and sludge treatment in the different scenarios (see Figure 3). In particular, it includes the demand of electricity and chemicals for operation of WWTP Altenrhein and the innovative NEXTGEN processes. Major flows of direct emissions into the environment are also accounted, such as effluent water quality of the WWTP, and gaseous emissions of wastewater treatment and sludge disposal. The avoided production of conventional products is subtracted as “avoided burden” in relation to the generated outputs in each scenario (electricity, heat, mineral fertilizer). The additional infrastructure required for the NEXTGEN scenario is also accounted in terms of material demand. For the baseline system, infrastructure already exists and will not change with introduction of the NEXTGEN system.

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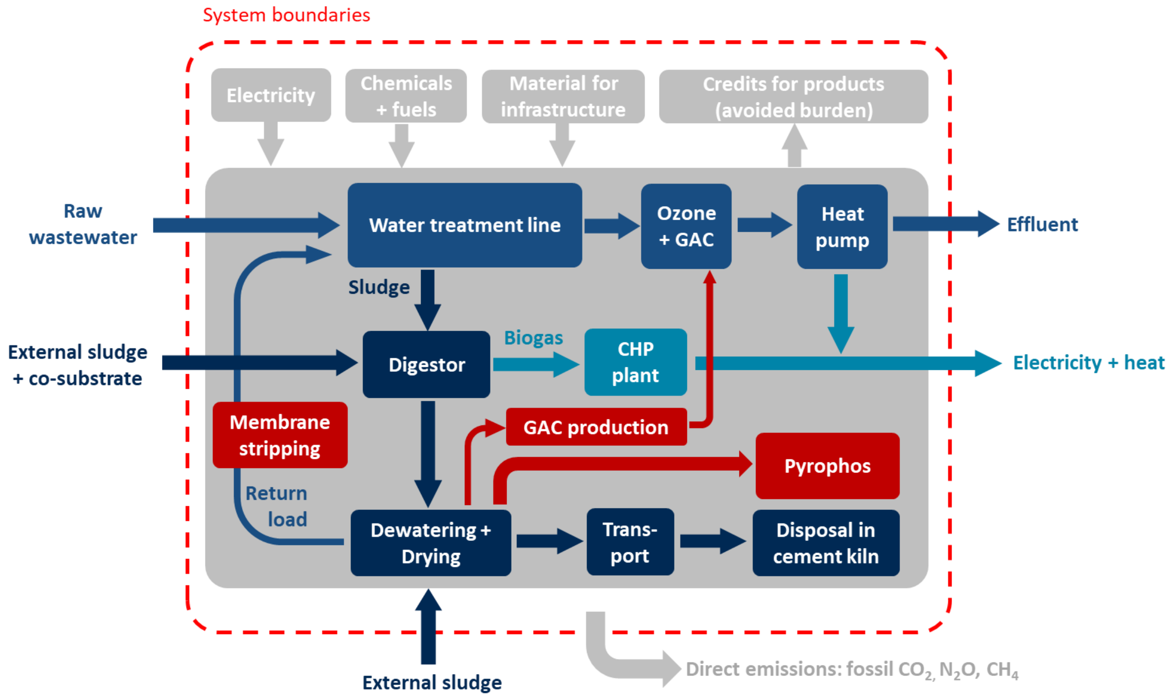

Figure 3: System boundaries of LCA at WWTP Altenrhein (in red: NEXTGEN technologies)

Allocation

Due to the multi-dimensional function of the systems under study, allocation of environmental impacts would be required if the functional unit is related to a specific singular product or service. However, the wide functional definition in this study includes all relevant services into one overarching system function. Therefore, allocation is not necessary, and all environmental impacts of the system are related to the operation of the entire system based on the functional unit ("per a").

Scenarios

This LCA compares five major scenarios:

- **Baseline:** this scenario represents mean operational data of WWTP Altenrhein for the reference year 2020, including both wastewater treatment and sludge treatment. It also includes disposal of dried sludge in a nearby cement kiln.
- **Stripping:** this scenario includes a full-scale membrane stripping unit for treatment of the centrate from dewatering. Relevant impacts of centrate treatment on the mainline WWTP and credits for recovered N product are also accounted.
- **Pyrophos (CH):** this scenario implements a full-scale Pyrophos® process for treatment of dried sludge to produce a PK fertilizer. Meat and bone meal (MBM) ash is added as input to the reactor to enhance the P and K content of the product and comply with the strict Swiss regulations on maximum heavy metal content in recycled fertilizers (ChemRRV, 2020). However, it is important to note that MBM ash is an external input into the process, so that this scenario is not directly comparable with the other scenarios.
- **Pyrophos (EU):** comparable to the previous scenario, a Pyrophos® process is implemented to convert the dried sludge to a PK fertilizer product. However, no

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MBM ash is added in this scenario, as EU regulations allow the utilization of the resulting PK fertilizer regarding its heavy metal content. Hence, it represents a generic "European" case of operating the Pyrophos® process, without the limitations of the Swiss regulation for recycled fertilizers.

- **GAC from sewage sludge:** this scenario reflects the production and regeneration of required GAC for tertiary wastewater treatment based on dried sewage sludge as input material. The regeneration frequency of renewable GAC is estimated in relation to the performance of conventional GAC as benchmark. In addition, a higher ozone dose is required to reach comparable removal of organic micropollutants with renewable GAC.

The size of the systems is related to the actual flows in WWTP Altenrhein in 2020 (Table 3). In total, 9.1 Mm³ of raw wastewater are treated at the site, together with 6000 t dry matter (DM) per year of external sludge and co-substrate. The membrane stripping unit treats 100% of the centrate from dewatering (67,500 m³/a). In the Pyrophos scenarios, the total amount of dried sludge (7,130 t/a) is used as input for the PK fertilizer production. In Swiss conditions, 4,742 t of MBM ash is added to the process. For the scenario using GAC from sewage sludge, a total amount of 122 t renewable GAC per year is required to reach an equivalent performance in removing organic micropollutants than using conventional GAC from hard coal.

Table 3: Scenarios for LCA and size of the systems in Altenrhein case study

Scenario and system	Size	Remarks
Baseline		
WWTP Altenrhein	9.1 Mio m³/a	Influent data of Altenrhein for 2020
External input for sludge line (sludge + co-substrate)	6,000 t DM/a	Details in Table 6
Stripping		
Membrane stripping for centrate	67,500 m³/a	Total centrate volume
Pyrophos CH/EU		
CH scenario	7,130 t dried sludge + 4,742 t MBM ash	Total mass of dried sludge mixed with MBM ash
EU scenario	7,130 t dried sludge	Total mass of dried sludge
GAC from sewage sludge		
Renewable GAC from sludge	122 t/a	More frequent regeneration and higher ozone dose to reach same performance than conventional GAC

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Data quality

Major input parameters for the LCA inventory are discussed below regarding data quality. An overview of data sources and data quality is provided in Table 4.

- Baseline: input data for WWTP Altenrhein is extracted from detailed reporting of operational data for the reference year 2020, and thus has high quality. Disposal of sludge in cement kiln is modelled based on generic KWB estimates (medium quality).
- Stripping: efficiency for N extraction and chemicals demand is extracted from full-scale data collected in previous projects (medium to good quality). Electricity demand, mass balances and direct emissions are based on full-scale data for an operational period at WWTP Altenrhein and are calculated by FHNW (high quality).
- Pyrophos: data for process efficiency, mass balances and product quality is based on results from pilot trials of CTU in NEXTGEN (medium to good quality). Electricity, heat and chemicals demand and production, and direct emissions are estimated by CTU based on design of comparable processes in previous projects (medium quality).
- GAC from sewage sludge: standing time, losses and required ozone dose are extrapolated from pilot trials by FHNW in comparison to conventional GAC. For production and regeneration of GAC, primary data of KWB for GAC production has been used in combination with FHNW data from pilot regeneration (e.g. make-up).
- Background data for production of electricity, chemicals, transport, fertilizers, and materials for infrastructure is taken from LCA database ecoinvent v3.8 (Ecoinvent, 2021).

Indicators for impact assessment

For the impact assessment, indicators are selected with a focus on three aspects: a) primary energy demand and greenhouse gas emissions as indicators for impacts from electricity, chemicals, and materials for infrastructure b) water quality parameters for N and P emissions as indicators for impacts from wastewater treatment effluent and c) acidification to account for direct gaseous emissions from wastewater treatment and sludge disposal.

In detail, the following indicator models are used for impact assessment:

- Cumulative energy demand (CED) of fossil and nuclear resources (VDI, 2012)
- Global warming potential (GWP) for a time horizon of 100a (IPCC, 2014)
- Freshwater eutrophication potential (FEP), marine eutrophication potential (MEP) and terrestrial acidification potential (TAP) from the ReCiPe method v1.13 (hierarchist perspective, without long-term emissions) (Huijbregts et al., 2017)

For system modelling and calculation of indicators, the LCA software UMBERTO® LCA+ has been used (IFU, 2018).

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Table 4: Data sources and quality for LCA of WWTP Altenrhein

Parameter/ Process	Data source	Data quality
Baseline		
Water quality	WWTP data (2020)	Good
Sludge data	WWTP data (2020)	Good
Electricity + chemicals	WWTP data (2020)	Good
Disposal in cement kiln	KWB model	Medium
Stripping		
Efficiency for N extraction	KWB estimate	Medium to good
Electricity + chemicals	FHNW (full-scale data) + KWB estimates	Medium to good
Mass balance (sludge)	FHNW (full-scale data)	Good
Direct emissions	FHNW (full-scale data)	Good
Pyrophos		
Efficiency + mass balance	CTU data (design + pilot trials)	Medium to good
Electricity + chemicals	CTU design data	Medium
Heat balance	CTU design data	Medium
Direct emissions	CTU design data	Medium
GAC from sewage sludge		
Standing time, losses, O_3 dose	FHNW (extrapolation of pilot trials)	Good
Production + regeneration	KWB data, FHNW for make-up	Medium to good
Background data	Ecoinvent database (v3.8)	Medium to good
Electricity	Swiss power mix	Good
Chemicals, materials	Europe or world market	Medium to good
GAC production	KWB data	Good
Fertilizer production	Swiss market mix	Good

Input data for LCA

Primary data

Inventory data for this study is provided by the WWTP operator (AVA, 2021) and the project partners FHNW and CTU based on results from full-scale operation, pilot trials and up-scaling of processes. Data gaps have been filled with available process data from previous projects and estimates by KWB.

Water quality

Water quality data includes raw wastewater flow to WWTP, WWTP effluent, and centrate for dewatering (Table 5). Baseline data is extracted from operational data for the reference year 2020 (AVA, 2021). For scenarios with Pyrophos (CH/EU) and renewable GAC, water quality is not affected. For the stripping scenario, N load in centrate is reduced by 85% as best estimate. It is assumed that 75% of N can be recovered as diammonium sulfate in the

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product (Böhler et al., 2018). 7% of N is emitted as NH_3 during pre-treatment (CO_2 stripping) and will end up in acidic scrubber water, while 3% is lost in sludge water. Potentially, these flows could also be internally recycled to the centrifuge and would increase the recovery potential further up to 85%, but this is not reflected in this study.

In total, N load in centrate (88 t N/a) is reduced to 15% of original value (12 t N/a), which decreases the total N load to the biological stage of the mainline WWTP from 386 t N/a to 310 t N/a. This amounts to a 20% reduction in N load to the biological stage, and this relative reduction is also estimated for the effluent water quality: in the stripping scenario, TN concentration in WWTP effluent is supposed to be reduced by 20% from 28 mg/L to 22 mg/L. In reality, this effect may be different due to operating strategies at the WWTP (e.g. aeration regime, tank volume for nitrification and denitrification) and thus has to be validated in full-scale. However, a reduced TN load to the biological stage offers the potential for a better denitrification with higher COD/N ratios, so an improvement in effluent quality can be expected here.

Table 5: Flow and quality of water for Altenrhein case study: raw wastewater, WWTP effluent, and centrate from dewatering for baseline and stripping scenario

Parameter	Unit	Raw wastewater	WWTP effluent	Centrate from dewatering	WWTP effluent	Centrate after stripping
		All scenarios	Baseline	Baseline	Stripping	Stripping
Volume	[Mm³/a]	9.1	9.15	0.067	9.15	0.061
COD	[g/m³]	579	11.2	1250	11.2	500
TSS	[g/m³]	207	1.4	490	1.4	50
Total N	[g/m³]	34	28	1300	22*	195#
Total P	[g/m³]	5.3	0.22	45	0.22	45
Source		WWTP data	WWTP data	WWTP data	*KWB estimate	#Calculated with stripping data

Sludge balance

Data of the sludge line for excess sludge from WWTP operation and external input of sludge and co-substrate is extracted from operational data of the WWTP, taking average values from 2018-2020 (AVA, 2021). Excess sludge from the WWTP amounts to 2,600 t dry matter (DM) per year, whereas external inputs are significantly higher with around 4,500 t DM/a of sludge and 1,500 t DM/a of co-substrate (Table 6). Biogas from sludge digestion amounts to 3.6 Mio Nm³/a with a methane content of 55%. After digestion, sludge is dewatered to 28% DM with centrifuges and then dried to 91% DM in a low-temperature belt dryer. Dried sludge for disposal amounts to 7130 t per year with a mean content of 69% volatile solids in dry matter.

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Table 6: Flow and quality of excess sludge from WWTP, external input as sludge or co-substrate, and dried sludge to disposal for Altenrhein case study

Parameter	Unit	Excess sludge	External raw sludge to digestor	Co-substrate to digestor	External digested sludge	External dewatered sludge	Dried sludge to disposal
		Baseline	Baseline	Baseline	Baseline	Baseline	Baseline
Mass	[t/a]	80,933	6,900	11,700	27,100	11,800	7,130
Dry matter (DM)	[%]	3.2	2.5	12.4	4.3	27	91
Volatile solids	[% of DM]	72	71	92	58	67	69
Total N	[% of DM]	5	2.9	6.9	4.7	5.7	7.2
Total P	[% of DM]	2.9	3.3	2	4.8	4	4
Source		WWTP data	WWTP data	WWTP data	WWTP data	WWTP data	WWTP data

Baseline data for sludge line is not changed within NEXTGEN scenarios, as the small sludge volume from pre-treatment of stripping (<30 t DM/a) is neglected here.

Disposal of dried sludge is usually done in a cement kiln (80 km truck transport), where the sludge is used as renewable fuel for the process. In Pyrophos scenarios, the dried sludge is treated with a combination of pyrolysis and fluidized bed incineration and addition of a potassium source to product a fertilizer product. Related mass balances have been estimated by project partner CTU based on pilot trials and up-scaling of the process to a full-scale unit. In the Pyrophos (CH) scenario for Swiss conditions, dried sludge is mixed with MBM ash (4,740 t/a) to enrich the product with P and K and reach strict heavy metal limits for recycled fertilizer products in Switzerland. This option produces 14,300 t/a of fertilizer with a P_2O_5 content of 15% and a K_2O content of 21% (Table 7). In the Pyrophos (EU) scenario, dried sludge can be processed without addition of MBM ash, producing 7,560 t/a of fertilizer product with 8% P_2O_5 and 12% K_2O. For both scenarios, P and K content in the fertilizer product is credited with an equivalent amount of substituted mineral fertilizer (Table 9).

Table 7: Mass balance for Pyrophos scenarios (CH and EU) for inputs and fertilizer products in Altenrhein case study

Parameter	Unit	Dried sludge to disposal	Meat and bone meal ash	Fertilizer product	Fertilizer product
		CH/EU	CH	CH	EU
Mass	[t/a]	7,130	4,740	14,300	7,560
Dry matter (DM)	[%]	91	100	100	100
P_2O_5	[t/a]	593	1,530	2,123	593
K_20	[t/a]	22	86	2,968*	872*
Source		WWTP data	CTU design	CTU design	CTU design

** including K from additive (Table 9)*

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Direct emissions of processes

Direct emissions of processes are accounted for the biological stage of the WWTP (N_2O, NH_3), the CHP plant (CH_4, NO_x, SO_2, N_2O), the centrifuge for sludge dewatering (CH_4), the co-incineration in cement kiln (N_2O), the stripping process (NH_3), and the Pyrophos process (NO_x, SO_2). CO_2 emissions from biogas use in CHP or incineration of dried sludge in cement kiln and Pyrophos process are expected to be of biogenic origin, so that no global warming potential is accounted for these emissions.

For the biological stage of the WWTP, NH_3 emissions are estimated to 0.6% of influent N load (Bardtke et al., 1994). For N_2O from biological nitrogen removal, a detailed monitoring campaign for the WWTP was done in previous projects for the baseline situation and the impact of lower N load with N stripping of the centrate (Böhler et al., 2016). As the WWTP is overloaded with N due to the high share of N load from centrate, the baseline emissions of N_2O amount to 1.8% of the N load to the biological stage (Gruber et al., 2020), which is high compared to typical emission factors at other WWTPs (Gruber et al., 2021). In a mitigation experiment, N_2O emissions of Altenrhein WWTP could be reduced by 80% if no centrate is added to the inflow (Gruber et al., 2020). As N load from centrate can only be reduced by 85% in this study, an overall reduction of 68% in emissions factor (80% x 85%) is assumed here. Finally, an N_2O emission factor of 0.6% is used for the biological stage for the stripping scenario, reducing the total N_2O emissions by 5830 kg/a.

For direct emissions of the CHP plant, emission data from a previous study is used (Ronchetti et al., 2002). A methane slip of 0.5% has been estimated for the CHP. For methane losses at the centrifuge, it is assumed that digested sludge is saturated with dissolved methane (20 mg/L CH_4 at 30°C) which is fully stripped in dewatering. For incineration of dried sludge in cement kiln, an N_2O emission factor of 100 g N_2O per ton dry matter is assumed. In the Pyrophos process, no N_2O emissions are accounted due to favourable incineration conditions for N_2O mitigation (info of CTU). For NO_x and SO_2, emission factors of 1.8 g and 0.18 g per kg input DM of dried sludge are expected for the Pyrophos off-gas after extensive gas cleaning.

For the stripping process, 7% of incoming N load is emitted as NH_3 during pre-treatment of centrate for CO_2 stripping. Off-gas from pre-treatment is further treated in an acidic scrubber, which can reduce NH_3 emissions by 99%.

Electricity, chemicals and material for infrastructure

Inventory data for electricity and heat demand and production of major processes are listed below (Table 8). Input data for WWTP operation is extracted from detailed process data of 2020 (AVA, 2021). Total electricity demand of the WWTP of 10.3 GWh/a can be satisfied by 75% with internal electricity production from CHP and photovoltaic modules. For the heat balance, the WWTP has a surplus heat of around 2 GWh/a, which can potentially be exported to the local district heating network.

In the stripping scenario, an additional 40 MWh/a of electricity is used by the stripping process. Thereof, 30 MWh/a are for the stripping unit itself (0.5 kWh/m³ centrate), and 10 MWh/a are estimated for concentrating the product with forward osmosis (data of FHNW). In the mainline, the lower N load (-75 t N/a) leads to savings in aeration energy, which are estimated to 55 MWh/a using typical oxygen balances for nitrification and denitrification (DWA, 2016a) and an effective electricity demand of 0.7 kWh/kg O_2. The stripping also requires heat (7.7 kWh/m³ centrate), which reduces the overall heat surplus by 469 MWh/a.

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For the Pyrophos scenarios, electricity and heat balance of the WWTP are not affected. The operation of the Pyrophos process requires electricity of around 1 GWh/a (140 kWh/t sludge input), but also produces electricity from off-gas heat in the range of 1.8 GWh/a. For the heat balance, the process has a net output of 12 GWh/a (1.9 MWh/t DM in sludge) which can be recovered and exported to the district heating network. If this heat is used internally for drying (e.g. in summer periods with little demand from district heating), electricity consumption of the heat pump could be reduced by 1.5 GWh/a (not considered here).

The scenario with GAC from sewage sludge requires more electricity for ozonation, as the required ozone dose is increased by a factor 3. Consequently, electricity demand for the water line increases by 961 MWh/a. Data for GAC production and regeneration is listed below with background data.

Table 8: Inventory data for electricity and heat for baseline and NEXTGEN scenarios in Altenrhein case study

Process	Unit	Baseline	Stripping	Pyrophos CH	Pyrophos EU	GAC from sewage sludge
Electricity						
WWTP (water line)	MWh/a	4,208	4,153	4,208	4,208	5,169
WWTP (sludge line)	MWh/a	3,041	3,081	3,041	3,041	3,041
Heat pump	MWh/a	3,020	3,020	3,020	3,020	3,020
Electricity from CHP	MWh/a	-6,955	-6,955	-6,955	-6,955	-6,955
Electricity from PV	MWh/a	-793	-793	-793	-793	-793
Stripping	MWh/a	-	41	-	-	-
Net balance at WWTP	MWh/a	2,521	2,507	2,521	2,521	3,482
Self-sufficiency WWTP	%	75	76	75	75	69
Pyrophos (in)	MWh/a	-	-	1,000	1,070	-
Pyrophos (out)	MWh/a	-	-	-1,811	-1,811	-
Heat						
Heat from CHP	MWh/a	-9,980	-9,980	-9,980	-9,980	-9,980
Heat from heat pump	MWh/a	-8,667	-8,667	-8,667	-8,667	-8,667
Heat to drier	MWh/a	14,350	14,350	14,350	14,350	14,350
Heat to digestor	MWh/a	1,689	1,689	1,689	1,689	1,689
Heat to auxiliary	MWh/a	549	549	549	549	549
Stripping	MWh/a	-	469	-	-	-
Net balance at WWTP	MWh/a	-2,059	-1,590	-2,059	-2,059	-2,059
Self-sufficiency	%	112	109	112	112	112
Pyrophos (net)	MWh/a	-	-	-12,162	-12,162	-

Inventory data for chemical demand and credited products are listed below for each scenario (Table 9). For the baseline WWTP, demand of $FeSO_4$ for P precipitation, polymer for sludge thickening and dewatering, liquid oxygen for ozonation, and conventional GAC for refilling the final filtration is extracted from operational data of 2020 (AVA, 2021). Products

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of the baseline scenario are the surplus heat (2 GWh/a) which can be exported to the local district heating network, and the dried sludge which is used to substitute fossil fuel (hard coal) in the nearby cement kiln. Substitution potential in the cement kiln is calculated via the heating value of dried sludge (8 MJ/kg) and the total mass (7130 t/a).

The stripping unit requires NaOH for pH adjustment (1 mol per mol N at membrane) and sulfuric acid for capturing NH_3 in the product (0.6 mol per mol N in product). Citric acid is required for regular membrane cleaning. The amount of additional polymer to remove suspended solids in pre-treatment is rather low (50 kg/a as active matter). The acid scrubber for the off-gas also requires some sulfuric acid (0.6 mol per mol N in off-gas). The stripping produces 855 t/a of DAS solution with 66 t N/a (7.7% N after concentration).

For the Pyrophos process, KOH is required as reductive potassium additive in high amounts. For off-gas cleaning, the process needs $NaHCO_3$, activated carbon, and NH_4OH, while natural gas is used during start-up. Besides the fertilizer products substituting mineral P and K fertilizer (cf. Table 7), the process also generates a significant amount of heat which is credited for district heating.

Table 9: Inventory data for chemicals and credited products for baseline and NEXTGEN scenarios in Altenrhein case study

Process	Unit	Baseline	Stripping	Pyrophos CH	Pyrophos EU	GAC from sewage sludge
Chemicals						
$FeSO_4$	t/a	180	180	180	180	180
Polymer (a.m.)	t/a	47,7	47,7	47,7	47,7	47,7
Oxygen (liquid)	t/a	126	126	126	126	378
GAC (regeneration)	t/a	41	41	41	41	122
NaOH (50%)	t/a	-	452	-	-	-
H_2SO_4 (96%)	t/a	-	286	-	-	-
Citric acid (100%)	t/a	-	0.64	-	-	-
KOH (100%)	t/a	-	-	3,408	1,013	-
$NaHCO_3$ (100%)	t/a	-	-	135	143	-
Activated carbon	t/a	-	-	7	5	-
NH_4OH (50%)	t/a	-	-	6	18	-
Natural gas	MWh/a	-	-	77	58	-
Credited products						
District heating	MWh/a	-2,059	-1,590	-14,221	-14,221	-2,059
Substitution of hard coal at cement kiln	MWh/a	-15,849	-15,849	-	-	-15,738
Substitution of mineral N fertilizer	t N/a	-	-66	-	-	-
Substitution of mineral P fertilizer	t P_2O_5/a	-	-	-2,123	-593	-
Substitution of mineral K fertilizer	t K_2O/a	-	-	-2,968	-872	-

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In the scenario with renewable GAC, more GAC material is required compared to the baseline using conventional GAC. From extrapolation of pilot trials, the expected standing time of GAC filters until regeneration is shorter with renewable GAC (2.1 a) than with conventional GAC (6.3 a). Hence, 3x more GAC material needs to be regenerated each year to reach an equivalent performance in removal of organic micropollutants with renewable GAC. As required ozone dosing is also threefold higher than the baseline, the amount of liquid oxygen increases by 252 t/a. On top, the dried sludge which is now used for production of renewable GAC (50 t/a of dried sludge) is no longer disposed in the cement kiln, which results in a slight reduction of the credits for disposal (-111 MWh/a).

Required material for infrastructure is roughly estimated for each scenario. For the stripping unit with pre-treatment, 5 t low-alloyed steel, 1 t stainless steel, and 1 t HDPE are needed. For the Pyrophos plant, 1000 m³ concrete, 180 t reinforcing steel, 100 t low-alloyed steel, 10 t stainless steel, and 10 t HDPE are required. For the GAC production, no additional infrastructure is required, as GAC production and regeneration takes place at an external location. Lifetime of the infrastructure is estimated to 15a for HDPE, stainless steel and low-alloyed steel, and 30a for concrete and reinforcing steel.

Background data

Background processes for production of electricity, chemicals, materials, transport, and fertilizer production are modelled with datasets from LCA database ecoinvent v3.8 (Ecoinvent, 2021). A full list of processes and related models is available in the annex (Table 57). Transport of materials is estimated by truck for chemicals (600 km), sludge of WWTP to cement kiln (80 km), and materials for infrastructure (200 km).

For production and regeneration of GAC, primary data of several GAC suppliers is used which has been compiled by KWB in previous studies (DWA, 2016b). For conventional GAC produced from hard coal, an input of 4 kg hard coal, 3.5 kg steam, and 0.1 kWh electricity is assumed per kg virgin GAC product. Emissions from hard coal combustion and transport of GAC from production sites in East Asia (16.000 km per ship and 600 km per truck) are also included. GAC regeneration needs 1.3 kWh natural gas and 0.1 kWh electricity per kg regenerated GAC. Losses during regeneration are assumed to 10% of the material, which has to be replaced by virgin GAC.

For renewable GAC from dried sludge, comparable production data is assumed for steam and electricity demand. However, no hard coal input and resulting emissions are needed, and transport distances are much lower (no ship transport). Input of dried sludge at 91% DM is 4 kg for each kg renewable GAC (=75% loss in activation).

During regeneration of renewable GAC, a loss of 10% of the material is assumed by FHNW based on pilot trials for regeneration. This loss has to be replaced by virgin material produced from dried sludge. With a total demand of 122 t renewable GAC per year, 12.2 t virgin GAC have to be produced from dried sludge, which requires 50 t/a dried sludge.

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LCA results

This chapter presents results of impact assessment, comparing the baseline situation with the NEXTGEN scenarios. Indicators are discussed separately and analyzed towards major contributors, important input parameters, and respective conclusions for the analysis.

Cumulative energy demand (CED)

Total net CED of the baseline amounts to -51 TJ/a (Figure 4). This number illustrates that the current operation at WWTP Altenrhein is actually energy-positive, meaning that more energy is produced on-site than is consumed by the WWTP operation. Major contributors for the gross primary energy demand of operation (42 TJ/a) are electricity for water line (34%), sludge line (24%) and heat pump (24%), followed by chemicals for operation (15%). Total energy credits from WWTP operation amount to -95 TJ/a and originate from produced electricity (27%), produced heat (7%) and especially from dried sludge disposal in cement kiln (65%). Both electricity production from biogas use and also the total amount of dried sludge are closely related to the high amount of external sludge input at the site. Hence, it can be concluded that WWTP Altenrhein has a total energy surplus mainly because it receives a high amount of external sludge and co-substrates, both of which import energy to the site in form of organic matter. This is in contrast to typical definitions of an "energy-positive WWTP", where the energy demand for wastewater treatment can be covered just by products from the process (= no import of substrates).

With the NEXTGEN scenarios, the energy balance either improves or is diminished (Figure 4): with membrane stripping, net CED is slightly increased to -50.8 TJ/a, while using GAC from sewage sludge raises net CED to -44 TJ/a. Only the scenarios with Pyrophos improve the net energy balance, with high benefits in the CH scenario (-160 TJ/a) and lower in the EU scenario (-66 TJ/a). These effects of NEXTGEN are analysed in detail below by focussing on the relative changes between baseline and the respective NEXTGEN scenario.

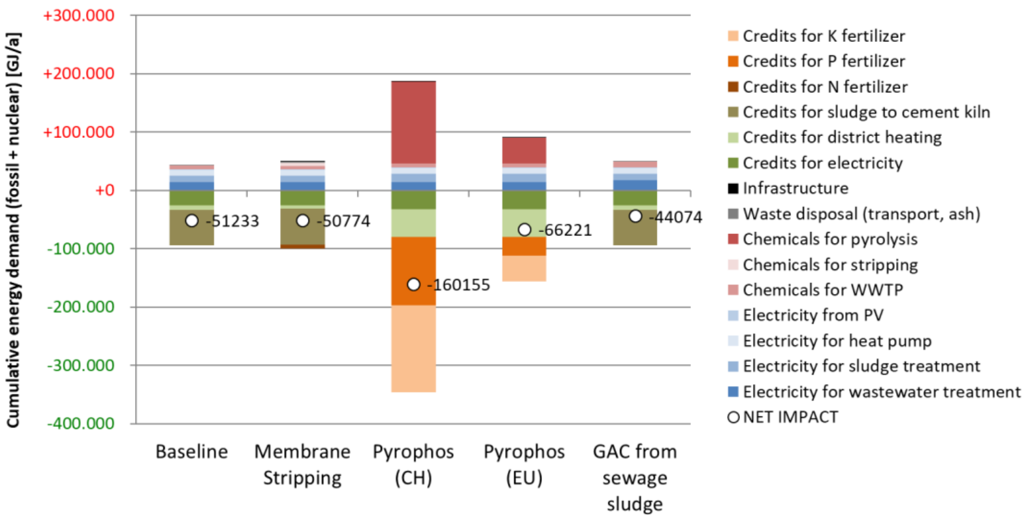

Figure 4: Cumulative energy demand of baseline and NEXTGEN scenario for Altenrhein WWTP

For the membrane stripping, the energy balance shows that additional credits for produced N fertilizer are almost neutralized mainly by chemicals (NaOH) required for the process (Figure 5). On top, stripping requires heat which can no longer be exported to the district heating, so some heat credits are lost. For the total electricity balance, the stripping scenario is actually beneficial, as saved electricity in mainline aeration is higher than electricity

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needed for stripping operation. However, the net CED shows that membrane stripping will add 458 GJ/a to the overall energy balance in total.

Using GAC from sewage sludge also has a negative impact on the net CED (+7159 GJ/a). While virgin GAC production with renewable sources saves primary energy in form of hard coal, the more frequent regeneration required for renewable GAC using natural gas neutralizes this benefit. On top, the higher ozone dose leads to additional demand for electricity and liquid oxygen, and this has a high impact on the overall energy balance of this scenario. Finally, dried sludge used as GAC raw material can no longer be used in the cement kiln, which reduces energetic credits from this route. It becomes obvious that in the present case study, dried sludge can either substitute hard coal as fuel in the cement kiln, or hard coal as raw material in GAC production. Although this is more efficient in GAC production (1 kg dried sludge substitutes 1 kg hard coal) than in cement kiln (1 kg dried sludge substitutes 0.3 kg hard coal), the more frequent regeneration of renewable GAC with natural gas and foremost the higher ozone dose off-set the benefits from using renewable raw materials and lead to an overall increase in net CED.

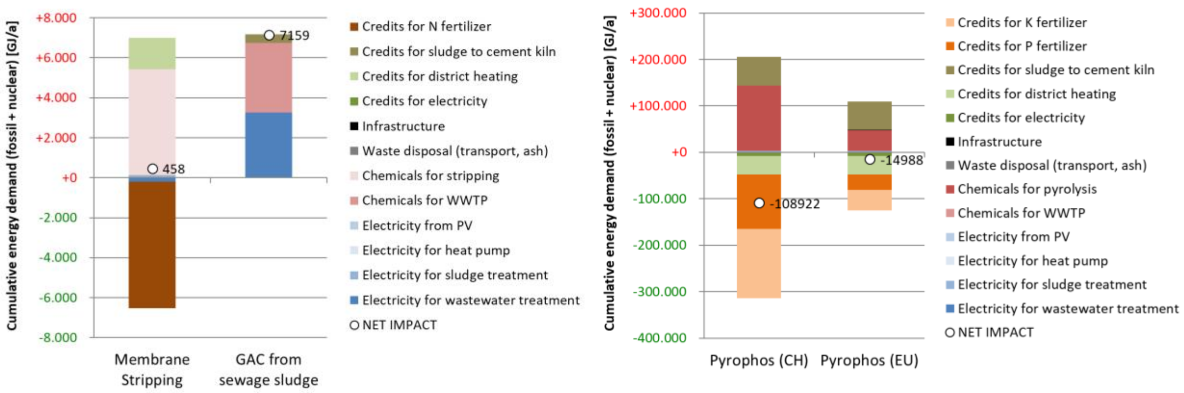

Figure 5: Changes in cumulative energy demand with NEXTGEN scenarios for Altenrhein WWTP (left: stripping and GAC from sewage sludge, right: Pyrophos CH and EU)

The Pyrophos scenarios have a high impact on the net energy balance (Figure 5): while energy is required for chemicals (mainly KOH) and credits of dried sludge disposal in cement kiln are lost, the process can recover both net electricity and heat, and also a high amount of P and K fertilizer. In the net energy balance, KOH input and credits for K fertilizer are in the same range and off-set each other. This is mainly due to the high energy footprint of the K fertilizer mix for Switzerland, which is used for K fertilizer credits in this study. Usually, KOH would have a higher energy demand for production (due to required caustic) than K fertilizer which is based on KCl input. The high energy demand of K fertilizer for Switzerland should be checked and validated in the LCA database. Energy content in dried sludge is recovered less efficient with Pyrophos, as lost credits in cement kiln (62 TJ/a) are higher than electricity output (-6 TJ/a) and excess heat (-41 TJ/a) of the Pyrophos process. Finally, the major energetic benefit of Pyrophos is the production of a plant-available P fertilizer and the substitution of the related amount of mineral P. This results in an overall benefit in net CED of -15 TJ/a for the EU scenario and -109 TJ/a in the CH scenario. For the latter scenario, it has to be kept in mind that MBM ash is added as an external substrate here and comes at no energetic cost.

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Global warming potential (GWP)

For GWP, results are closely related to energy inputs and outputs, but also to other products and direct emissions of processes. The net GWP of the baseline scenario amounts to -2607 t CO_2e/a (Figure 6). For GWP, the impact of credits from sludge disposal are even more important (89% of total credits) than for CED, which is mainly due to the high CO_2e footprint of the substituted hard coal in the cement kiln. In contrast, electricity demand and production at the WWTP are not so relevant for the GWP: the Swiss power mix has a low CO_2e footprint (39 g CO_2e/kWh), so that this factor has a low impact in GWP. Direct emissions of N_2O from the biological treatment of nitrogen in the water line also add substantially to the GWP of WWTP operation (75% of gross CED). Overloading of WWTP with a high share of N load from centrate leads to a high N_2O emission factor, and consequently to a high contribution of this powerful GHG gas to the net GWP balance.

In the NEXTGEN scenarios, net GWP can be substantially reduced with membrane stripping (-4074 t CO_2e/a) and Pyrophos (CH scenario: -8080 t CO_2e/a). For the Pyrophos EU scenario, net GWP increases to -1695 t CO_2e/a, while the use of renewable GAC from sludge increases it to -2400 t CO_2e/a. Again, the changes in GWP with NEXTGEN are analysed in detail below to track the most important effects of each scenario compared to the baseline.

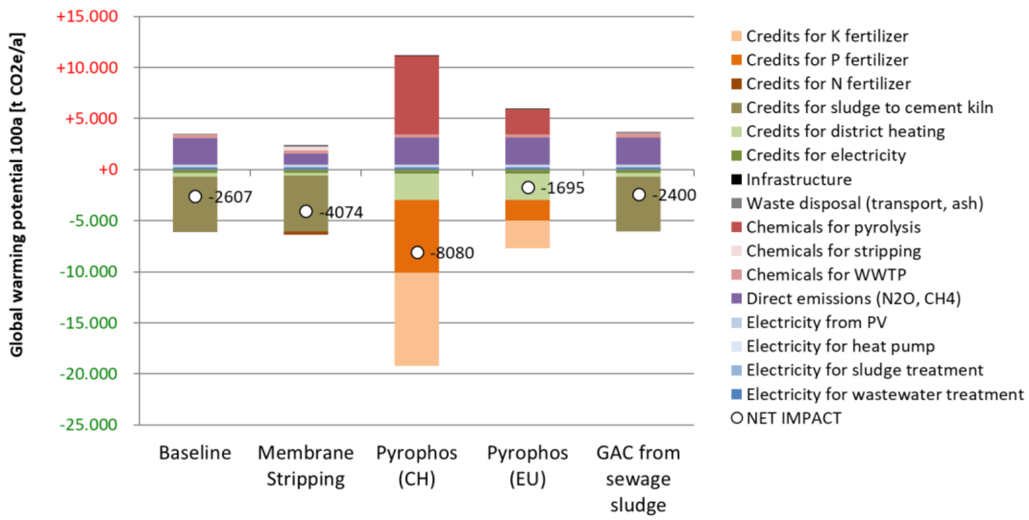

Figure 6: Global warming potential of baseline and NEXTGEN scenario for Altenrhein WWTP

For membrane stripping, it becomes obvious that the major benefit in GWP comes from the reduction of direct N_2O emissions of biological N removal in the water line (Figure 7). While credits for N fertilizer are more than off-set by chemical and heat demand of the stripping process, the lower N load to the mainline leads to a major reduction of 5.8 t N_2O/a or 1540 t CO_2e/a. In fact, this benefit of membrane stripping for the GWP balance is particularly high for WWTP Altenrhein, because the plant is overloaded with N and suffers from high N_2O emissions. This has to be considered when transferring the results of this LCA to other locations. It has been, however, also a strong motivation for WWTP Altenrhein to implement the stripping process at their site and improve their GHG balance.

The scenario with renewable GAC has a negative impact on net GWP, increasing it by 207 t CO_2e/a (Figure 7). While production and regeneration of renewable GAC has lower net GWP compared to conventional GAC, the higher ozone dose with electricity and oxygen demand and also the lost credits in cement kiln off-set this advantage and lead to a significant additional GWP for this scenario. Focussing on the use of sludge as GAC raw material, the

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use of dried sludge in cement kiln is better for the total GHG balance than substituting hard coal in the GAC production process if the renewable GAC has to be regenerated more often.

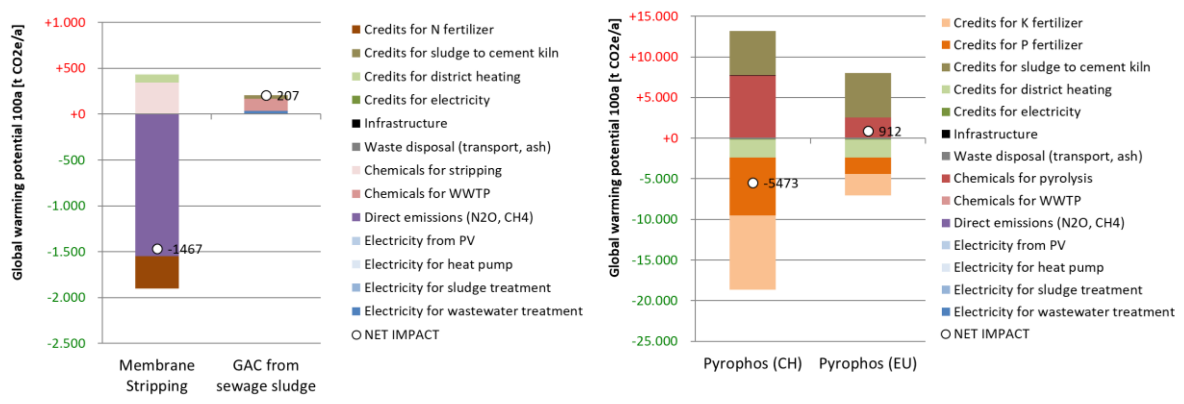

Figure 7: Changes in global warming potential with NEXTGEN scenarios for Altenrhein WWTP (left: stripping and GAC from sewage sludge, right: Pyrophos CH and EU)

For the Pyrophos scenarios, the GWP balance shows that the energetic use of dried sludge in cement kiln yields more benefits (5447 t CO_2e/a) than the energy recovered in Pyrophos in the form of electricity and heat (sum of 2318 t CO_2e/a). On top, GWP credits for mineral P and K fertilizer are partially neutralized by chemical needs for the process (KOH), given the high CO_2e footprint of K fertilizer in Switzerland according to the LCA database. Nevertheless, the CH scenario with external input of MBM ash still has a substantial benefit for GWP (-5473 kg CO_2e/a) due to the high amount of P and K fertilizer recovered. In contrast, the EU scenario increases net GWP by 912 t CO_2e/a (Figure 7): here, the benefits of P/K recovery are outweighed by the inferior use of the energetic potential of dried sludge. These results illustrate that the use of dried sludge as input for nutrient recovery processes is always in competition to the "pure" energetic use of this substitute fuel, and that the overall GHG balance is mainly driven by the efficiency of its energetic use at the specific location. In this regard, using dried sludge for the Pyrophos process is not competitive to disposal in a cement kiln especially in Switzerland, as the energetic products of Pyrophos come with a lower GWP credit (low CO_2e of Swiss electricity and district heating) than the use in a cement kiln (high CO_2e of hard coal, independent of the location).

Freshwater eutrophication potential (FEP)

FEP of the baseline scenario amounts to 1.7 t P-eq/a, which mainly originate from P emissions with WWTP effluent (Figure 8). Some credits in FEP come with the sludge disposal in the cement kiln, as substitution of hard coal decreases potential P emissions in coal mining. The NEXTGEN scenarios do not impact P effluent of the WWTP, so that membrane stripping and GAC from sludge both have a comparable FEP to the baseline (1.7 t P-eq/a).

In the Pyrophos scenarios, FEP is affected by chemical production (KOH) and substitution of mineral P/K fertilizer. Moreover, these scenarios lose the FEP credit of hard coal substitution in the cement kiln. Substitution of mineral P fertilizer with NEXTGEN products obviously reduces P losses into the environment from mining of P rock. Production of mineral K fertilizer is associated with KCl mining: here, direct emissions of P are not relevant, but the high energy use during KCl processing introduce some indirect P emissions in the life-cycle of mineral K fertilizers and chemicals. Overall, the Pyrophos CH scenario reduces FEP by around 100 kg P-eq/a with its high substitution of mineral P fertilizer, whereas the EU scenario increases FEP by 230 kg P-eq/a (Figure 8).

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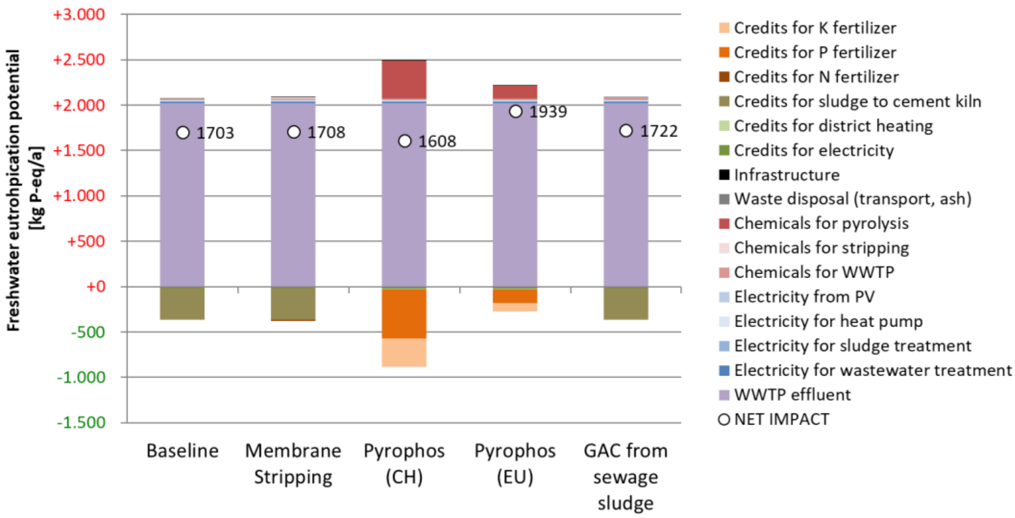

Figure 8: Freshwater eutrophication potential of baseline and NEXTGEN scenarios for Altenrhein WWTP

Marine eutrophication potential (MEP)

MEP of all scenarios is completely dominated by direct N emissions with WWTP effluent (Figure 9). MEP of the baseline accounts for 262 t N-eq/a, which is not changed significantly with NEXTGEN scenarios for Pyrophos or renewable GAC. However, membrane stripping will decrease MEP of the system by almost 54 t N-eq/a, mainly due to the better WWTP effluent quality. As the current WWTP is overloaded with N, a reduction of N load from the centrate will most probably lead to a lower TN concentration in the WWTP effluent. However, this effect has to be supported by a suitable operational regime at the WWTP (aeration setpoints, anoxic volume for denitrification) and should be validated with primary data from the WWTP once the stripping unit is operated continuously.

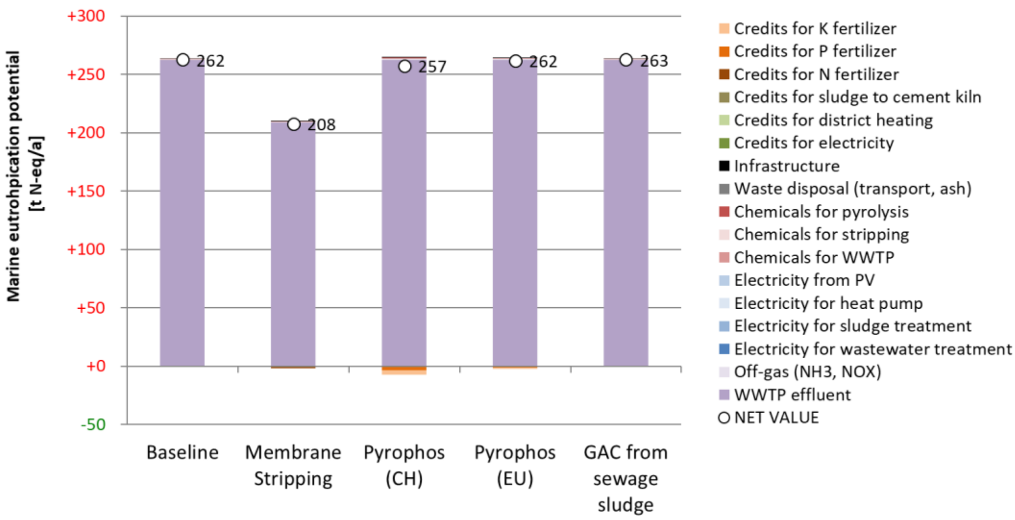

Figure 9: Marine eutrophication potential for baseline and NEXTGEN scenarios for Altenrhein WWTP

Terrestrial acidification potential (TAP)

TAP of the baseline scenario amounts to -11 t SO_2e/a, mainly due to high credits for hard coal substitution in cement kiln (-30 t SO_2e/a) (Figure 10). These credits off-set some life-cycle emissions from WWTP operation, but also direct emissions of NH_3 at the WWTP (17 t SO_2e/a). It has to be noted that these NH_3 emissions are estimated with a generic emission factor for activated sludge WWTPs in this study, which is based on the incoming N load.

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For the stripping scenario, the production of chemicals (NaOH, but also H_2SO_4) causes some additional emissions of acidifying gases and increases net TAP by 3 t SO_2e/a compared to the baseline. The Pyrophos scenarios increase TAP by 15 t SO_2e/a (CH) and 34 t SO_2e/a (EU), mainly because credits from hard coal substitution in cement kiln are lost and KOH has a high energy-related TAP in production. The substitution of conventional GAC with renewable GAC from sludge increases TAP by +2 t SO_2e/a compared to the baseline. Overall, differences in TAP scores of the different scenarios are mostly due to fuel-related emissions in the life-cycle of chemicals and products, and not due to direct emissions on-site.

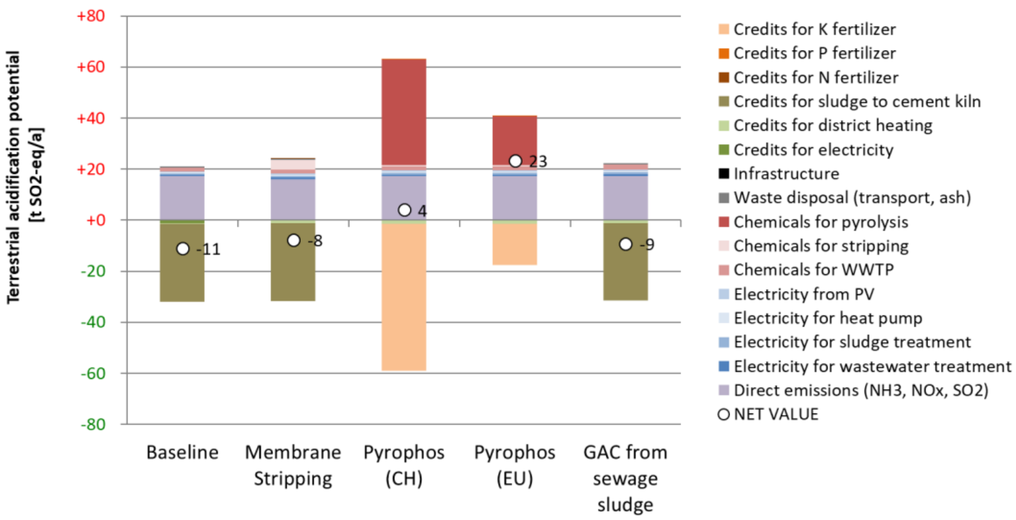

Figure 10: Terrestrial acidification potential for baseline and NEXTGEN scenarios for Altenrhein WWTP

Interpretation and conclusions

Table 10 gives a summary on the net environmental impacts for all calculated impact categories and scenarios for the Altenrhein case study. From the LCA, the following conclusions can be drawn:

- The **current operation of WWTP Altenrhein** is already **energy-positive in its primary energy balance**, meaning that energy value in outputs of the WWTP (heat and dried sludge) is higher than energy required for WWTP operation (electricity + heat). This is mainly due to the high input of external sludge and co-substrates, providing a significant import of organic matter to the system. Most important for the good energy balance is the heating value of the dried sludge, which can be valorised in the nearby cement kiln as substitute fuel. Consequently, **WWTP Altenrhein also has a positive GHG balance**, with high credits from sludge disposal off-setting the operational GHG emissions and also the relatively high N_2O emissions from biological treatment.
- **Membrane stripping** can recover 66 t nitrogen fertilizer per year from the centrate at the cost of additional chemicals and heat. **Energy balance of nitrogen recovery is slightly negative**, as more energy is used for heat and chemicals for stripping than can be saved in mainline aeration and fertilizer production. However, N stripping

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leads to a major reduction of N return load to the mainline, which sharply decreases high N_2O emissions from biological N removal. Overall, **stripping will significantly improve the total GHG balance** of the plant (-1,500 t CO_2e/a), and can also lead to better effluent quality in total nitrogen.

- Producing a PK fertilizer from dried sludge with the **Pyrophos® process** can recycle phosphorus in sludge (~ 260 t P/a) in form of a plant-available fertilizer. The process can also **improve the energy and GHG balance** of the plant. Although energy credits for disposal of dried sludge in the cement kiln are lost, the Pyrophos® process can valorise the heating value of dried sludge into surplus electricity and heat. If sludge is processed together with meat and bone meal ash, the overall GHG balance will improve due to the high amount of recycled P. Operating Pyrophos® only on dried sludge is not beneficial for the GHG balance, as fertilizer and energy output saves less GHG emissions than the use of dried sludge as substitute fuel in the cement kiln.
- Using dried sludge as a **renewable raw material for granular activated carbon** production does **not improve the energy and GHG balance** of the plant. Although the production of fresh GAC from sludge saves on fossil resources such as hard coal, the more frequent regeneration of renewable GAC using natural gas off-sets this benefit in the life cycle of the product. On top, renewable GAC requires a higher ozone dose (3x) to reach a comparable removal of micropollutants to conventional GAC, which adds a significant demand of electricity and liquid oxygen for WWTP operation. Finally, dried sludge used for GAC production can no longer be valorised as substitute fuel in the cement kiln, resulting in lower energy and GHG credits for sludge disposal.

Table 10: Summary of net environmental impacts for WWTP Altenrhein: baseline and NEXTGEN scenarios

Scenario		Base-line	Stripping	Pyrophos (CH)*	Pyrophos (EU)	GAC from sewage sludge
Products of NEXTGEN#	1/a		66 t N	260 t P + 18 t K	260 t P + 18 t K	122 t GAC
Cumulative energy demand (non-renewable)	TJ/a	-51.2	-50.8 (+1%)	-160.2 (-213%)	-66.2 (-29%)	-44 (+14%)
Global warming	t CO_2-eq/a	-2607	-4074 (-56%)	-8080 (-210%)	-1695 (+35%)	-2400 (+8%)
Freshwater eutrophication	t P-eq/a	1.7	1.7 (+-0%)	1.6 (-6%)	1.9 (+14%)	1.7 (+1%)
Marine eutrophication	t N-eq/a	262	208 (-21%)	257 (-2%)	262 (+-0%)	263 (+1%)
Terrestrial acidification	kg SO_2-eq/a	-11	-8 (+25%)	4 (+137%)	23 (+313%)	-9 (+16%)

** additional input of 4,500 t meat and bone meal ash   #originating from wastewater + sludge*

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Overall, the LCA results show that the environmental footprint of WWTP Altenrhein is already quite low in energy and GHG emissions, generating valuable products such as district heat and dried sludge as fuel for the cement kiln. However, NEXTGEN solutions can still help to improve the situation: membrane stripping in the centrate can help to alleviate operational problems from high N return load, is beneficial for the overall GHG balance and can produce a renewable N fertilizer. The Pyrophos® process can recycle P in sludge and also improves the GHG balance, but only when high amounts of other P-rich inputs are processed together with the sludge. The production and use of renewable GAC from sludge is feasible, but competes with the use of sludge as substitute fuel at the cement kiln and is not favourable for the GHG balance given the more frequent need for regeneration and also the higher required ozone dose.

The analysis illustrates that NEXTGEN solutions for nutrient, energy and material recycling can be beneficial for the overall environmental footprint, but need to be efficient in operation and integrated intelligently into the overall WWTP situation. A detailed analysis of the individual WWTP and its operating environment seems to be required to ensure that potential environmental benefits of a circular economy approach can actually be realized. A direct transfer of the results of this LCA to other WWTPs is not possible, as the situation in Altenrhein is quite specific (e.g. function as local sludge centre, high N return load, drying of sludge with heat from heat pump and valorisation in cement kiln) and has a high impact on the outcomes of this LCA.

Input data for this LCA is mainly based on full-scale and pilot trials, but also relies in part on estimates by the project partners. More operational results and primary data of larger systems is required to validate the conclusions from this LCA. Important factors for LCA outcomes are the efficiency of membrane stripping (N yield into product), the energy balance of the Pyrophos® process, and the long-term performance of renewable GAC in comparison to conventional products after regeneration and in relation to ozone dosing upstream.

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Braunschweig (DE): nutrient and energy recovery in municipal wastewater treatment

The WWTP in Braunschweig has a design capacity of 275’000 pe, but does currently treat a raw wastewater load equivalent to 380’000 pe with an average annual volume of 21 Mm^3 wastewater. This overload results in periodic challenges to meet effluent discharge standards, e.g. for nitrogen. The treatment plant consists of primary sedimentation and activated sludge treatment including enhanced biological removal of nitrogen and phosphate. About 50 % of the treated wastewater is used for irrigation of agricultural fields, while another 50 % are stored in infiltration fields and finally discharged to the receiving water body of the Aue-Oker-Channel.

The sludge from primary sedimentation and the excess sludge from activated sludge treatment is digested in an anaerobic treatment step in order to reduce its dry matter and to generate methane, which is used for energy production in CHP plants. The digested sludge is mixed with the irrigation water to supply nutrients to the plants in the growing season and dewatered and disposed in winter. As agricultural disposal of sludge will be banned in Germany in the near future, a nutrient recovery system has been implemented to continue the concept of nutrient recycling and also lower the nitrogen return load to the WWTP. The recovery system in the sludge water from dewatering consists of struvite precipitation and harvest and ammonia stripping and sorption. In addition, a unit for thermal hydrolysis of excess sludge has been installed to enhance methane production in the digesters and also use synergies with nutrient recovery in terms of higher nutrient loads in sludge water (Figure 11).

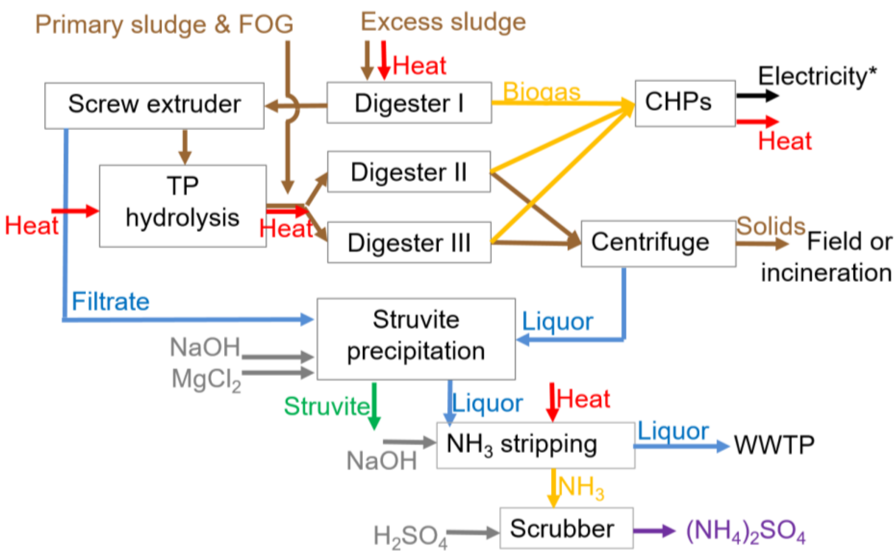

Figure 11: Sludge treatment scheme with thermal hydrolysis, struvite precipitation and NH3 stripping at the Braunschweig WWTP

The present study assesses the environmental effects for this system in different operational modes based on full-scale data and extrapolations. The sludge water from the centrifuge has not used in the nutrient recovery scheme, due to high dry matter loads. Only the filtrate

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from the screw extruder has been used so far, resulting in lower nutrient recovery yields so far.

Goal and scope definition

The goal of this LCA is to analyse potential environmental impacts of the WWTP Braunschweig-Steinhof with different innovations for sludge and sludge water treatment realised within the NextGen project. In detail, the following aspects will be analysed:

- Integration of a thermal hydrolysis of pre-dewatered digested excess sludge in combination with a nutrient recovery system (struvite and ammonium sulphate solution) from sludge water.
- Different options to generate steam for the thermal hydrolysis by biogas or off-gas heat from the CHP
- Systems are analysed for the existing sludge disposal route (irrigation in summer and dewatering and disposal in winter) and a potential future route (year-round dewatering and mono-incineration).

This LCA serves as an example for WWTP dealing with high nitrogen loads in the sludge centrate, while simultaneously targeting to increase biogas yield and recover nutrients to increase nutrient use-efficiency from wastewater. The target group of this study consists primarily of the WWTP operators (e.g. SEBS for Braunschweig), but also planers and engineers and other relevant stakeholders (such as farmers or AVB).

Function/ Functional Unit

The function of the system under study is “to provide wastewater treatment according to the legal requirements” including all processes related to this function. The functional unit of this LCA is defined via the annual organic load of the WWTP calculated in population equivalents (pe) of the WWTP (“per pe and year” or “$[pe \cdot a]^{-1}$”).

System boundary

As this LCA analyses the entire system of wastewater and sludge treatment and disposal, the system boundary includes the complete WWTP, the wetlands for polishing the effluent and also the distribution network for reused water to agriculture, up to the point of water irrigation on the fields. Water and nutrients delivered to agriculture are accounted as credit equivalent for avoided mineral fertilisers and pumping groundwater. Potential field emissions of nutrient reuse are accounted as well as avoided emissions from mineral fertilisers. Biogas is utilised in a CHP and electricity is accounted. Heat is reused in the WWTP as far as possible, however excess heat in the summer month is not accounted. Finally, the system boundary includes background process for production of electricity, chemicals, fuels and materials (see Figure 12).

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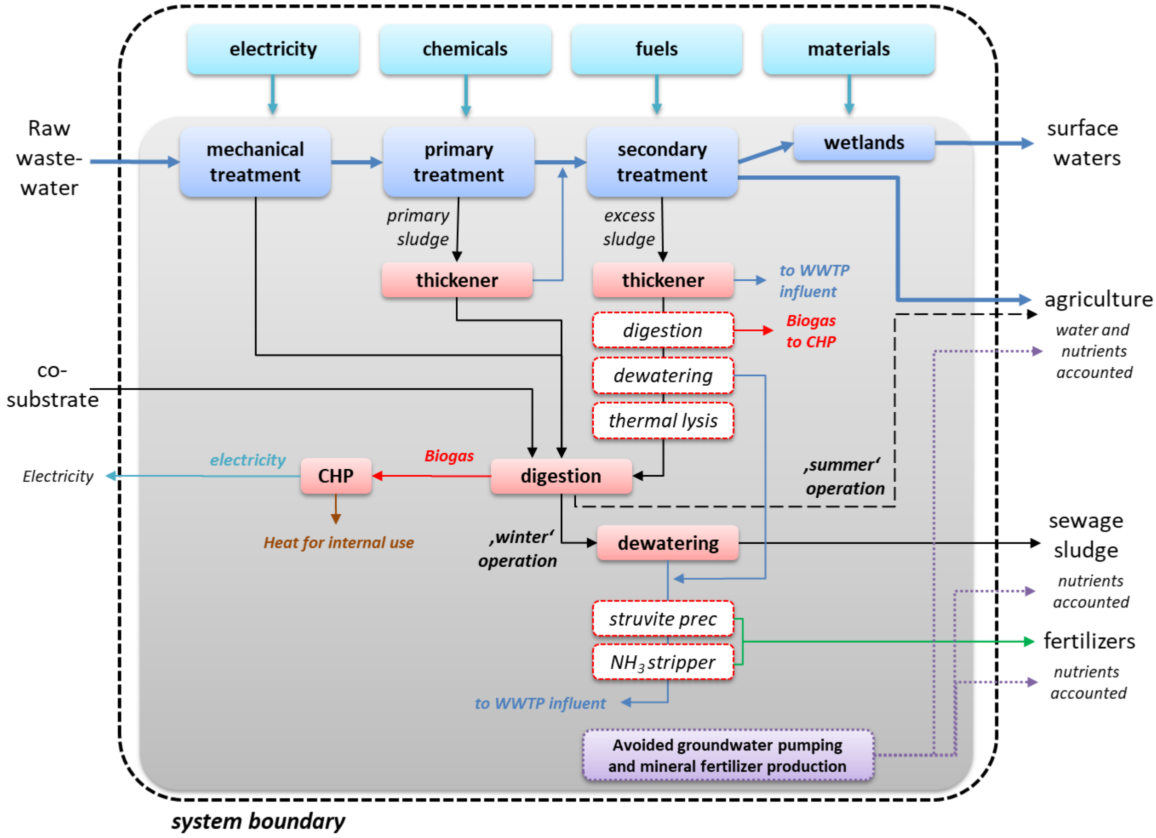

Figure 12: System boundary and scope of the LCA study Braunschweig: baseline plant layout with NEXTGEN technologies in dashed boxes

Allocation

Although the WWTP delivers several functions (wastewater treatment, and water, energy and nutrient recovery), all efforts (e.g. energy consumption) and benefits (e.g. replacement of mineral fertiliser and water delivery) are related to the function of wastewater treatment and its functional unit. So, no allocations are required. Water and nutrients delivered to agriculture are accounted with credits using specific factors with regards to avoided groundwater use for irrigation and avoided mineral fertiliser use (avoided burden approach).

Scenarios

The scenarios have been selected to show environmental benefits and drawbacks of the innovative technologies in different operational modes. The specific scenarios are listed below:

- <u>**Mid-term scenarios (current sludge disposal)**</u>
  1. **Baseline:** This is the scenario prior to the implementation of the NextGen scheme including sludge valorisation via irrigation in summer and sludge valorisation in co-incineration or agriculture in winter
  2. **NG (Steam Gen.):** This is the scenario including excess sludge digestion, pre-dewatering and thermal hydrolysis of pre-dewatered digested excess sludge followed by digestion of hydrolysed excess sludge and primary sludge (so called DLD – digestion, lysis digestion). Both sludge waters (e.g. filtrate from pre-dewatering and centrate from final dewatering) are mixed and fed into nutrient recovery, which consists of struvite precipitation and harvesting and ammonia stripping and

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scrubbing as ammonium sulphate. The steam needed for the thermal hydrolysis is generated by a steam generator using biogas as energy source.

3. **NG (HT CHP):** This scenario is similar to '2. NG (Steam Gen.)', but the steam for the thermal hydrolysis is generated using the high temperature heat from the CHP. Thus, the entire biogas from the digesters is valorised in the CHP and generates more electricity.
4. **NG (Struvite max):** This scenario is also based on 2. NG (Steam Gen.)', but without a provisional struvite precipitation step before final dewatering. This will transfer more ortho-phosphate into the centrate and maximize struvite production.

- **Long-term scenarios (mono-incineration)**
  5. **Baseline:** This scenario is based on scenario '1. Baseline', however the sludge is dewatered year-round and sludge is valorised in a mono-incinerator.
  6. **NG (Steam Gen.):** This scenario is based on scenario '2. NG (Steam Gen.)', however the sludge is dewatered year-round and sludge is valorised in a mono-incinerator.
  7. **NG (HT CHP):** This scenario is based on scenario '3. NG (HT CHP)', however the sludge is dewatered year-round and sludge is valorised in a mono-incinerator.
  8. **NG (Struvite max):** This scenario is based on scenario '4. NG (Struvite max)', however the sludge is dewatered year-round and sludge is valorised in a mono-incinerator.

Data quality and limitations of this study

Major input parameters for the LCA inventory are discussed below regarding data quality and uncertainties and limitations. An overview of data sources and data quality is provided in Table 11.

- **Water and sludge quality and quantities:** All relevant data for water and sludge quality and quantities were provided by the WWTP operator SEBS for 2019. The quantities of certain main- and side streams were calculated based on specific key performance parameters of several aggregates. The data quality is assumed to be good or very good.
- **Key performance parameters, energy and chemical consumption of the innovative technologies:** Parameters as removal efficiency, biogas yield, harvesting efficiency, dry matter results, electricity, heat, natural gas, polymer and chemical consumption had been provided by the WWTP operator SEBS based on full-scale data in selected operation modes during commissioning. The specific consumptions were used to estimate overall consumption yields and volumes. The data quality is assumed to be good or very good.
- **Background data** are discussed for all LCA studies in the annex (Table 57).

Normalisation

Normalisation reveals the contribution of the WWTP in relation to the total environmental footprint of each EU-27 citizen. The normalisation factors are listed in the annex (Table 58).

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Table 11: Parameters, data source and estimated data quality

Parameter/ Process	Data source	Data quality
WWTP - Baseline		
Water quality and quantity	WWTP operator (Siemers, 2021)	very good
Measured sludge and sludge liquor quality parameters	WWTP operator (Siemers, 2021)	very good
Sludge and sludge liquor quantities (volume & loads)	Calculated based on (Siemers, 2021)	good
Energy and chemical consumption	WWTP operator (Siemers, 2021)	very good
Heat balance (CHP, external gas)	Estimated based on (Siemers, 2021)	medium-good
Gaseous emissions from fields/wastewater, heavy metals	Estimated based on Literature (ATV, 2000; EEA, 2016; Eionet, 2017b; Kraus et al., 2019; Parravicini et al., 2016; ReCiPe, 2008)	medium
Nutrient recovery scheme		
Measured sludge and sludge liquor quality parameters	WWTP operator (Siemers, 2021)	good
Sludge and sludge liquor quantities (volume & loads)	Estimated based on (Siemers, 2021)	medium-good
Energy and chemical consumption	WWTP operator (Siemers, 2021)	good
Heat balance (CHP, steam generator, external gases)	Estimated based on (Siemers, 2021)	medium-good

Indicators for impact assessment

For the impact assessment, indicators are selected with a focus on four aspects: a) primary energy demand and greenhouse gas emissions as indicators for impacts from electricity and chemicals b) water quality parameters for N and P emissions as indicators for impacts from wastewater treatment effluent c) acidification to account for direct gaseous emissions from wastewater treatment and sludge disposal and d) human toxicity to assess potential contaminants in recovered nutrient products.

In detail, the following indicator models are used for impact assessment:

- Cumulative energy demand (CED) of fossil and nuclear resources (VDI, 2012)
- Global warming potential (GWP) for a time horizon of 100a (IPCC, 2014)
- Freshwater eutrophication potential (FEP), marine eutrophication potential (MEP), terrestrial acidification potential (TAP) and human toxicity potential (HTP) from the ReCiPe method v1.13 (hierarchist perspective, without long-term emissions) (Huijbregts et al., 2017)

For system modelling and calculation of indicators, the LCA software UMBERTO® LCA+ has been used (IFU, 2018).

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Input data for LCA

Primary data

The inventory data for this LCA study were provided by the WWTP operator (Siemers, 2021) and complemented with estimates based on previous studies (Kraus et al., 2016; Kraus et al., 2019). The sludge and sludge water quantities and qualities for the baseline scenario (5.) is shown in Table 12, whereby for the baseline scenario (1.) 36 % of the digested sludge is irrigated in agriculture, resulting in only 12’000 m³ dewatered sludge and 95’000 m³ centrate.

Table 12: Sludge and sludge water data for baseline scenario (5.)

Parameter	Primary sludge	Excess sludge	Digested sludge	Dewatered sludge	Parameter	Centrate
Volume [m³]	82’000	80’000	170’000	20’000	**Volume [m³]**	150’000
DM [%]	5.0	6.6	3.4	23.0	**SS [mg/L]**	4’000
oDM [% DM]	88	79	73	79	**COD [mg/L]**	1’220
TN [g N/kg DM]	39	102	127	103	**TN [mg/L]**	1’330
TP [g P/kg DM]	9	35	40	43	**TP [mg/L]**	40

The sludge and sludge water quantities and qualities for the NextGen scenario (6.) and (7.) is shown in Table 13 whereby for the corresponding scenarios (2.) and (3.) also 36 % of the digested sludge is irrigated in agriculture, resulting in only 10’000 m³ dewatered sludge and 60’000 m³ centrate.

Table 13: Sludge and sludge water data for NEXTGEN scenario (6.) and (7.)

Parameter	Digested Excess sludge	Pre-dewatered excess sludge	Digested sludge	Dewatered sludge	Parameter	Filtrate	Centrate
Volume [m³]	80’000	24’000	110’000	16’000	**Volume [m³]**	56’000	94’000
DM [%]	4.5	13.0	4.4	25.0	**SS [mg/L]**	550	2’400
oDM [% DM]	69	68	70	70	**COD [mg/L]**	1’350	2’400
TN [g N/kg DM]	137	114	116	97	**TN [mg/L]**	15’00	1’200
TP [g P/kg DM]	53	47	45	44	**TP [mg/L]**	450	150
					PO_4-P [mg/L]	380	40

The sludge and sludge water quantities and qualities for the NextGen scenario (8.) without provisional struvite precipitation in the digested sludge is shown in Table 14 whereby for the corresponding scenarios (4.) also 36 % of the digested sludge is used via irrigation in agriculture, resulting in only 11’000 m³ dewatered sludge and 59’000 m³ centrate.

A detailed inventory on electricity and chemical consumption for the baseline scenario is provided in Figure 13.

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Table 14: Sludge and sludge water quantities and qualities for NextGen scenario (8.)

Parameter	Digested Excess sludge	Pre-dewatered excess sludge	Digested sludge	Dewatered sludge	Parameter	Filtrate	Centrate
Volume [m³]	80’000	24’000	110’000	17’000	**Volume [m³]**	56’000	93’000
DM [%]	4.5	13.0	4.4	23.0	**SS [mg/L]**	550	2’400
oDM [% DM]	69	68	70	70	**COD [mg/L]**	1’350	2’400
TN [g N/kg DM]	137	114	116	97	**TN [mg/L]**	15’00	1’200
TP [g P/kg DM]	53	47	45	40	**TP [mg/L]**	450	310
					PO_4-P [mg/L]	380	200

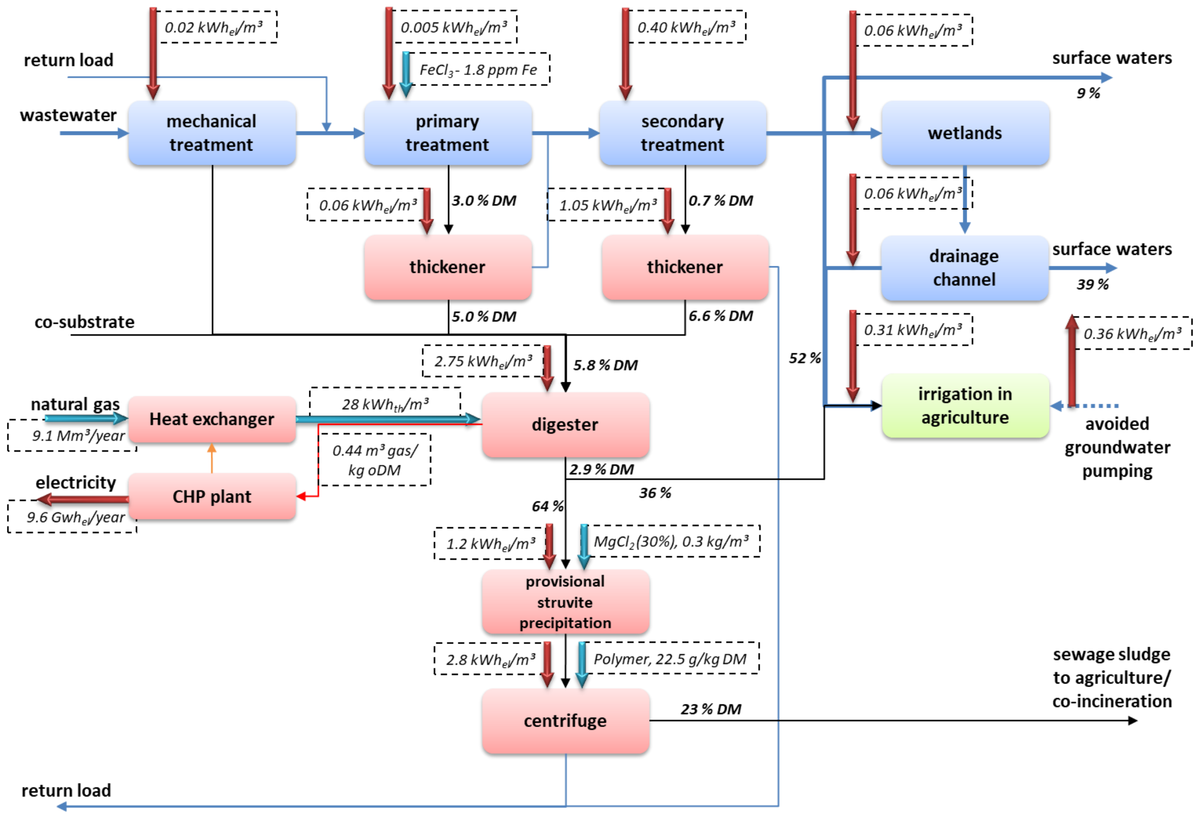

Figure 13: Simplified inventory for electricity and chemical consumption for the baseline scenario (1.)

For the other scenarios (2.-4. and 6.-8.) excess sludge is digested (0.36 m³ gas/kg oDM) separately with a final DM content of 4.5 %, and then pre-dewatered in a screw-press to 13 % DM using 1 kWh_{el}/m^3 and 20 g POL/kg DM. The pre-dewatered digested excess sludge is hydrolysed in a thermal hydrolysis using 1.8 kWh_{el}/m^3 and 130 kg steam/m³. Hydrolysed excess sludge is mixed with primary sludge and digested again (0.43 m³ gas/kg oDM) to a final DM of 4.4%. Digested sludge is then dewatered to 25 % DM using 18 g POL/ kg DM in a centrifuge. This higher dewatering yield and lower polymer consumption was observed in operation, verifying the positive effect of hydrolysis treatment on dewaterability described in literature.

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Both sludge waters, from the screw press and the centrifuge are united and treated in the struvite reactor and the ammonia stripper. The struvite reactor consumes about 1.3 kWh_{el}/m^3, 1 L NaOH (50%)/m^3 and 2.3 L $MgCl_2$ (25%)/m^3. Ortho-Phosphate is precipitated with an efficiency and harvested of 95 %. The ammonia stripper consumes about 1 kWh_{el}/m^3, 9 kWh_{th}/m^3 and 3.3 L NaOH (50%)/m^3. The scrubber consumes about 1.4 L H_2SO_4 (96%)/m^3 sludge water. The efficiency for ammonium removal is also about 95 %.

For the scenarios 2., 4., 6. and 8., steam is generated via a steam generator using biogas. Logically this biogas cannot be used in the CHP to generate electricity and heat. Within the scenarios 3. and 7. this steam is generated via a heat exchanger using the high temperature off-gas heat from the CHP. The heat balances containing heat supply (CHP, steam generated from biogas) and heat demand (digesters, stripper, buildings and thermal hydrolysis) are assessed per month to consider seasonal distribution (Kleyböcker et al., 20222). Heat deficits (in winter months) are covered by natural gas. The balances are shown in Figure 14, Figure 15 and Figure 16.

The aggregated annual inventory data is shown in Table 15.

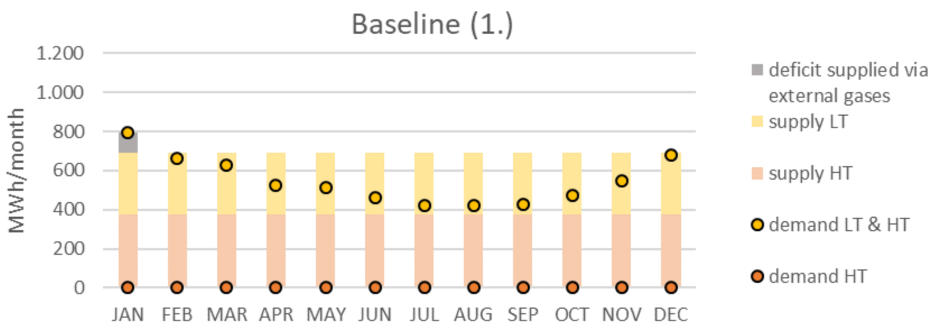

Figure 14: Heat balance for the Baseline scenario (1.)

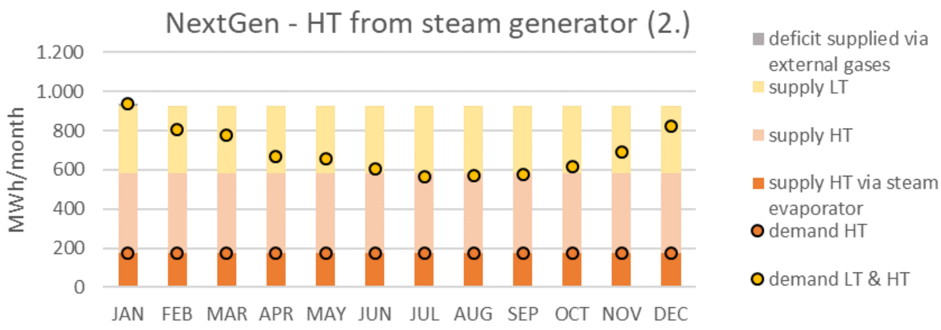

Figure 15: Heat balance for the NextGen – HT from steam generator (2.)

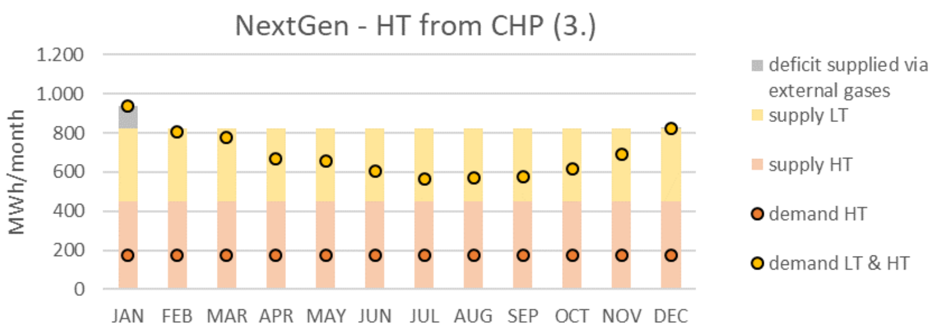

Figure 16: Heat balance for NextGen – HT from CHP (3.)

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Table 15: Annual inventory data (only consumables) for the WWTP

Inventory parameter and unit (annual values)	Mid-term scenarios (current sludge disposal)				Long-term scenarios (mono-incineration)			
	1. Baseline	2. NG (Steam Gen.)	3. NG (HT CHP)	4. NG (Struvite max)	5. Baseline	6. NG (Steam Gen.)	7. NG (HT CHP)	8. NG (Struvite max)
Electricity wastewater treatment [MWh]	8’696	8’609	8’609	8’608	8’797	8’639	8’639	8’638
Electricity sludge treatment [MWh]	2’333	2’771	2’771	2’684	2’595	3’027	3’026	2’889
Electricity effluent distribution [MWh]	4’666	4’663	4’663	4’663	4’654	4’655	4’655	4’655
Electricity credit CHP [MWh]	-9’036	-9’798	-10’795	-9’797	-9’073	-9’848	-10’850	-9’846
Electricity credit avoid. GW pumping [MWh]	-1’166	-1’166	-1’166	-1’166	-1’166	-1’166	-1’166	-1’166
polyacrylamide [t]	85	131	131	131	133	164	164	164
$FeCl_3$ (14 %) [t]	745	783	783	773	751	799	799	786
$MgCl_2$ (25%) [t]	38	308	308	484	61	325	325	587
NaOH (50%) [t]	0	763	763	757	0	993	993	983
H_2SO_4 (96%) [t]	0	299	299	297	0	389	389	385
Natural gas [m^3]	13’868	2’159	15’438	2’069	14’186	5’306	15’791	5’165
Sludge production [t OS]	14’109	11’721	11’721	12’744	22’456	18’469	18’469	20’078
Struvite production [t] (5 % N, 12 % P)	0	142	142	242	0	143	143	294
ASL production [t] (9 % N)	0	1’546	1’546	1’474	0	1’983	1’983	1’875
Electricity coverage WWTP by CHP [%]	**58%**	**61%**	**67%**	**61%**	**57%**	**60%**	**66%**	**61%**
P accounted via water & sludge irrigation [t P]	**88**	**84**	**84**	**84**	**10**	**11**	**11**	**11**
P recovered via struvite [t P]	**0**	**18**	**18**	**31**	**0**	**18**	**18**	**37**
P recovery rate via struvite [%]	**0%**	**7%**	**7%**	**13%**	**0%**	**8%**	**8%**	**16%**
N accounted via water and sludge irrigation [%]	**91**	**76**	**76**	**76**	**29**	**26**	**26**	**26**
N recovered via struvite & ASL [t N]	**0**	**149**	**149**	**148**	**0**	**189**	**189**	**188**
N recovery rate via struvite & ASL [%]	**0%**	**10%**	**10%**	**10%**	**0%**	**13%**	**13%**	**13%**

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Heavy metals in sludge are calculated based on estimates from concentrations from the baseline scenario whereby the heavy metal load in sludge is kept constant independent from the sludge quantity, which varies due to the degree of digestion in the scenarios. The heavy metals in struvite as well as in avoided conventional P-Fertiliser are considered as well (see Table 16) based on literature values. Sludge has a relative P-Fertiliser efficiency of 95 %, whereby struvite and conventional P-Fertiliser have 100 % P efficiency.

Table 16: Heavy metals per phosphate in sludge (Baseline scenario), Struvite and Conventional fertiliser

Metal, Unit	Sludge (Baseline)	Struvite	Conventional Fertiliser
Cd [mg/kg P_2O_5]	15	0.6	53
Cr [mg/kg P_2O_5]	329	14	348
Cu [mg/kg P_2O_5]	2880	69	101
Hg [mg/kg P_2O_5]	6.6	0.8	2.4
Ni [mg/kg P_2O_5]	312	14	91
Pb [mg/kg P_2O_5]	424	14	20
Zn [mg/kg P_2O_5]	9919	124	807

In terms of direct emissions from the sewage treatment plant and the agricultural fields, various emission factors from literature are assumed. Direct N_2O and NH_3 emissions from secondary treatment are estimated to 0.3% for N_2O and 0.6% for NH_3 of the N influent into secondary treatment. For the field emissions for sludge irrigation and valorisation the respective emissions are significantly higher (around 1% for N_2O and 10% for NH_3) based on the N applied. Only 25 % of N in sludge is assumed to have a relative N-fertiliser effect. In contrast the field emissions for mineral fertilisers and ASL are assumed with lower emissions (respectively 0.8 % for N_2O and 2.5 % for NH_3). Nitrate and Phosphate emissions into receiving waters from fields are assumed to be similar (7.3% of N and 5.3% of P).

Background data

Background data for production of electricity, chemicals, materials and transport are based on ecoinvent database v3.6, namely shown in the annex (Table 57).

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LCA results

Cumulative energy demand (CED)

The cumulative energy demand of non-renewable resources for the scenarios is shown in Figure 4. The baseline scenarios require in sum 72 MJ/(pe a) for the current sludge disposal and 81 MJ/(pe a) for year-round dewatering and mono-incineration. The efforts and credits are mainly influenced by electricity consumption in wastewater treatment, water pumping to the irrigation fields and sludge treatment (efforts) and electricity recovery from the CHP and the incinerator and avoided groundwater pumping for irrigation (credits). In terms of different sludge disposal pathways, heat recovery from the mono-incinerator increases credit from sludge disposal compared to electricity from the co-incinerator and nutrient credits in agriculture, when the sludge valorisation scheme is changed in the future. However, the higher overall energy demand for scenario (5.) occurs from additional electricity and polymer consumption due to year-round sludge dewatering.

The NextGen-scenarios slightly increase or decrease the CED by -13 to +18 MJ/(pe a), depending mainly on the way of steam generation for the thermal hydrolysis (see Figure 18). Using biogas to generate steam (scenarios 2., 4., 6. and 8.), the additional biogas from TH used in the CHP to gain electricity is comparably low (+ 8 %), as most of this additional biogas (80 %) is utilised for steam generation. This additional energy recovery is also off-set by the additional electricity and chemical demand in sludge treatment (pre-dewatering including polymer, hydrolysis) and the lower energy recovery from sludge disposal in the incinerator due to the reduced heating value of the sludge. If the steam is generated from the high temperature heat from the CHP via heat exchangers, significant more biogas can be utilised in the CHP, resulting in a higher electricity credit and the overall system reveals savings (scenario 3. and 7.).

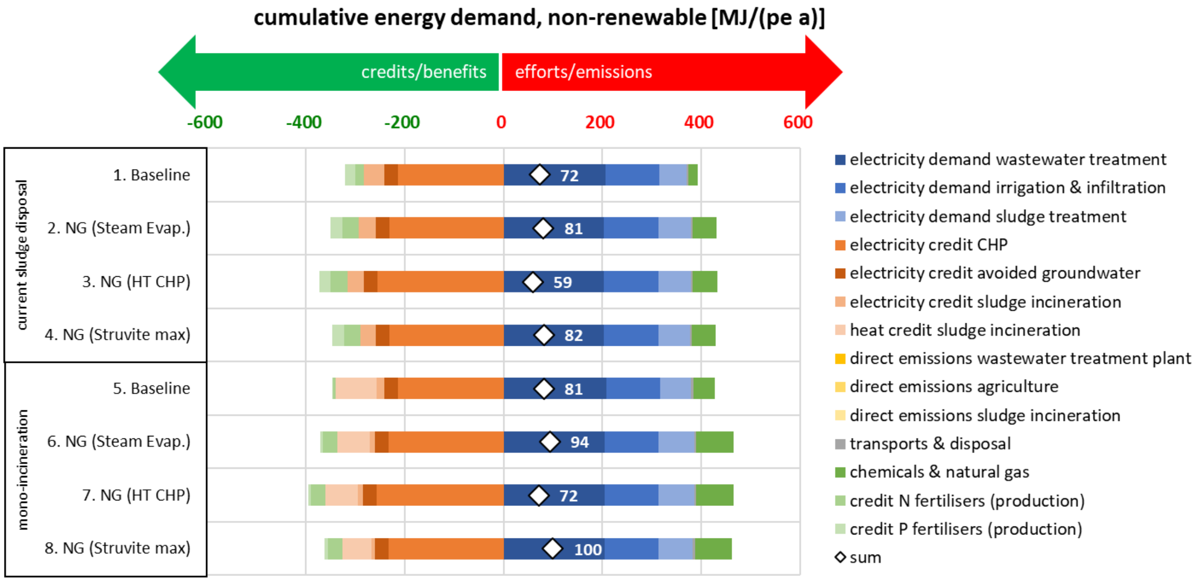

Figure 17: Non-renewable cumulative energy demand for the Braunschweig WWTP

While a significant energy credit is accounted for the recovered N fertiliser, corresponding efforts for chemicals (mainly caustic soda for pH increase prior ammonia stripping and sulfuric acid for ammonia scrubbing) compensate these credits. Normally, heat is also here

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an important factor, however most of the heat needed for the scrubber can be utilised by heat generated from the CHP.

Maximizing the struvite yield (scenario 4. and 8.) is associated with slightly higher credits for recovered P fertiliser, however the lower dewaterability due to present ortho-phosphate species results in a lower sludge heating value of dewatered sludge and higher efforts in sludge drying. In comparison of scenario (2.) and (4.) or (6.) and (8.) it becomes apparent that the higher P yield is energetically unfavourable, due to resulting lower dewaterability.

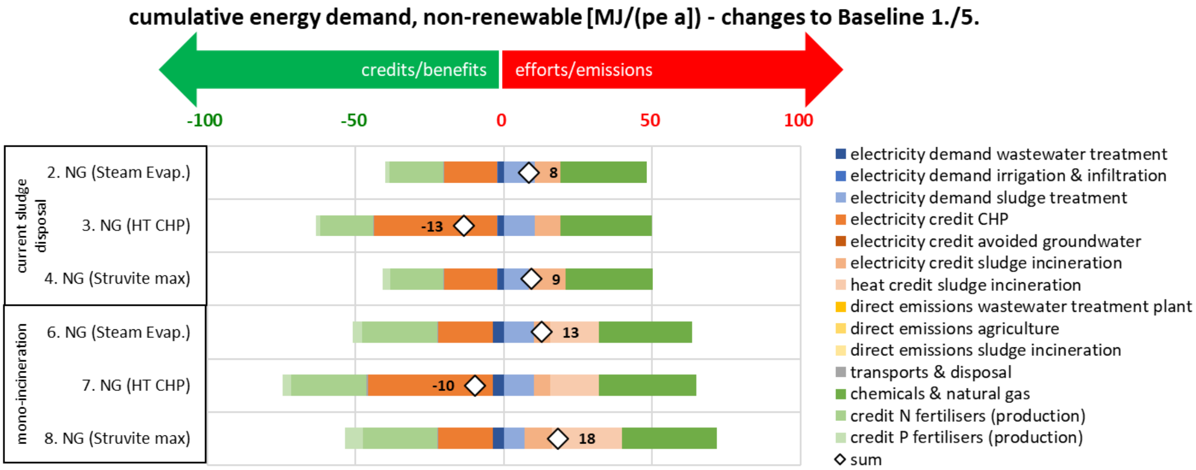

Figure 18: Changes for the non-renewable cumulative energy demand for the Braunschweig WWTP compared to their specific Baseline 1. or 5.

Global warming potential (GWP)

The GWP principally shows similar results to the cumulative energy demand when comparing the scenarios (see Figure 58). This results from a high share of fossil energy in the non-renewable cumulative energy demand and thereby corresponding CO_2 emissions. However, additionally direct N_2O emissions from the WWTP and from sludge and nitrogen valorisation in agriculture or from the mono-incinerator contribute significantly (with about 25%) to the overall GWP assuming the electricity mix from German power mix of 2017 used in this study. The GWP of the baseline scenarios is estimated to 14.9 kg CO_2-Eq/(pe a) for the current sludge disposal and to 16.2 kg CO_2-Eq/(pe a) for the mono-incinerator. The NextGen-scenarios slightly increase or decrease the GWP by -1.9 to +0.2 kg CO_2-Eq/(pe a), depending again on the way of steam generation for the thermal hydrolysis (see Figure 20).

The effects on the GWP via indirect emissions are quite similar to the findings described for the CED. The effect of chemicals is lower for GWP, due to the low CO_2 footprint of sulfuric acid production compared to its fossil energy demand (elemental sulphur from crude oil/natural gas). Each NextGen-scenario reduces the direct emissions of the system: less N_2O comes from the secondary treatment due to lower N return load, and less N_2O comes from sludge or fertiliser valorisation or from the incinerator due to lower N content in the sludge after enhanced digestion. This reduction of direct emissions will be crucial in the future when targeting climate neutrality: the indirect emissions for electricity, heat and chemicals will decline due to a more renewable energy mix in Germany. Therefore, the direct emissions will become more relevant for the net GWP. The reduction of emissions and more targeted application of reactive N species (as mineral fertilisers) can thereby play a crucial role for climate neutrality in sewage treatment.

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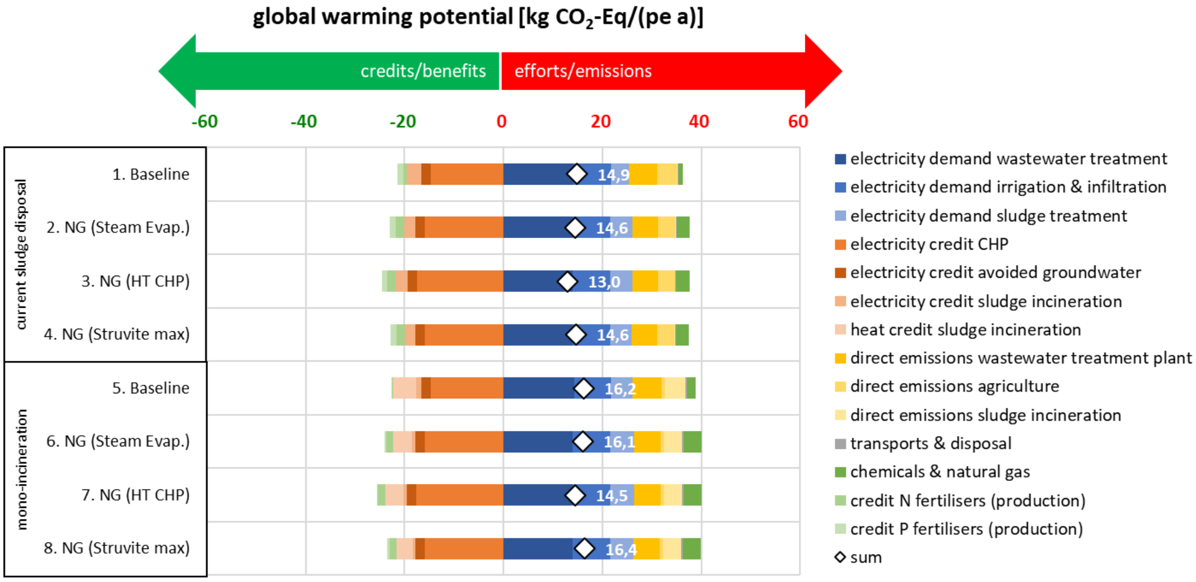

Figure 19: Global warming potential for the Braunschweig WWTP

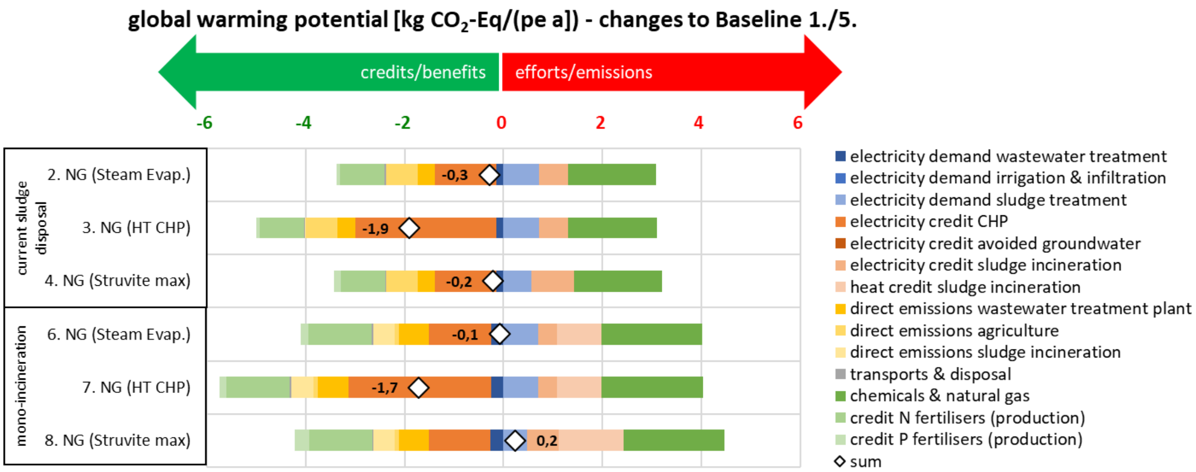

Figure 20: Changes for the global warming potential for the Braunschweig WWTP compared to their specific Baseline 1. or 5.

Terrestrial acidification potential (TAP)

The terrestrial acidification potential (Figure 10) is strongly affected by direct ammonia emissions, mainly due to sludge valorisation in agriculture. The NextGen scheme increases the conversion of organic N into ammonia in digestion and thereby reduces the nitrogen content in sludge, resulting in lower ammonia emissions in agriculture. The switch towards mono-incineration significantly reduces ammonia emissions, as sludge N with low use efficiency and high N losses is no longer applied to the fields.

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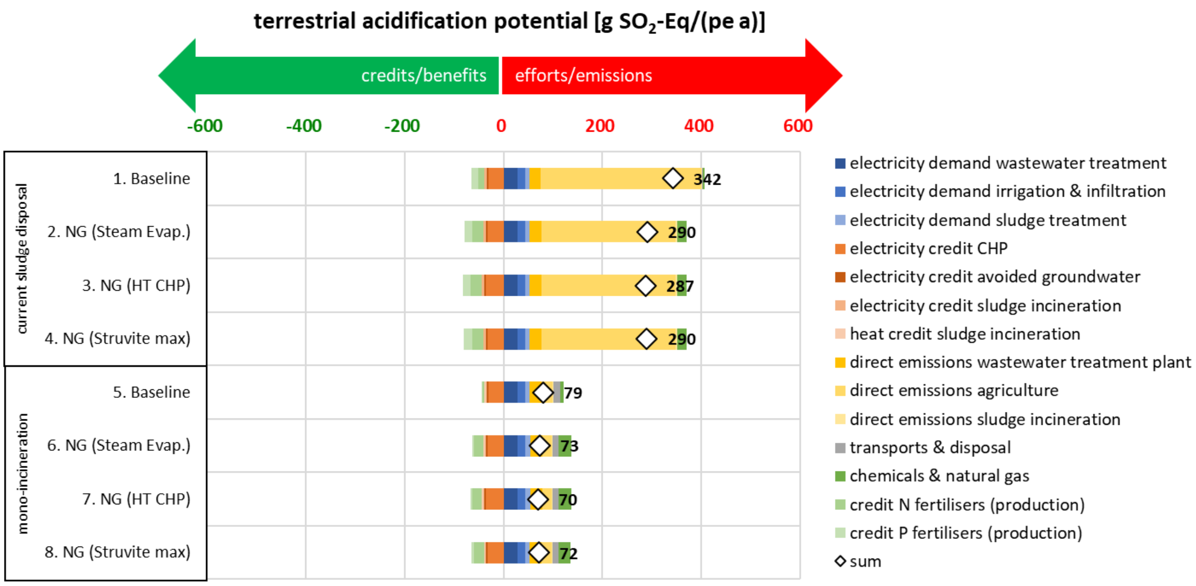

Figure 21: Terrestrial acidification potential for the Braunschweig WWTP

Freshwater eutrophication potential (FEP)

The freshwater eutrophication potential (see Figure 8) is highly influenced by the phosphate concentration in the WWTP effluent. Effects on freshwater water bodies via direct emissions from sludge valorisation level out with substituted conventional phosphate fertilisers and their corresponding emissions due to the high P fertilising efficiency of sludge. The phosphate effluent concentration is not affected by the NextGen scheme, since the baseline scenario already contains a provisional struvite precipitation removing ortho-Phosphate from the return load. The slight increase in direct emissions occurs due to organic P species in the centrate from the final dewatering step due to a poor degree of separation regarding dry matter. These organic P species cannot be removed via struvite precipitation, whereas the TP return load increases.

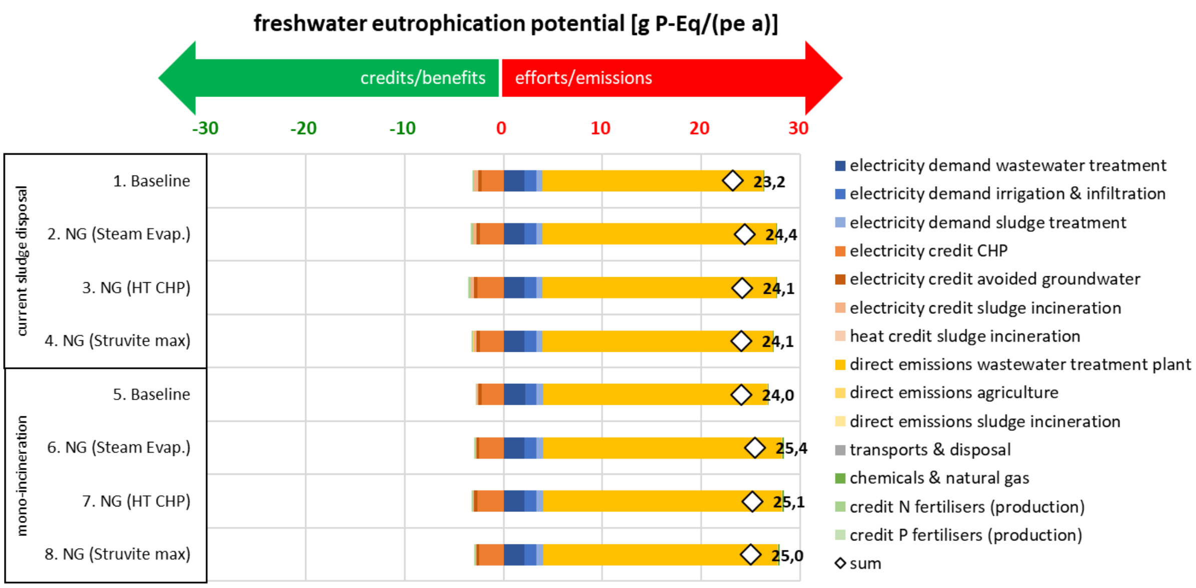

Figure 22: Freshwater eutrophication potential for the Braunschweig WWTP

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Marine eutrophication potential (MEP)

The marine eutrophication potential (see Figure 9) is affected by the N effluent concentration and mainly nitrate emissions from sludge or fertiliser valorisation in agriculture, which are associated with poor N fertilising efficiency rates of sludge. The transfer from agricultural sludge valorisation towards incineration underlines the poor N fertilising efficiency of sludge, resulting in a reduction of MEP with full mono-incineration of sludge. Secondly the NextGen schemes are reducing the ammonium in the return load via stripping and scrubbing, resulting in a further decrease of N species entering secondary treatment and thereby improving the N effluent concentration of the WWTP (- 11 % N).

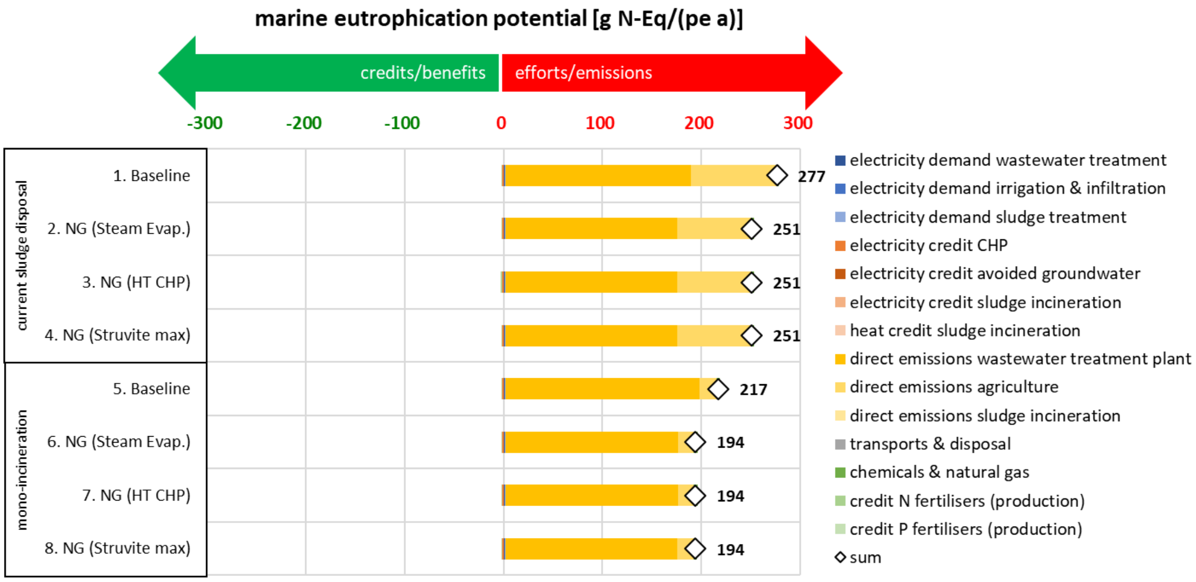

Figure 23: Marine eutrophication potential for the Braunschweig WWTP

Human toxicity potential (HTP)

Human toxicity potential (see Figure 24) is mainly influenced by input of heavy metals on agricultural soils. It decreases for the NextGen schemes especially in combination with the end of sludge application in agriculture. The direct emissions in agriculture are calculated as a net balance between actual heavy metal loads in nutrient products (sludge, struvite) and avoided conventional P fertiliser.

For the current sludge disposal schemes, the heavy metals in sludge end up on soil, whereas corresponding metal loads from substituted conventional fertilisers are avoided. With increase of the recovery rates of struvite with low heavy metal content, this credit for avoided conventional fertilizers increases. If sludge is not recycled to arable land, the heavy metals in recovered water contribute mainly to the HTP score. Due to avoided heavy metals in mineral fertilisers scenario 5. is thereby relatively equal to scenario 1., hence the impact mainly evoked due to zinc emissions from sludge valorisation are replaced by an impact mainly evoked by cadmium emissions from conventional fertilisers. Due to higher recovery rates of struvite with low heavy metal content, the total score for human toxicity potential then decreases.

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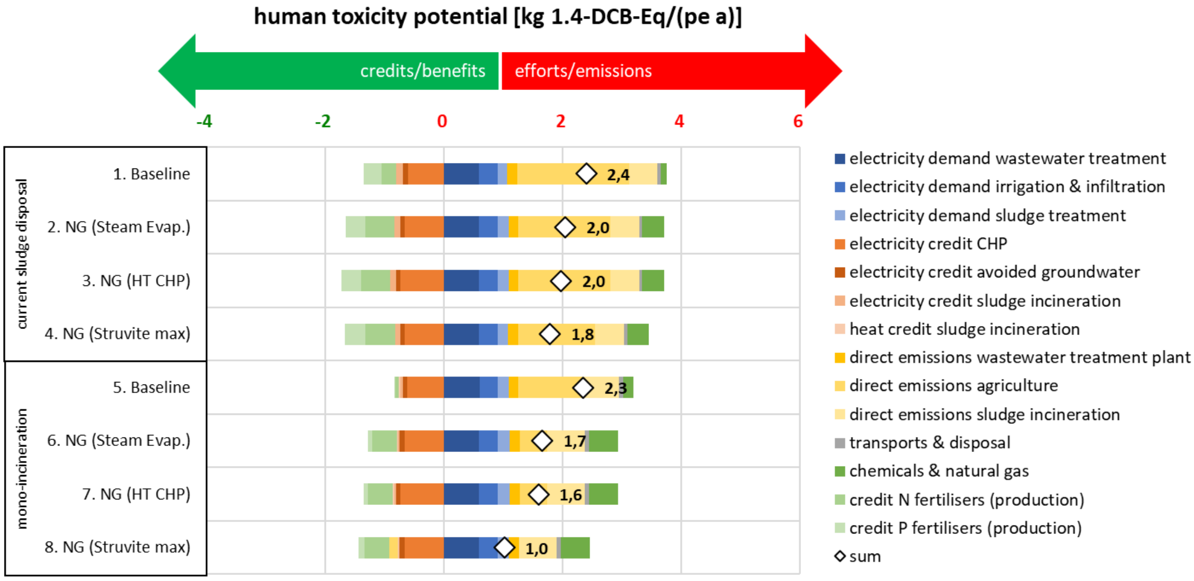

Figure 24: Human toxicity potential for the Braunschweig WWTP

Normalisation

The net score for each impact category per pe and year is related to the normalisation data per citizen and year to show the relative contribution of the system under study to the total environmental impact per person (see Figure 25).

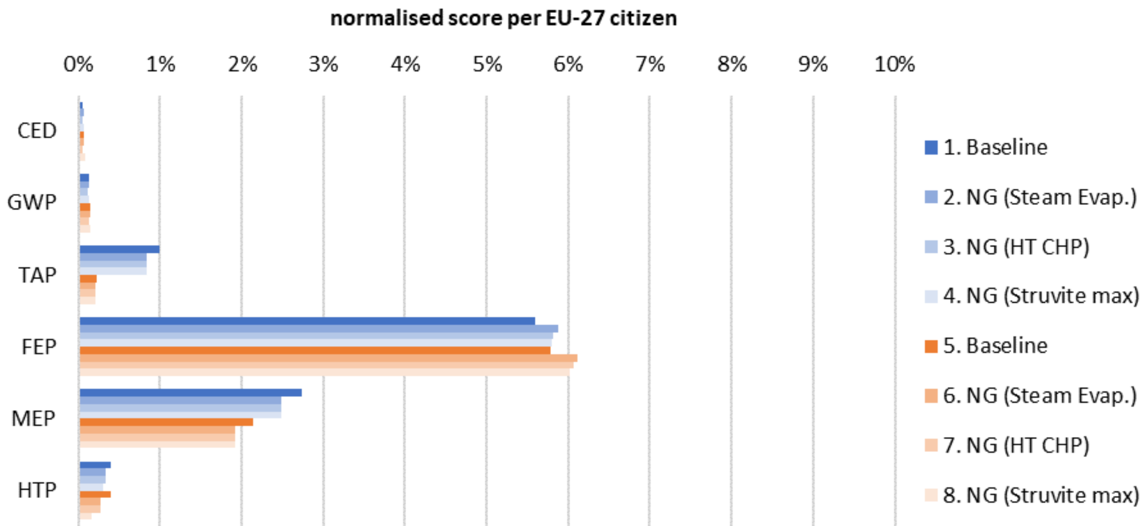

Figure 25: Normalised score for all impact categories per average EU-27 citizen

Energy-related indicators such as CED and GWP contribute approximately only 0.1 % to the total impact per citizen and year, meaning that sewage treatment has only a marginal contribution. For TAP in terms of sludge valorisation in agriculture and HTP (heavy metals) the contribution is a bit higher (0.2 – 1 % for TAP and 0.2 – 0.4 % for HTP). A relevant contribution of sewage treatment is in terms of phosphate and nitrogen species emitted to water bodies as a consequence of the treatment plant effluent. This contribution is about 6 % for FEP (phosphate species) and around 2 % for MEP (nitrogen species). According to the normalised results, it appears to be justified to invest a bit more energy if it is possible to reduce eutrophication.

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Interpretation and conclusions

Table 10 gives a summary on the net environmental impacts and benefits for all calculated impact categories and scenarios. It can be observed that the NextGen-scheme has benefits in most scenarios for global warming potential, acidification potential, marine eutrophication potential (due to improved N management) and to a decrease of human toxicity potential (heavy metal management). Increases in the freshwater eutrophication potential are minor, while the cumulative energy demand increases more significantly in some scenarios, mainly due to the increased use of chemicals (caustic soda, sulfuric acid and polymer).

Table 17: Summary of net environmental impacts and benefits for all impact categories for the Braunschweig WWTP. Percentual numbers relating to their specific Baseline 1. or 5..

Impact category	Mid-term scenarios (current sludge disposal)				Long-term scenarios (mono-incineration)			
	1. Baseline	2. NG (Steam Gen.)	3. NG (HT CHP)	4. NG (Struvite max)	5. Baseline	6. NG (Steam Gen.)	7. NG (HT CHP)	8. NG (Struvite max)
Products of NEXTGEN [1/a]		18 t P 149 t N 762 MWh	18 t P 149 t N 1759 MWh	31 t P 148 t N 761 MWh		18 t P 189 t N 775 MWh	18 t P 189 t N 1777 MWh	37 t P 188t N 773 MWh
CED [MJ/(pe a)]	72.4	80.9 (+12%)	59.0 (-19%)	81.7 (+13%)	81.2	93.9 (+16%)	71.6 (-12%)	99.5 (+23%)
GWP [kg CO_2-Eq/(pe a)]	14.9	14.6 (-2%)	13.0 (-9%)	14.6 (-2%)	16.2	16.1 (-1%)	14.5 (-11%)	16.4 (+1%)
TAP [kg SO_2-Eq/(pe a)]	0.34	0.29 (-15%)	0.29 (-16%)	0.29 (-15%)	0.08	0.07 (-8%)	0.07 (-12%)	0.07 (-10%)
FEP [kg P-Eq/(pe a)]	0.02	0.02 (+5%)	0.02 (+4%)	0.02 (+4%)	0.02	0.03 (+6%)	0.03 (+5%)	0.02 (+4%)
MEP [kg N-Eq/(pe a)]	0.28	0.25 (-9%)	0.25 (-9%)	0.25 (-9%)	0.22	0.19 (-11%)	0.19 (-11%)	0.19 (-11%)
HTP [kg 1,4-DCB-Eq/(pe a)]	2.39	2.04 (-15%)	1.97 (-18%)	1.79 (-25%)	2.35	1.66 (-29%)	1.59 (-32%)	1.02 (-57%)

The following aspects can be summarized:

- All **NextGen schemes** are able to **recover nutrients with a net-zero CO_2e footprint** – direct N_2O emissions are reduced. A further reduction of the CO_2 footprint could be achieved by utilisation of excess heat in summer for the stripper to reduce caustic soda consumption.
- **Recovery of HT Heat from the CHP** could **improve the CO_2 and energy footprint**; however, this scenario suffers from high investment costs. The use of biogas for steam generation increases the energy demand, hence almost all of the additional biogas produced is needed for steam generation. Additionally, the demand for polymer in pre-dewatering and the reduced heating value in sludge incineration increase the energy demand overall.

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- All NextGen schemes generally **reduce emissions of reactive nitrogen species** (N_2O from wastewater treatment and sludge incineration, NH_3 from sludge irrigation and N species in the effluent causing eutrophication). The energy efficiency of the stripping process is dependent from the exact operational stripping parameters. Thereby the consumption of caustic soda is crucial for the energy and CO_2 footprint. If excess heat is available, higher stripping temperatures may reduce the caustic soda consumption and therefore reduce the energy and CO_2 footprint. It should be investigated whether a slightly lower N recovery rate of 80 % without dosing caustic soda is more sufficient compared to the current operation.
- The energy efficiency of the struvite process is related to the PO_4-P concentration in the sludge water. Higher phosphate concentrations resulting in higher yields, while electric energy for the reactor is similar for low and high phosphate concentrations. In the overall assessment, **a lower struvite yield and higher dewaterability due to provisional pre-dewatering magnesium dosing is beneficial from an energy and CO_2e footprint** compared to a high struvite yield.
- The combination of struvite and ammonium sulphate recovery is recommended to avoid unintended struvite scaling in the stripping column. The DLD treatment involving thermal hydrolysis increases the N load in sludge water, which is favourable for the overall N recovery yield, however thereby increased efforts for chemicals as caustic soda are relevant for the energy footprint.
- **Sludge incineration will reduce NH_3 emissions** compared to sludge valorisation in agriculture, however less P will be recycled to arable land and a higher overall energy demand and CO_2 footprint is resulting.
- The recovered products, **struvite and ammonium sulphate will reduce the input of heavy metals into environment** compared to sludge valorisation in agriculture or the use of conventional fertilisers.

Input data for this LCA had been derived from full-scale operation in a dedicated monitoring campaign. Some estimates in terms of gaseous emissions (N_2O from the WWTP) had been undertaken. These assumptions should be refined in further assessments. Other important factors influencing the results of this LCA are related to the degradation ratio in the digestor in combination with dewaterability and following sludge disposal treatment. The overall energy and carbon footprint for our technologies in the WWTP are influenced by the assumptions taken for sludge disposal in terms of different incinerators or agricultural valorization.

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Tossa de Mar (ES): water reuse with regenerated membranes

Tossa de Mar is a town located in the south of Costa Brava in the province of Girona in Catalonia, Spain. In this coastal town, the population in the summer months is 5 times higher than the permanent residents (12,000) due to high touristic activity, resulting in challenges for seasonal water supply and wastewater treatment.

In terms of water supply the city is connected to the water network of the southern zone of Consortio Costa Brava (CCB). Besides local wells in the Tossa valley ("Tossa wells") a high share (>50 %) of the freshwater demand is imported via a long-distance water network. The imported water is sourced from the Tossa Lloret Drinking Water Treatment Plant (Tossa Lloret DWTP) and the Tordera Seawater Desalination Plant using a reverse osmosis (Tordera SWRO). Part of the produced water from both plants is pumped across hills into the Tossa valley, while both plants also supply water for other municipalities (e.g. Lloret de Mar, Blanes, Alt Maresme). Due to increasing water scarcity in the region, there is competition on available drinking water resources. The annual drinking water demand of Tossa de Mar is around 1.45 Mm^3/year. About 0.7 Mm^3/year is produced locally from the Tossa Wells, while 0.75 Mm^3/year are imported via the water network (0.7 Mm^3/year from Tossa Lloret DWTP and 0.05 Mm^3/year from Tordera SWRO) – see Figure 26.

In the Tossa de Mar wastewater treatment plant (Tossa de Mar WWTP), 0.81 Mm^3/year of raw wastewater are collected and treated in secondary treatment. The secondary treatment sufficiently removes solids and COD, while the nitrogen removal is limited due to the low sludge age and a lack of treatment capacity, especially in the summer months with high load from the touristic population (Figure 27). To reduce the drinking water demand, a reclaimed water network was installed in the early 2000s together with a tertiary treatment at the WWTP to make use of purified wastewater. This Tossa de Mar water recycling plant (Tossa de Mar WRP) consists of coagulation, filtration, UV disinfection and chlorination. In summer, the reclaimed water is used for irrigation of public areas.

However, tertiary treatment is not running at full capacity in recent years. Moreover, it is planned to extent the water reuse scheme towards private irrigation, so additional reclaimed water in higher quality is needed to comply with the higher standards for private use. Therefore, a new tertiary treatment scheme was investigated in NEXTGEN using regenerated RO membranes instead of sand filtration. These membranes reached their end-of-life in seawater desalination, but can still be reused in wastewater treatment. This treatment ensures higher water quality in terms of chemical and microbial parameters, and allows private irrigation with the reclaimed water.

However, replacing drinking water only for irrigation has a limited substitution potential, and further steps could be taken to alleviate stress on local water resources. Therefore, another potential scenario was investigated to re-infiltrate reclaimed water into the ground and thus reduce stress on the aquifer in Tossa de Mar ("indirect reuse"). For this strategy, it is necessary to improve secondary and tertiary treatment of the WWTP to sufficiently remove ammonium and salinity to protect the aquifer. In this final development about 30 % of the incoming wastewater could be reclaimed, representing around 17 % of the overall water demand of Tossa de Mar.

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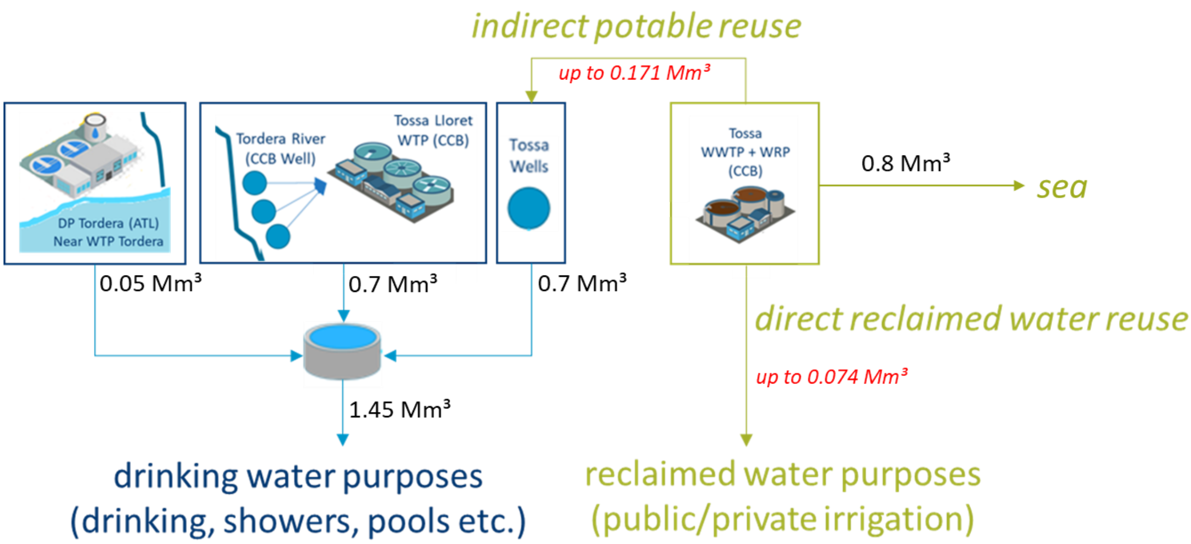

Figure 26: Overview of drinking water and wastewater and potential reclaimed water resources and their usage at Tossa de Mar: green arrows and red numbers show potential in future scenarios

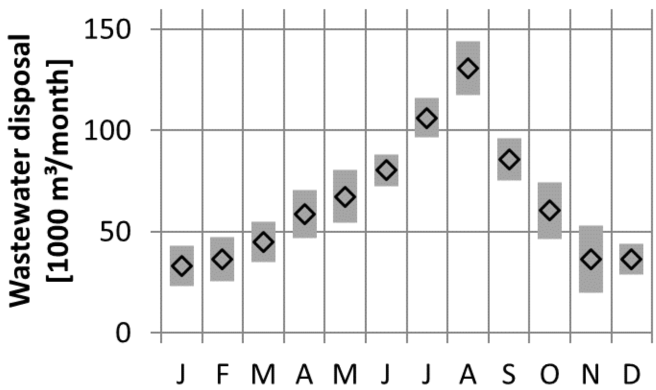

Figure 27: Seasonal distribution of wastewater production with peak in summer (June-Sept)

Goal and scope definition

The goal of this LCA is to analyse potential environmental impacts of the reuse scheme at WWTP Tossa de Mar with different water reclamation technologies and strategies demonstrated within NEXTGEN. In detail, the following aspects will be analysed:

- The current tertiary treatment with coagulation, filtration, UV disinfection and chlorination treating a part of the secondary effluent in the summer months for public irrigation
- The tertiary treatment demonstrated within the NextGen project with coagulation, membrane filtration with regenerated RO membranes, and chlorination treating a part of the secondary effluent in the summer months for public and private irrigation
- An improved secondary treatment at the WWTP resulting in low ammonium levels, combined with NEXTGEN water reuse scheme with regenerated membranes. This scheme will allow public and private irrigation with reclaimed water in the summer months, and additional treatment in winter (RO + advanced oxidation) as pre-treatment for infiltration to recharge the aquifer with reclaimed water.

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For each water reuse scenario corresponding freshwater provided by other sources will be substituted by reclaimed water.

The LCA serves as an example for municipalities suffering from water scarcity and dealing with the seasonal effects of tourism on water management with varying influent volumes and loads during the year. The target group of this study consists primarily of the local WWTP and WRP operators (CCB), but also planers and engineers of water reuse schemes.

Function/ Functional Unit

The function of the system under study is "to provide wastewater treatment according to the legal requirements" including all processes related to this function. The functional unit of this LCA is defined via the annual organic load of the WWTP calculated in population equivalents (pe) of the WWTP ("per pe and year" or "$[pe \cdot a]^{-1}$").

System boundary

As this LCA analyse the entire system of wastewater treatment and management, the system boundary includes the complete WWTP and WRP including the water reuse. Corresponding drinking water saved, due to the implementation of water reuse schemes is considered as avoided burden. Finally, the system boundary includes background process for production of electricity, chemicals, fuels and materials (see Figure 28).

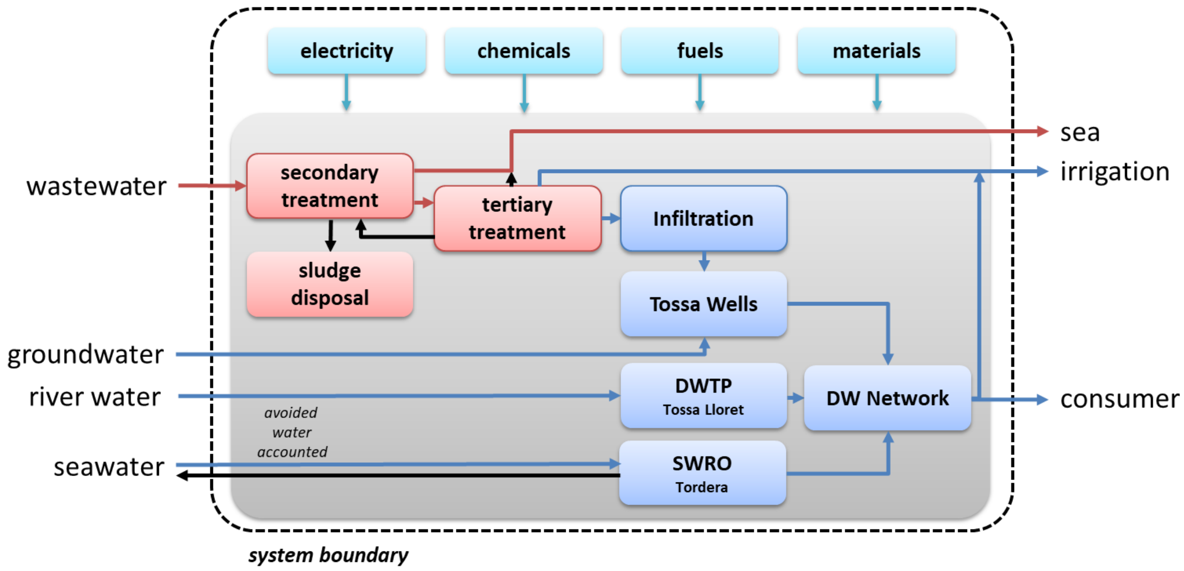

Figure 28: System boundary and scope of the LCA study Tossa de Mar

Allocation

Although the WWTP delivers several functions (wastewater treatment and water reclamation), all efforts (e.g. energy and chemical consumption) and benefits (e.g. avoided drinking water production) are related to the function of wastewater treatment and its functional unit. No allocations are required. Water is accounted with credits using specific factors with regard to drinking water production and delivery (avoided burden approach).

Scenarios

The scenarios have been selected to show environmental benefits and drawbacks of the technologies and operational modes. The specific scenarios are listed below:

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1. **Baseline:** This scenario represents the existing secondary treatment at the WWTP Tossa de Mar without any water reclamation.
2. **Current Tertiary**: This scenario represents the existing secondary treatment at the WWTP Tossa de Mar with the current tertiary treatment with coagulation, filtration, UV disinfection and chlorination. The reclaimed water production is 60’000 m^3/year. This volume is provided during June to September for irrigation in public areas (assumption of demand by CCB). A corresponding volume of drinking water is saved, assuming constant production shares from Tossa Lloret DWTP and Tordera SWRO.
3. **NextGen:** This scenario represents the existing secondary treatment at the WWTP Tossa de Mar with the tertiary treatment developed in NEXTGEN with coagulation, filtration with regenerated RO membranes, and chlorination. The reclaimed water production is assumed to 74’400 m^3/year calculated from WWTP dry weather flow and membrane capacity. This volume is provided during June to September for public or private irrigation. A corresponding volume of drinking water is saved, assuming constant production shares from Tossa Lloret DWTP and Tordera SWRO.
4. **Future:** This scenario represents an upgraded secondary treatment at WWTP Tossa de Mar, including higher capacity for a year-round removal of ammonium, which is a pre-condition for extending water reuse to water infiltration.
    a. In summer, the reclaimed water production capacity is 74’400 m^3/year treated with NEXTGEN technology and used for public or private irrigation. A corresponding volume of drinking water and its production with constant production shares from Tossa Lloret DWTP and Tordera SWRO is saved.
    b. Additionally, the reclaimed water production capacity is assumed to 171’900 m^3/year treated via regenerated membranes, reverse osmosis (reducing also salinity) and advanced oxidation process using hydrogen peroxide. The volume is calculated based on the available dry weather flow of the WWTP in winter and membrane capacity. This water is infiltrated and recovered via the Tossa wells. A corresponding volume of drinking water and its production with constant production shares from the Tossa Lloret DWTP and the Tordera SWRO is saved.

Data quality and limitations of this study

Major input parameters for the LCA inventory are discussed below regarding data quality and uncertainties and limitations. An overview of data sources and data quality is provided in Table 18.

- Water quality and quantities: All relevant data for water quality and quantities were provided by the WWTP operator CCB for 2014-2019. The data quality is assumed to be very good.
- Key performance parameters, energy and chemical consumption: Parameters as removal efficiency, electricity, polymer and chemical consumption had been provided by the WWTP operator CCB and EUROCAT. The annual consumptions were used to calculate specific consumption and estimate the overall consumptions for the specific scenarios.

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The data quality is assumed to be medium or good. In terms of the future scenario, data from a full-scale membrane tertiary treatment in Torelle (Belgium) was used to estimate the electricity and chemical consumption as well as expert knowledge to estimate the consumables for the AOP. This data is assumed as medium quality.

- Background data are discussed for all LCA studies in the annex (Table 57**).**

Table 18: Parameters, data source and estimated data quality

Parameter/ Process	Data source	Data quality
WWTP - Baseline		
Water quality and quantity	WWTP operator (CCB, 2019)	very good
Energy and chemical consumption	WWTP operator (CCB, 2019)	good
Gaseous emissions from WWTP	Literature (ATV, 2000; Parravicini et al., 2016)	Low-medium
Tertiary Treatment		
Energy and chemical consumption (Scenario 2./3.)	WWTP operator (CCB, 2019; Serra, 2021)	medium
Energy and chemical consumption (Scenario 4.)	Literature (Kraus et al., 2016; Van Houtte, 2016)	medium
Drinking Water Treatment		
Energy and chemical consumption	WWTP operator (CCB, 2019; Sala, 2022; Serra, 2021)	medium

Normalisation

Normalisation reveals the contribution of the WWTP in relation to the total environmental footprint of each EU-27 citizen. The normalisation factors are listed in the annex (Table 58).

Indicators for impact assessment

For the impact assessment, indicators are selected with a focus on three aspects: a) primary energy demand and greenhouse gas emissions as indicators for impacts from electricity, and chemicals b) water quality parameters for N and P emissions as indicators for impacts from wastewater treatment effluent and c) acidification to account for direct gaseous emissions from wastewater treatment and sludge disposal.

In detail, the following indicator models are used for impact assessment:

- Cumulative energy demand (CED) of fossil and nuclear resources (VDI, 2012)
- Global warming potential (GWP) for a time horizon of 100a (IPCC, 2014)
- Freshwater eutrophication potential (FEP), marine eutrophication potential (MEP), and terrestrial acidification potential (TAP) from the ReCiPe method v1.13 (hierarchist perspective, without long-term emissions) (Huijbregts et al., 2017)

For system modelling and calculation of indicators, the LCA software UMBERTO® LCA+ has been used (IFU, 2018).

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Input data for LCA

Primary data

An overview of the water treated in tertiary treatment, the quantity of reclaimed water and changes for the different water sources is provided in Table 19. The water recovery rate is below 10 % with the current tertiary treatment and can be increased towards 30 % in the future scenario.

Table 19. Water treated in tertiary treatment, reclaimed water, changes for drinking water sources and recovery and substitution rates for the different scenarios

Inventory parameter and unit (annual values)	1. Baseline	2. Current Tertiary	3. NextGen	4. Future
Feed of tertiary treatment [m³]	0	62’176	93’000	372’000
Reclaimed water from Tossa WWTP [m³]	0	60’000	74’400	246’300
DW from Tossa Wells [m³]	0	0	0	+171’900
DW from Tossa Lloret DWTP [m³]	0	-56’000	-69’400	-229’800
DW from Tordera SWRO [m³]	0	-4’000	-5’000	-16’500
Water recovery rate compared to secondary influent of Tossa WWTP [%]	0%	7%	9%	30%
Water substitution rate compared to total drinking water demand [%]	0%	4%	5%	17%

The water quality and quantity of the baseline scenario including tertiary treatment using water from the existing secondary treatment is shown in Table 20. The secondary treatment has limited N and P removal. Nitrogen in the effluent is almost only present as ammonium, due to the low sludge age in secondary treatment and insufficient nitrification capacity.

Table 20: Water quantity and quality data of baseline scenario (secondary), current and NEXTGEN tertiary treatment for irrigation with existing secondary treatment

Parameter	Summer influent (Jun-Sep)	Summer effluent secondary	Effluent current tertiary	Effluent NEXTGEN tertiary	Winter influent (Oct-May)	Winter effluent secondary
Volume [m³]	416’000	413’000	60’000	74’400	394’000	392’000
SS [mg/L]	296	9	5	0.9	240	10
COD [mg/L]	736	45	44	43	583	35
TN [mg/L]	83	31	31	9	64	30
TP [mg/L]	9	4	4	0.8	8	3

Water quality and quantity of the future scenario including tertiary treatment is shown in Table 21. Nitrogen in the effluent of the secondary treatment is almost only present as nitrate.

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Table 21: Water quantity and quality data of future scenario (upgraded secondary treatment), and tertiary treatment for irrigation and infiltration

Parameter	Summer influent (Jun-Sep)	Summer effluent secondary	Tertiary water for irrigation	Winter influent (Oct-May)	Winter effluent secondary	Tertiary water for infiltration
Volume [m³]	416’000	434’000*	74’400	394’000	499’000*	171’900
SS [mg/L]	296	9	0.9	240	9	0.1
COD [mg/L]	736	43	43	583	31	1.0
TN [mg/L]	83	17	5	64	13	1.2
TP [mg/L]	9	0.9	0.2	8	0.8	0.03

secondary effluent is higher than influent due to backwash of UF treated in secondary treatment

The electricity consumption for secondary treatment and sludge treatment is estimated with 0.6 kWh/m³ and can be reduced in the future with a new aeration system to 0.5 kWh/m³ while the effluent quality can be improved especially in terms of ammonium.

The current tertiary treatment uses about 8.5 ppm Al for coagulation and additional phosphorus removal, while filtration requires 0.04 kWh/m³. The UV disinfection also requires 0.04 kWh/m³ and finally 14.5 ppm Cl are used for chlorination. In contrast, the NEXTGEN tertiary treatment with regenerated membranes requires 0.24 kWh/m³ for membrane filtration, 8.5 ppm Al for coagulation and additional chemicals in smaller amount for membrane cleaning (citric acid, sodium bisulfide, sodium hypochlorite and hydrochloric acid). Residual chlorine is realised via chlorination similar to the current tertiary treatment. This treatment is also used as pre-treatment for RO in the future scenario. Here, RO requires 0.58 kWh/m³ and additional chemicals (citric acid, sodium bisulfide, sulfuric acid, ammonium chloride and caustic soda) are needed. The AOP requires 0.05 kWh/m³ and 10 ppm hydrogen peroxide (50 %). The resulting annual quantities for all scenarios are shown in Table 22.
To estimate the avoided burden for drinking water production, a corresponding inventory for the different drinking water resources was also estimated based on operator data. The specific consumption of electricity and chemicals per m³ for the different drinking water resources are shown in Table 23.

Background data

Background data for production of electricity, chemicals, materials and transport are based on ecoinvent database v3.6, namely shown in the annex (Table 57).

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Table 22: Annual inventory data (only consumables) for the WWTP and WRP at Tossa

Inventory parameter and unit (annual values)	1. Baseline	2. Current Tertiary	3. NextGen	4. Future
Electricity secondary and sludge treatment [kWh]	493'600	494'300	496'800	428'400
Electricity tertiary treatment [kWh]	0	4'600	23'000	197'600
polyacrylamide [kg]	3'100	3'100	3'100	2'700
Citric acid (40 %) [kg]	0	0	1'600	7'200
HCl (32 %) [kg]	0	0	100	500
$AlCl_3$ (45 %) [kg]	0	5'800	8'700	34'700
$NaHSO_3$ (39 %) [kg]	0	0	700	3'200
NaOCl (15 %) [kg]	0	12'300	45'900	45'900
NH_4Cl (50 %) [kg]	0	0	0	900
NaOH (29 %) [kg]	0	0	0	1'000
H_2SO_4 (78 %) [kg]	0	0	0	4'800
H_2O_2 (50 %) [kg]	0	0	0	1'700

Table 23: Specific consumables for different drinking water resources at Tossa

Inventory parameter and unit	DW Tossa Wells	DW Tossa Lloret DWTP	DW Tordera SWRO
Electricity DWTP [kWh/m³]	0.04	0.35	2.65
Electricity for pumping [kWh/m³]	0	0.85	0.90
NaOCl (15 %) [ppm Cl]	0.2	0	0
Cl gas [ppm Cl]	0	2.0	0
CO_2 liquid [ppm CO_2]	0	0	40.5
Citric acid (40 %) [mg/L]	0	0	3.33
$FeCl_3$ (40 %) [mg/L]	0	0	0.32
$Ca(OH)_2$ (solid) [mg/L]	0	0	32.5
NaHS (39 %) [mg/L]	0	0	26.8
NaOH (29 %) [mg/L]	0	0	13.8

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LCA results

Cumulative energy demand (CED)

The cumulative energy demand of non-renewable resources for the scenarios in shown in Figure 29. The baseline scenario require in sum 346 MJ/(pe a), which is due to electricity consumption for wastewater aeration with >90 %. Implementing a tertiary treatment, the energy demand decreases in the overall balance. On the one hand the additional electricity consumption and chemical demand of tertiary treatment increase the gross energy demand. On the other hand, corresponding drinking water (and its supply) is saved by using reclaimed water. Here, it is of major importance which drinking water resource is replaced by reclaimed water for public (and private) irrigation. In Figure 29 a proportional replacement from the DWTP Tossa Lloret or even the energy-intensive SWRO Tordera is assumed. Water from both resources needs to be pumped into the Tossa Valley via several storage tanks, requiring 0.85 kWh/m³ just for water delivery to Tossa de Mar. The water from SWRO additionally requires a very high electricity consumption in its production.

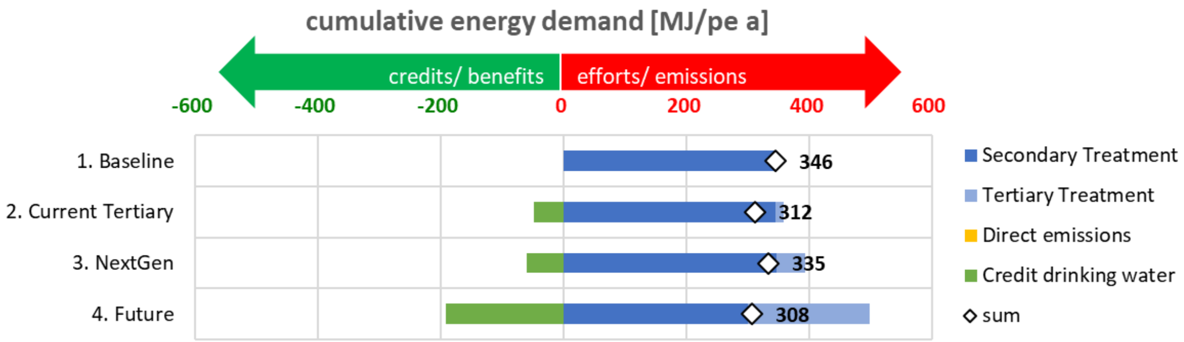

Figure 29: Non-renewable cumulative energy demand for the Tossa de Mar WWTP & WRP

In terms of energy the current tertiary has advantages compared to the NEXTGEN scheme with regenerated membranes, since the specific electricity and chemical consumption in tertiary treatment is lower, while the water recovery rate compared to the membrane scheme is higher and a higher quantity of drinking water can be replaced by reclaimed water. However, this energy balance does not consider water quality aspects: reclaimed water quality is higher with NEXTGEN than with the existing tertiary treatment.

For the future scenario including an upgraded WWTP, the net energy balance is further improved. The electricity demand in secondary treatment is reduced due to new aerators. As a higher quantity of water is treated in tertiary treatment and the infiltration in winter requires an energy intensive RO process, the energy demand for tertiary treatment increases significantly. However, due to the correspondingly high water savings from external water resources, such as the Tossa Lloret DWTP and the Tordera SWRO, the net energy demand can be reduced towards 308 MJ/(pe a).

Global warming potential (GWP)

The GWP shows similar results to the CED in terms of indirect emissions due to electricity and chemical consumption. However, direct N_2O emissions have a crucial role in the GWP. Based on literature data (Parravicini et al., 2016), it is assumed here that high N_2O emissions from secondary treatment correspond with low N removal efficiency. Hence, the current secondary treatment with poor N removal (50%) in summer leads to a high contribution of N_2O to GWP (1% of influent N to N_2O). Therefore, net GWP varies for scenarios 1.-3. with existing

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secondary treatment between 34-37 kg CO_2-eq/(pe a). With the future WWTP scheme, secondary treatment is improved and nitrogen is removed with higher efficiency, which results in lower direct N_2O emissions. The overall footprint for the future scenario is thus only 22 kg CO_2-eq/(pe a). It should be pointed out that N_2O emission factors are based on literature, so these results are affected with high uncertainty.

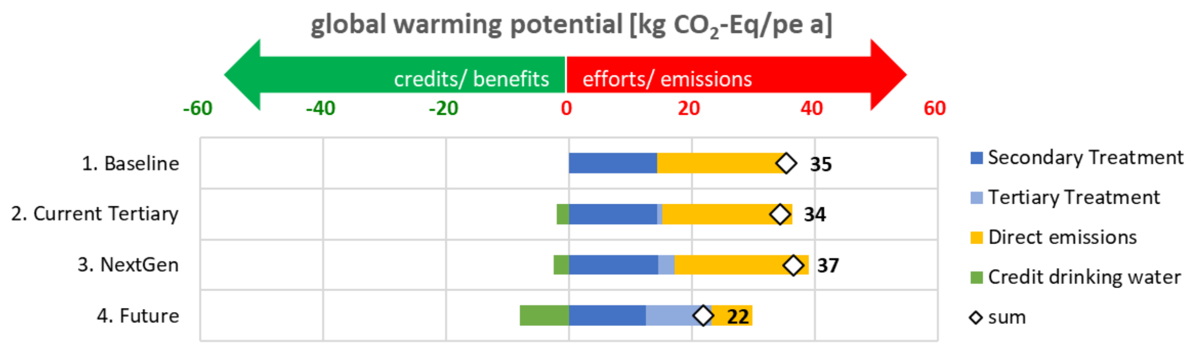

Figure 30: Global warming potential for the Tossa de Mar WWTP & WRP

Terrestrial acidification potential (TAP)

Besides some indirect SO_2 and NH_3 emissions due to electricity and chemicals production, the TAP is strongly affected by direct ammonia emissions in secondary treatment (Figure 31). The net footprint is relatively constant for all scenarios. The sludge/ sludge compost application was excluded from the scope of this LCA and would increase ammonia emissions in a similar share for all scenarios.

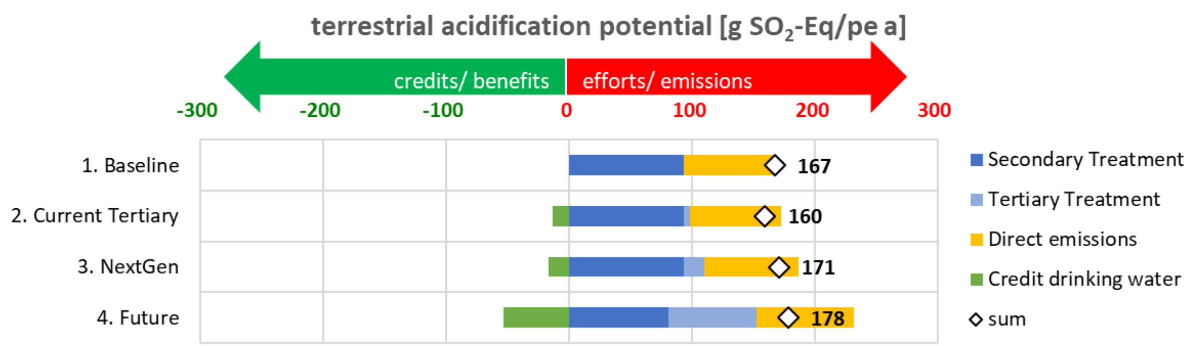

Figure 31: Terrestrial acidification potential for the Tossa de Mar WWTP & WRP

Freshwater eutrophication potential (FEP)

The FEP is influenced by the phosphate concentration in the tertiary treated water used for irrigation or aquifer recharge, causing potential freshwater eutrophication (Figure 32). As secondary treated water is discharged in the Mediterranean Sea in the baseline scenario, direct emissions of phosphate are not accounted in terms of FEP. The current tertiary treatment shows the lowest phosphate removal rate compared to the other tertiary treatment using membranes, so a significant increase in FEP is expected for the existing scheme. The high phosphate elimination in scenario 3. and 4. result in a low FEP as compared to the baseline, although significant amounts of reclaimed water might impact the local freshwater bodies. In general, the FEP net value for all scenarios is comparably low, hence most of the non-removed phosphate is discharged in the sea. Furthermore, the application of sludge compost with high P amounts was excluded here.

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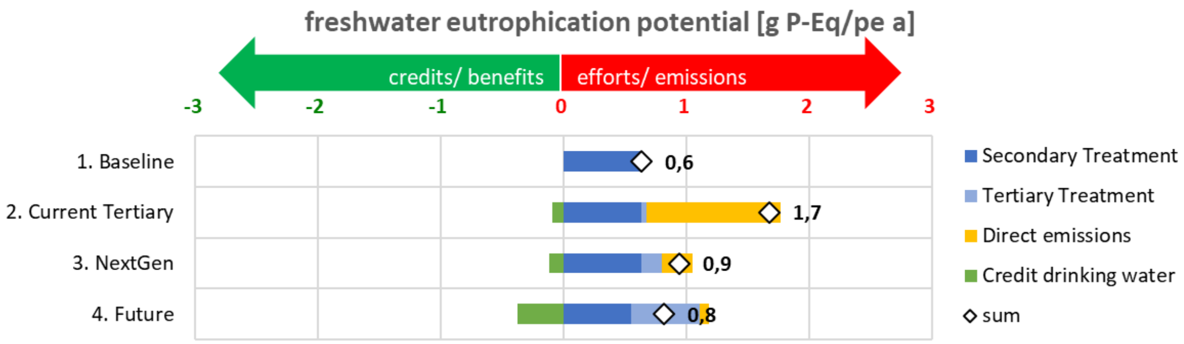

Figure 32: Freshwater eutrophication potential for the Tossa de Mar WWTP & WRP

Marine eutrophication potential (MEP)

In terms of the marine eutrophication potential (see Figure 33), the insufficient nitrogen removal of the current secondary treatment becomes apparent. For the baseline scenario and the other scenarios relying on the current secondary treatment the MEP is around 2.6-2.9 kg N-Eq/(pe a). The effluent is the only relevant contributor. For the future scenario with improved secondary treatment and an targeted N elimination rate of 80 % in secondary treatment, the MEP is reduced to 1.0 kg N-Eq/(pe a). Again, nitrogen in cooperated into sludge and potentially relevant emissions in terms of marine eutrophication from sludge are excluded from the scope of the study.

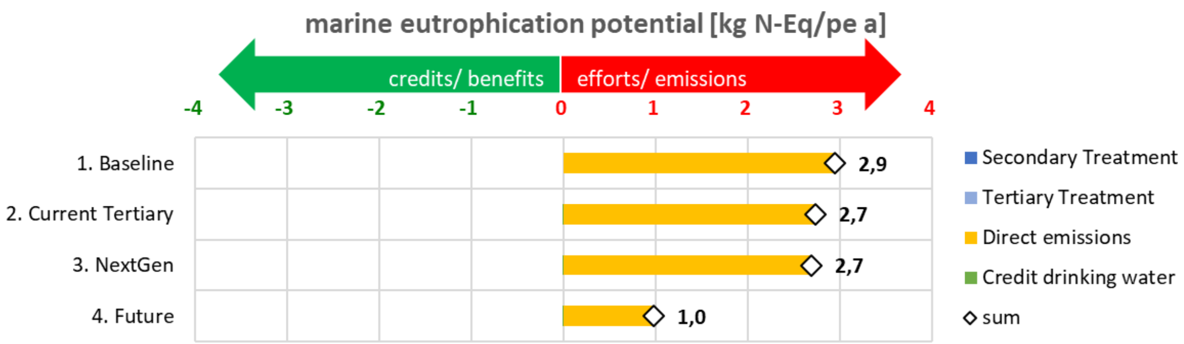

Figure 33: Marine eutrophication potential for the Tossa de Mar WWTP & WRP

Normalisation

The net score for each impact category per pe and year is related to the normalisation data per citizen and year to show the relative contribution of the system under study to the total environmental impact per person (see Figure 34).

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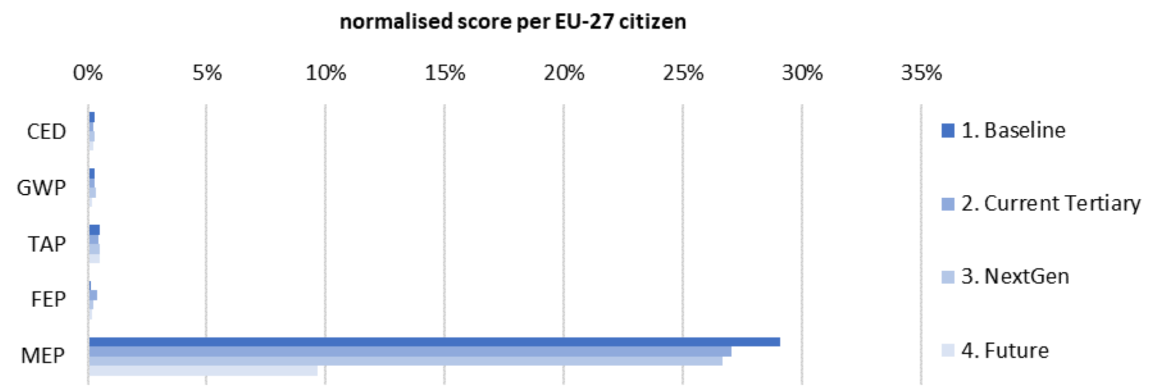

Figure 34: Normalised score for all impact categories per average EU-27 citizen

All indicators except MEP contribute around 0.2-0.5 % to the to the total impact per citizen and year, meaning that sewage treatment has only a marginal contribution. In terms of freshwater eutrophication potential this is due to the fact, that the phosphate in the effluent is mostly discharged into the sea. The normalisation stresses particularly the relevance of nitrogen removal which is around 25-30 % for the current secondary treatment with insufficient nitrogen removal and is reduced towards 10 %, when a state-of-the-art secondary treatment would be implemented.

Interpretation and conclusions

Table 24 gives a summary on the net environmental impacts and benefits for all calculated impact categories and scenarios. It can be observed that the NEXTGEN scheme with the new tertiary treatment has benefits in energy demand, acidification and marine eutrophication. A minor increase is detected for GHG emissions. However, this strongly relates to the question which drinking water resource is replaced by reclaimed water. If water import into the Tossa Valley from external sources is reduced, a decrease also in global warming potential is likely. The future scenario shows significant savings for almost all impact categories due to the higher quantity of drinking water replaced by reclaimed water and due to avoidance of emissions of nitrogen species (such as N_2O for global warming and NH_4^+/NO_3^- for marine eutrophication). The freshwater eutrophication increases for all reuse scenarios, since residual phosphate loads in reclaimed water will potentially affect freshwater resources compared to the baseline scenario, where they cause no harm when discharged into the sea.

Table 24: Summary of net environmental impacts and benefits for all impact categories for the Tossa de Mar WWTP & WRP

Impact categories	1. Baseline	2. Current Tertiary	3. NextGen	4. Future
Products of NEXTGEN [1/a]		60,000 m³ water	74,400 m³ water	246,300 m³ water
CED [MJ/(pe a)]	345.9	312.0 (-10%)	334.5 (-3%)	307.6 (-11%)
GWP [kg CO_2-Eq/(pe a)]	35.3	34.4 (-3%)	36.6 (+4%)	21.9 (-38%)
TAP [kg SO_2-Eq/(pe a)]	0.17	0.16 (-5%)	0.17 (+2%)	0.18 (+7%)
FEP [kg P-Eq/(pe a)]	0.001	0.002 (+165%)	0.001 (+49%)	0.001 (+29%)
MEP [kg N-Eq/(pe a)]	2.95	2.74 (-7%)	2.70 (-8%)	0.98 (-67%)

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The following aspects can be summarized:

- **Water reuse is associated with environmental savings** for almost all impact categories except freshwater eutrophication. The savings are depending on the respective water resource and its energy intensity in production that is replaced by reclaimed water.
- The **NEXTGEN scheme using regenerated membranes** is able to provide a higher level of water quality compared to the current tertiary treatment. Although the water recovery rate of this treatment train is lower compared to the current tertiary treatment, **higher quantities of water can be recycled** due to higher demand, as the reuse purpose can be extended from public irrigation only to public and private irrigation.
- LCA shows cumulative efforts and causal effects of water reuse in the supply chain of electricity and chemicals, but it **does not illustrate reclaimed water quality** in terms of required chemical or microbial quality for public and private irrigation or infiltration.
- However, it has become apparent during the analysis that the **electrical conductivity and ammonium species in WWTP effluent are crucial** aspects to deal with before infiltration can be a potential scenario for an indirect potable reuse scheme. The suggested treatment train in the future scenario consisting of an upgraded secondary treatment to deal with ammonium and a hybrid-membrane scheme to reduce salinity addresses these effects and is able to **reduce environmental impacts when the reclaimed water replaces drinking water imports.**

Input data for this LCA is mainly based on full-scale data from local water and wastewater treatment facilities, and pilot trials for the NEXTGEN technology. Data gaps are closed with estimates. Further operational data from long term operation would be required to validate the conclusions from this LCA. Important factors for the LCA outcomes are the electricity consumption of several treatment steps and the assumptions regarding N removal in the WWTP. In terms of an exact assessment of the carbon footprint, N_2O emissions from the secondary treatment should be measured to verify the outcomes of this study.

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La Trappe (NL): nature-based treatment and water recovery from brewery wastewater

This case study investigates different options for treatment of brewery wastewater from a brewery at Koeningshoven Abbey close to Tilburg in the Netherlands. As it is a Trappist monastery since the 19th century, the site is called “La Trappe” brewery. Apart from the treatment of wastewater from the brewing process with innovative technology, advanced treatment of water for recycling to the brewery in a water reuse concept is also investigated in the NEXTGEN project.

The brewery at Koeningshoven produces a variety of beers and also other products, and generates wastewater that has to be treated before discharge. For this purpose, an innovative biological wastewater treatment system has been installed at the site in 2018. The concept was originally designed by project partner BIOPOLUS and is called BioMakery. The process is based on a modular and functional reactor-based ecological engineering, using a “metabolic network reactor” (MNR) with a combination of fixed-bed biofilm and higher plants to treat the brewery wastewater (Figure 35). The MNR system is designed to reach required discharge standards and even provide an effluent quality to enable water reuse for local irrigation of farmland.

Figure 35: Metabolic network reactor in the BioMakery concept for wastewater treatment at La Trappe brewery

In the frame of NEXTGEN, several activities have been carried out at the site:

- The innovative **MNR process** was operated for a longer term to check its performance in terms of process stability and effluent quality. However, due to the CoViD19 pandemic in 2020-2022, the operation of the brewery was not continuous, and support for MNR operation could not be provided by the project partners due to travel restrictions. Consequently, the system was still under optimization in 2022 and could not produce reliable long-term data for a sound assessment. Hence, this study

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relies on design assumptions from BIOPOLUS for the MNR process complemented by available data from the local operators.

- In parallel, pilot trials have been carried out on-site by project partner SEMiLLA to enhance reuse of water and nutrients from the brewery wastewater with advanced technology. Using a **capillary nanofiltration membrane**, MNR effluent was treated to produce a product water with high quality that is suitable for reuse within the brewery, e.g. as process water for cleaning. This would enable the reduction of freshwater demand of the brewery, and eventually the expansion of the brewing capacity without additional freshwater needs.
- A **photobioreactor** was also tested by project partner SEMiLLA in lab and pilot scale to produce biomass from the brewery wastewater by growing purple bacteria. This biomass contains valuable proteins and could be used for various purposes such as fish fodder or fertilizer. Although the trials successfully proved the general feasibility of the concept, reasonable up-scaling of this technology for implementation at the brewery was not possible. Finally, it was decided not to assess this technology in the frame of LCA, as suitable data for prospective full-scale operation at La Trappe could not be provided.

Both the MNR process and the advanced treatment with membranes for water reuse will be assessed with LCA in this study. Based on the findings in full-scale and pilot trials, the concepts are evaluated in their environmental impacts compared to different benchmarks of brewery wastewater treatment using conventional technology (“baseline”). Benchmark technologies for brewery wastewater treatment are aerobic processes with activated sludge operated as a sequencing batch reactor (SBR), or anaerobic processes with upflow sludge beds such as enhanced granular sludge bed systems (EGSB) followed by a aerobic post-treatment.

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Goal and scope definition

The goal of this LCA is to analyse potential environmental impacts of different innovative processes for treatment of brewery wastewater at the Koeningshoven brewery near Tilburg (NL). It will compare the impacts of the NEXTGEN innovations to conventional concepts for brewery wastewater treatment as a baseline. In detail, the following aspects will be analysed in the LCA:

- Impacts of operation and infrastructure for wastewater treatment and sludge disposal
- Impacts of operation and infrastructure for membrane treatment for water reuse
- Credits for avoided production of mineral fertilizer, electricity or heat, and process water for the brewery

This LCA serves as an example for on-site wastewater treatment in a small to medium brewery, including potential recycling of water for internal reuse. The target group of this study consists primarily of professionals dealing with planning and operation of industrial wastewater treatment plants for breweries, such as plant operators, engineering companies, and researchers in this field.

Function/ Functional Unit

The function of the systems under study is the treatment of brewery wastewater according to the quality required for its discharge. The LCA includes all relevant processes related to this function. The total annual influent amounts to 52,500 m^3 (150 m^3/d at 350 days per year). Consequently, the functional unit is defined as "treatment of 52,500 m^3 brewery wastewater for a period of one year" ("per a"). The amount of raw wastewater treated in the system is defined based on information of the operator (Table 27).

System boundaries

This LCA includes all relevant processes for wastewater and sludge treatment in the different scenarios (see Figure 36). In particular, it includes the demand of electricity and chemicals for operation of the systems, including the innovative NEXTGEN processes. Major flows of direct emissions into the environment are also accounted, such as effluent water quality of the wastewater treatment process, and gaseous emissions of wastewater treatment and sludge disposal. The avoided production of conventional products is subtracted as "avoided burden" in relation to the generated outputs in each scenario (electricity, heat, mineral fertilizer, recycled water). The infrastructure required for each scenario is also accounted in terms of material demand.

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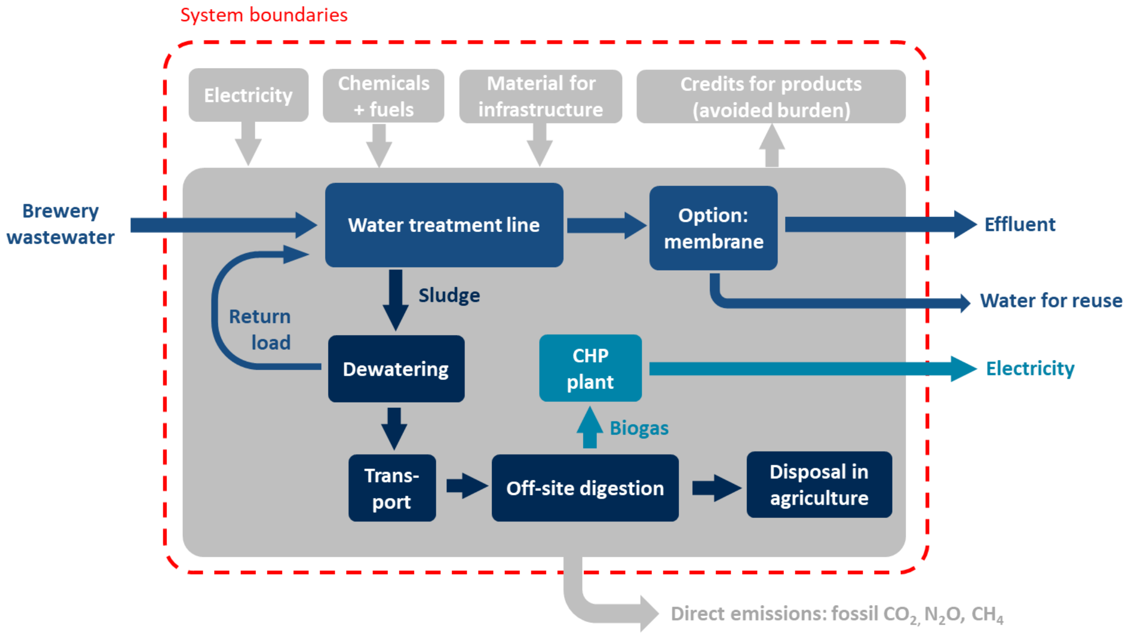

Figure 36: System boundaries of LCA at LaTrappe brewery

Allocation

Due to the one-dimensional function of the systems under study, allocation of environmental impacts is not required. All environmental impacts of the system are related to the operation of the entire system based on the functional unit ("per a").

Scenarios

This LCA compares five major scenarios for brewery wastewater treatment:

- **MNR:** this scenario includes the operation of the metabolic network reactor for wastewater treatment. After equalization and pH control in an influent buffer tank, raw wastewater is treated in the MNR system, which consists of a series of aerated tanks with an attached biofilm. After the MNR, solids are separated in a compact dissolved air flotation (DAF) unit followed by a microfilter. DAF operation is supported by dosing coagulant and flocculant upstream. Treated water is discharged to a local canal. Excess sludge from DAF is stored and dewatered on-site with a belt filter press before being transported to a nearby digestor for stabilisation and biogas recovery. Finally, digested sludge is applied on farmland to recycle residual nutrients and organic matter. Credits from sludge disposal for energy and nutrient recovery are accounted with substituting conventional products.
- **MNR + NF:** this scenario includes the MNR system as in the first scenario, and adds a capillary nanofiltration membrane as a post-treatment step after the MNR. The recovered permeate has a high quality and can be reused within the brewery as process water (e.g. for cleaning). The membrane is operated on purpose with low water recovery, so that the retentate of the membrane still complies with the effluent discharge limits, and can be discharged to the canal as before. Credits for substituted freshwater at the brewery are also accounted.

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- **SBR:** this scenario as a benchmark for a conventional aerobic treatment of brewery wastewater. It includes a sequencing batch reactor (SBR) with an activated sludge process, followed by a microfilter to guarantee a high effluent quality. Sludge disposal is comparable to the MNR scenario.
- **EGSB + SBR:** this scenario is a benchmark for anaerobic treatment of brewery wastewater. After pre-treatment of the wastewater with a coarse filter to remove residual solids, an enhanced granular sludge bed (EGSB) reactor converts part of the organic matter into biogas, which can be recovered and used for heating at the brewery. After the EGSB, an aerobic post-treatment step in an SBR and a microfilter are required to reach the defined effluent quality standards. Again, sludge disposal is comparable to the MNR scenario.

The size of the systems is scaled to the actual flows at Koeningshoven brewery in early 2022 (Table 25). In total, 150 m³ of raw wastewater are treated at the site per day. Accounting for 350 operational days per year, a total annual volume of 52,500 m³ of wastewater is treated in each scenario. The existing MNR system was originally designed to treat a maximum capacity of 450 m³ of wastewater per day. However, the actual load of the system in early 2022 was only 150 m³ per day, as the brewery was not operating at full capacity. Together with project partner DeDommel, it was decided to assess each scenario for the actual wastewater load of 150 m³/d in the present study. To guarantee a fair comparison between scenarios, relevant process data for the over-sized MNR system was adjusted to reflect an optimised operation of equipment (e.g. blowers, DAF) according to the original design load.

Table 25: Scenarios for LCA and size of the systems in LaTrappe case study

Scenario and system	Size	Remarks
MNR		
Metabolic network reactor	150 m³/d	Existing system at LaTrappe (designed for 450 m³/d)
MNR + NF		
Metabolic network reactor + nanofiltration membrane	150 m³/d	Pilot trials with NF membrane in NEXTGEN
SBR		
Sequencing batch reactor	150 m³/d	Benchmark for aerobic treatment of brewery wastewater
EGSB + SBR		
Enhanced granular sludge bed reactor + SBR as post-treatment	150 m³/d	Benchmark for anaerobic treatment of brewery wastewater

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Data quality

Major input parameters for the LCA inventory are discussed below regarding data quality. An overview of data sources and data quality is provided in Table 26.

- MNR: input data for MNR operation was provided by BIOPOLUS based on process modelling for effluent water quality, nutrient dosing and sludge production (SUMO software) and design assumptions for equipment (electricity). Unfortunately, long-term data for stable process performance and related demand for energy/chemicals could not be collected during the project, as the system still experienced operational issues in 2022. Chemical demand is extrapolated from operator data (acid or caustic for pH control) or from supplier information (coagulant and flocculant for DAF and dewatering).
- NF: data for operation of capillary nanofiltration was provided by SEMiLLA based on results of pilot trials (water quality, water recovery). Electricity and chemicals demand of NF stage was estimated by SEMiLLA based on other studies of capillary NF design.
- SBR: data for SBR operation and infrastructure was generated by KWB based on various design guidelines for activated sludge plants and brewery wastewater treatment. Water quality and nutrient dosing was estimated from mass balancing, whereas electricity demand is based on design assumptions for different aggregates and process steps.
- EGSB + SBR: data for EGSB operation is based on supplier information and literature for water quality, electricity and chemicals demand. Biogas yield and direct emissions of CH_4 are estimated based on literature. Downstream SBR after EGSB is modelled from design guidelines in analogy to SBR scenario.
- Sludge disposal: data for treatment of dewatered sludge in a nearby digestor, related energy output from biogas and nutrient credits for agricultural disposal of digested sludge are estimated based on previous studies of KWB.
- Background data for production of electricity, chemicals, transport, fertilizers, and materials is taken from LCA database ecoinvent v3.8 (Ecoinvent, 2021).

Indicators for impact assessment

For the impact assessment, indicators are selected with a focus on three aspects: a) primary energy demand and greenhouse gas emissions as indicators for impacts from electricity, chemicals, and materials for infrastructure b) water quality parameters for N and P emissions as indicators for impacts from wastewater treatment effluent and c) acidification to account for direct gaseous emissions from wastewater treatment and sludge disposal.

In detail, the following indicator models are used for impact assessment:

- Cumulative energy demand (CED) of fossil and nuclear resources (VDI, 2012)
- Global warming potential (GWP) for a time horizon of 100a (IPCC, 2014)
- Freshwater eutrophication potential (FEP), marine eutrophication potential (MEP) and terrestrial acidification potential (TAP) from the ReCiPe method v1.13 (hierarchist perspective, without long-term emissions) (Huijbregts et al., 2017)

For system modelling and calculation of indicators, the LCA software UMBERTO® LCA+ has been used (IFU, 2018).

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Table 26: Data sources and quality for LCA of LaTrappe case study

Parameter/ Process	Data source	Data quality
MNR		
Water quality + sludge	SUMO model (BIOPOLUS)	Medium to good
Electricity	BIOPOLUS design data	Medium to good
Chemicals	Supplier data + KWB estimates	Medium
Infrastructure	Design data for existing system	Good
MNR + NF		
Water quality	Pilot trials (SeMilla)	Good
Electricity + chemicals	SeMilla design based on literature	Medium
Infrastructure	KWB estimate for NF	Medium
SBR		
Water quality + sludge	Design guidelines for SBR	Medium to good
Electricity + chemicals	KWB estimate + supplier data	Medium to good
Infrastructure	KWB estimate based on design	Medium to good
EGSB + SBR		
Water quality + sludge	Supplier and literature data	Medium to good
Electricity + chemicals	Supplier data	Medium to good
Biogas yield + emissions	Literature	Medium
Infrastructure	KWB estimate based on design	Medium to good
Sludge disposal for all scenarios		
Electricity + chemicals	KWB estimate	Medium to good
Credits for electricity and nutrients	KWB estimate	Medium to good
Background data	Ecoinvent database (v3.8)	Medium to good
Electricity	NL power mix	Good
Chemicals, materials	Europe or world market	Medium to good
Fertilizer production	NL market mix	Good

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Input data for LCA

Primary data

Inventory data for this study is mainly provided by the project partners BIOPOLUS, SEMiLLA and DeDOMMEL based on process design and operation of the systems on-site. KWB provided data for benchmark scenarios based on design guidelines and literature or supplier data (Exner, 2023). Data gaps have been filled with available process data from previous projects and estimates by KWB.

Water quality

Water quality data includes raw wastewater influent, and effluent of the respective scenarios (Table 27). Raw influent data is defined by project partner DeDommel based on actual volume and influent quality sampling in spring 2022. Due to frequent and high variation of measured TSS concentration in the influent buffer (impact of high TSS from dewatering centrate and sludge accumulation in buffer tank), this parameter has been adjusted to reflect the actual TSS load coming from the brewery.

MNR effluent quality after DAF and MF is predicted by BIOPOLUS using modelling software for biological wastewater treatment (SUMO, 2022). Retentate quality of the NF membrane after MNR is calculated based on retention data from pilot trials of capillary NF and estimated water recovery into permeate (25%). Permeate of NF amounts to 13,125 m³/a and meets quality criteria for reuse as process water in the brewery. SBR effluent quality is calculated based on relevant design guidelines (DWA, 2009; 2010; 2016a) and nutrient balances (Exner, 2023). Effluent of EGSB to SBR is estimated from supplier data, whereas final SBR is also calculated based on SBR design guidelines (Exner, 2023). All effluents in the different scenarios comply with the local discharge limits for the brewery.

Table 27: Flow and quality of water for LaTrappe case study: raw wastewater and effluent of the different scenarios

Parameter	Unit	Raw wastewater	MNR effluent	MNR + NF effluent	SBR effluent	EGSB + SBR effluent	Discharge limits
		All scenarios	MNR	MNR + NF	SBR	EGSB + SBR	All
Volume	[m³/a]	52,500	52,500	39,375*	52,500	52,500	
COD	[g/m³]	3,725	84	111*	85	79	125
TSS	[g/m³]	438	3.1	4.1*	3.6	2.1	10
Total N	[g/m³]	46	1.5	1.7*	1.9	1.3	10
Total P	[g/m³]	5.1	0.2	0.3*	0.6	0.3	1
Source		DeDOMMEL	BIOPOLUS	SEMiLLA	KWB	KWB	DeDOMMEL

** Retentate of NF membrane is more concentrated than original MNR effluent (25% water recovery of NF feed into permeate)*

Sludge balance

Data of excess sludge production for all scenarios is calculated based on modelling or design guidelines comparable to water quality (Table 28). For the MNR process, the amount of dry matter (DM) of excess sludge is predicted by the SUMO model. DM of excess sludge from SBR is calculated from design guidelines, whereas sludge DM from EGSB is estimated from literature (Exner, 2023). Final DM content of excess sludge after dewatering in belt filter press is estimated to 22% DM for all scenarios, except for sludge from pre-treatment of

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EGSB which is directly dewatered in a screw press to 15% DM. Total mass of the sludge to be disposed is then calculated from total DM and dewatering result.

Nutrient content in the sludge is estimated to 5% nitrogen in DM for all sludges, whereas P content is calculated based on a closed P mass balance (P input = P output in effluent or sludge). Nutrient credits from sludge disposal (cf. Table 9) are calculated based on nutrient content in sludge and estimated efficiencies for mineral fertilizer substitution (N: 50% and P: 80%).

Table 28: Flow and quality of excess sludge in each scenario for LaTrappe case study

Parameter		MNR	MNR + NF	SBR	EGSB + SBR		Remark
		MNR	MNR + NF	SBR	Pre-treatment	EGSB + SBR	
Mass	[t/a]	275	275	272	95	80	calculated via DM
Dry matter (DM)	[%]	22	22	22	15	22	KWB estimate
	[t/a]	60.6	60.6	59.9	14.3	17.6	Model or design guidelines
Total N	[% of DM]	5	5	5	5	5	KWB estimate
Total P	[% of DM]	2.8	2.8	1.7	0.1	1.4	P mass balance
Source		BIOPOLUS	BIOPOLUS	KWB	KWB	KWB	

Direct emissions of processes

Direct emissions of processes are accounted for the biological stage of the WWTP (CH_4 in EGSB scenario) and biogas incineration in a heater (CH_4, NO_x, SO_2, N_2O). For the anaerobic process of EGSB, it is assumed that the effluent is almost saturated with CH_4 at 25°C (20.5 mg/L CH4), which is transferred to the downstream SBR. This dissolved fraction amounts to 1125 kg/a CH_4 or 3.5% of the total CH_4 produced in the EGSB. In the SBR, it is assumed that 50% of the dissolved CH4 is stripped to the atmosphere and counted as direct emission in this study. The remaining 50% of dissolved CH_4 are consumed by methanotrophic microorganisms in the SBR, and are thus not emitted to atmosphere.

Potential emissions of N_2O from biological nitrogen conversion are not accounted in the present study. The composition of brewery wastewater shows a very high COD/N ratio (~ 80) compared to municipal wastewater, so no targeted denitrification is required to reach N effluent limits. In contrast, mineral nitrogen has to be dosed into the process to allow for sufficient nutrient supply to the biomass (see below and Table 31). Overall, it is very difficult to predict potential N_2O emissions from biological treatment of brewery wastewater, as most available knowledge of N_2O emission factors relate to municipal wastewater. In addition, it seems not feasible to predict any difference between scenarios of this study in terms of N_2O emissions, so it was decided to neglect these emissions for all scenarios.

For direct emissions of biogas incineration, emission data from a previous study is used (Ronchetti et al., 2002) with a methane slip of 0.5%. On top, 0.5% of biogas is flared and does not contribute to heat credits.

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Electricity, chemicals and material for infrastructure

Inventory data for electricity demand of major processes are listed below (Table 29). Electricity demand for MNR operation is estimated by BIOPOLUS based on installed equipment on-site, calculating via installed load, run time per day, and load factor of each unit. To account for actual underloading of the existing system (designed for 450 m^3/d, but loaded with 150 m^3/d), higher specific efficiencies for aeration and DAF operation are taken from BIOPOLUS calculations at full design load. Overall, MNR operation requires 3.3 kWh/m^3 of electricity, mainly for aeration (64%), pumping and mixing (15%), and sludge separation and dewatering with DAF and belt filter press (15%).

The NF membrane stage requires 0.19 kWh/m^3 influent based on information from SEMiLLA. The low water recovery (25%) and the relatively low inlet pressure (3 bar) for the capillary NF lead to a comparably low electricity demand for this stage. On top, more electricity for pumping is required to deliver the reused water from the NF stage to the brewery (2 bar).

Table 29: Inventory data for electricity demand and energy credits for scenarios of LaTrappe case study

Process	Unit	MNR	MNR + NF	SBR	EGSB + SBR	Remark
Electricity						
Pre-treatment	MWh/a	-	-	-	10.1	
Aeration	MWh/a	109.0	109.0	93.3	16.1	
Pumping + mixing	MWh/a	26.0	31.2	31.5	44.7	
Sludge separation + dewatering	MWh/a	24.3	24.3	11.8	8.9	i.a. DAF, MF, belt filter press
Auxiliary	MWh/a	11.7	11.7	11.1	11.9	i.a. chemical dosing, off-gas air filter
Membrane	MWh/a	-	10.1	-	-	0.19 kWh/m^3_{in}
Total	MWh/a	171.0	186.3	147.6	91.8	All units
Total	kWh/m^3	3.3	3.5	2.8	1.7	In relation to influent wastewater
Biogas from external sludge digestion						
Electricity credit	MWh/a	-24.2	-24.2	-23.9	-12.2	Net output of sludge digestion
Biogas from anaerobic treatment						
Heat credit	MWh/a	-	-	-	-425	From biogas of EGSB

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For the SBR scenario, total electricity demand is calculated to 2.8 kWh/m³ using typical efficiencies and cycle time (Exner, 2023). Again, the driving factor is the aeration demand (63%) followed by pumping and mixing (22%). Electricity for SBR aeration is calculated based on predicted oxygen demand (DWA, 2016a) and a specific oxygen transfer efficiency of 2 kg O_2/kWh for fine bubble aeration, using an alpha factor of 0.6.

For the EGSB+SBR scenario, total electricity demand for water treatment amounts to 1.7 kWh/m³ (Exner, 2023), with major contributions from pumping and mixing (49%) followed by aeration in SBR (18%).

Electricity credits from sludge digestion are calculated to 400 kWh per ton DM in sludge according to previous studies of KWB (Remy et al., 2021). This number already represents a net electricity output where electricity produced from biogas via CHP plant is partially off-set by electricity needs for digestor operation and final dewatering.

Credits for biogas from EGSB are calculated based on typical methane yields for anaerobic treatment of brewery wastewater (0.29 Nm³/kg COD in), resulting in a total methane volume of 50,300 Nm³ per year. From the total methane produced, losses with dissolved CH_4 in effluent are deducted (3.5%, see above). Use of recovered biogas in a heating system in the brewery at 90% thermal efficiency yields credits of 425 MWh/a of heat, which can substitute an equivalent amount of heat from natural gas.

Inventory data for chemical demand and credited products are listed below for each scenario (Table 30). Polymer for sludge dewatering in belt filter press (4 kg active matter per ton DM) and final dewatering after external digestion (8 kg active matter per kg DM to digestor) is accounted in each scenario. For pH control of incoming raw wastewater, both caustic and sulfuric acid are used based on information by the operator.

For the MNR scenario, nutrients have to be dosed upstream of the biological treatment to balance the unfavourable COD/N/P ratio of the wastewater and enable sufficient growth of the biomass. According to SUMO modelling by BIOPOLUS, a total amount of 2 t N and 1.5 t P per year are required on average, which are dosed here as urea and mineral P. DAF operation needs dosing of coagulant (FeCl3) and polymer, which is assumed here based on supplier information with additional safety factors. For NF operation in the MNR+NF scenario, additional chemicals are used for membrane cleaning (NaOH, citric acid, NaOCl) according to information from SEMiLLA.

For SBR operation, nutrient deficits have been calculated with design rules for activated sludge plants (DWA, 2016a), resulting in slightly different dosing of additional N (+ 2.3 t/a) and P (+ 1 t/a) compared to the MNR scenario. No nutrient dosing is required in the EGSB+SBR scenario, as the anaerobic process has a lower biomass yield and consequently a lower nutrient demand. The downstream SBR process after the anaerobic stage operates with a suitable COD/N/P ratio for aerobic processes, as most of the COD has been removed in the anaerobic EGSB. To minimize H_2S content in the recovered biogas, $FeCl_2$ is dosed upstream of EGSB to convert sulphur into iron sulphide.

Credits for each scenario are accounted for nutrients in sludge, and recovered process water in the scenario MNR+NF. Nutrient content in sludge is estimated with a fixed factor of 5% N in DM for nitrogen, while phosphorus content is calculated from a mass balance of P input (raw wastewater and dosed nutrients) and output with effluent. From the total nutrient

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content in sludge, 50% of N and 80% of P are accounted as readily plant-available to substitute an equivalent amount of mineral fertilizer (NL mix of mineral N/P fertilizers).

In the water reuse scenario MNR+NF, a total volume of 13,125 m³ per year is recovered as process water for the brewery with NF permeate. This water can substitute an equivalent volume of freshwater which would normally be used at the brewery (e.g. for bottle washing, cleaning). The avoided burden of water production is accounted here with an LCA dataset for water production from groundwater without further treatment.

Material demand for infrastructure is calculated based on a detailed inventory of tanks, pipes and process units for each scenario (Exner, 2023). Resulting total masses of selected materials are listed below (Table 31). Lifetime of the infrastructure is estimated to 15a for machinery, and 30a for buildings and tanks.

Table 30: Inventory data for chemicals and credited products for scenarios of LaTrappe case study

Process	Unit	MNR	MNR + NF	SBR	EGSB + SBR	Remarks
Chemicals						
$FeCl_2$ (30%)	kg/a	-	-	-	480	For sulfide control in biogas
$FeCl_3$ (40%)	kg/a	5068	5068	-	-	Supplier data for DAF
Polymer for DAF	kg am/a	630	630	-	-	Supplier data + security factor
Polymer for belt press	kg am/a	256	256	239	73	Supplier data
Polymer (external)	kg am/a	484	484	479	269	Dewatering after digestor
NaOH (50%)	kg/a	4590	4590 + 48 (NF)	4590	4590	For pH control in influent buffer
H_2SO_4 (96%)	kg/a	3350	3350	3350	3350	For pH control in influent buffer
NaOCl (10%)	kg/a	-	150	-	-	For membrane cleaning
Citric acid (60%)	kg/a	-	77	-	-	For membrane cleaning
Urea (as N)	kg/a	2030	2030	2275	-	For nutrient supply of aerobic biomass
Mineral P	kg/a	1470	1470	1015	-	For nutrient supply of aerobic biomass
Credited products						
Mineral N fertilizer	kg N/a	1517	1517	1485	776	50% of N in sludge
Mineral P fertilizer	kg P/a	1380	1380	807	200	80% of P in sludge
Recycled process water	m³/a	-	13,125	-	-	NF permeate

am: active matter

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Table 31: Inventory data for infrastructure materials for scenarios of LaTrappe case study

Process	Unit	MNR	MNR + NF	SBR	EGSB + SBR	Remarks
Materials						
Concrete	t	667	703	695	664	Tanks, building
Reinforcing steel	t	66	69	60	57	Tanks, building
Stainless steel	kg	164	264	426	2,378	e.g. EGSB reactor
Iron	kg	832	932	562	573	Pumps
HDPE	kg	139	139	67	67	Pipes
PP	kg	1,400	1,400	305	1,511	Pipes
PVC	kg	-	-	-	173	Pipes
GRP	kg	410	610	40	2,040	e.g. DAF, EGSB reactor
Glass	t	22	22	-	-	Glasshouse for MNR
Sand-lime bricks	t	52.8	52.8	-	-	Glasshouse for MNR

Background data

Background processes for production of electricity, chemicals, materials, transport, and fertilizer production are modelled with datasets from LCA database ecoinvent v3.8 (Ecoinvent, 2021). A full list of processes and related models is available in the annex (Table 57). Transport of materials is estimated by truck for chemicals (150 km), sludge of WWTP to local digestor (10 km) and disposal to farmland (10 km), and materials for infrastructure (100 km).

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LCA results

This chapter presents results of impact assessment, comparing the baseline situation using conventional technologies for WWT with the NEXTGEN scenarios. Indicators are discussed separately and analyzed towards major contributors, important input parameters, and respective conclusions for the analysis.

Cumulative energy demand (CED)

Total net CED of the MNR amounts to -1572 GJ/a (Figure 4). Major contributions to CED come from electricity consumption (70%), followed by nutrient dosing (16%), chemicals for operation (9%) and infrastructure (5%). Sludge disposal generates CED credits with recovered biogas and also some nutrient recycling, off-setting around 24% of CED from the system.

Adding an NF stage for water reuse, CED increases by 4% or 65 GJ/a. In comparison to MNR, a conventional SBR system for aerobic treatment of brewery wastewater has a lower CED of around 1302 GJ/a, which is 17% less than for the MNR system. Changing to an anaerobic treatment, the net CED is even negative, with a net energy benefit of -1290 GJ/a from the system.

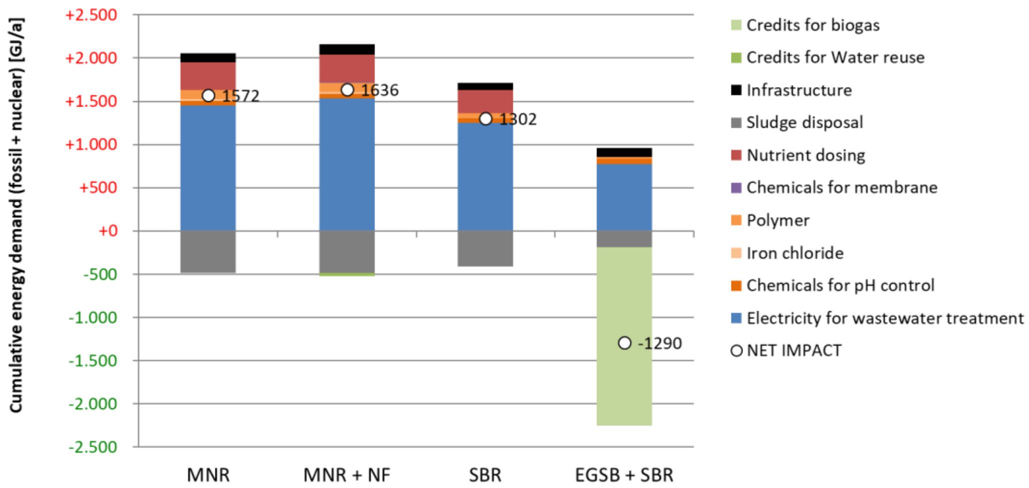

Figure 37: Cumulative energy demand of NEXTGEN scenarios for LaTrappe brewery

The increase of CED with adding an NF stage is mainly due to additional electricity required for NF operation (Figure 5). Additional infrastructure for the membrane stage and piping also adds to the CED. Chemicals for NF cleaning play only a minor role in the overall CED. The efforts for water reuse are partially compensated by avoided water production at the brewery, which can off-set 35% of additional CED. However, it becomes clear that water reuse from MNR effluent needs more energy (7.6 MJ/m³) than the existing water supply in the brewery from “clean” groundwater (2.7 MJ/m³).

Compared to the MNR, an SBR system will decrease electricity consumption by 14% (cf. Table 8), mainly due to more efficient aeration and no need for an energy-intensive DAF system. While oxygen demand for COD removal is comparable between MNR and SBR, aeration efficiency seems better in SBR due to higher tank depth (SBR: 4.5m, MNR: 3m). On top, SBR operation needs less chemicals than MNR (no polymer and $FeCl_3$ for DAF operation, less P dosing).

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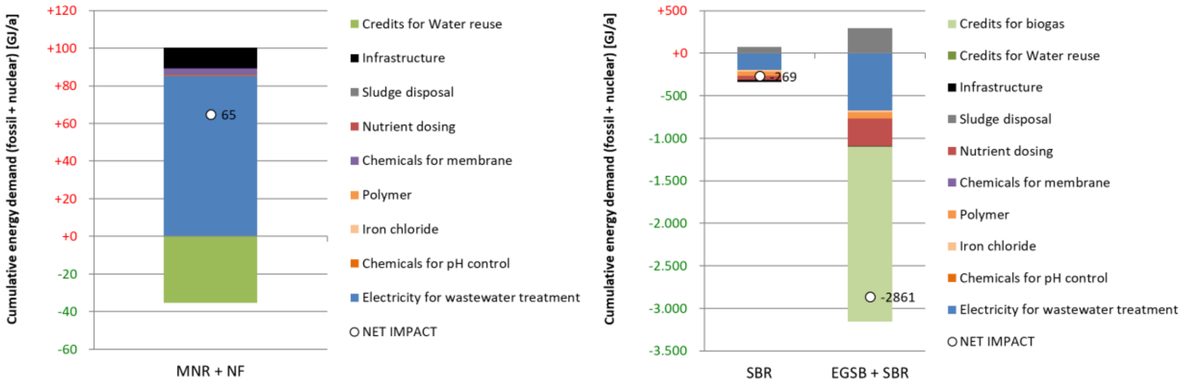

Figure 38: Changes in cumulative energy demand compared to MNR scenario for LaTrappe brewery (left: MNR+NF, right: SBR and EGSB+SBR)

For the anaerobic EGSB system, lower electricity demand (-46% to MNR) and no nutrient dosing contribute to a lower CED compared with MNR and SBR. However, the major energetic benefit of this scheme is the high amount of biogas produced from the organic load, which can be used for heat generation at the brewery and yields credits of 39 MJ/m³ of wastewater. Overall, the high energy recovery can fully compensate the energy demand of wastewater treatment, resulting in an energy-positive scheme with net energy output for the brewery.

Global warming potential (GWP)

For GWP, results are closely linked to energy inputs and outputs of the systems, as fossil fuels used in energy or chemical production mainly contribute to GHG emissions. The net GWP of the MNR system amounts to -105 t CO_2e/a (Figure 6), with contributions from electricity (74%), nutrient dosing (12%), other chemicals (7%) and infrastructure (7%). Credits from sludge disposal can off-set 23% of total GWP of the system.

With water reuse in scenario MNR-NF, net GWP increases by 6% (6 t CO_2e/a) compared to MNR. The SBR system reduces net GWP by -18%, while the anaerobic EGSB generates net GWP credits with -31 t CO_2e/a.

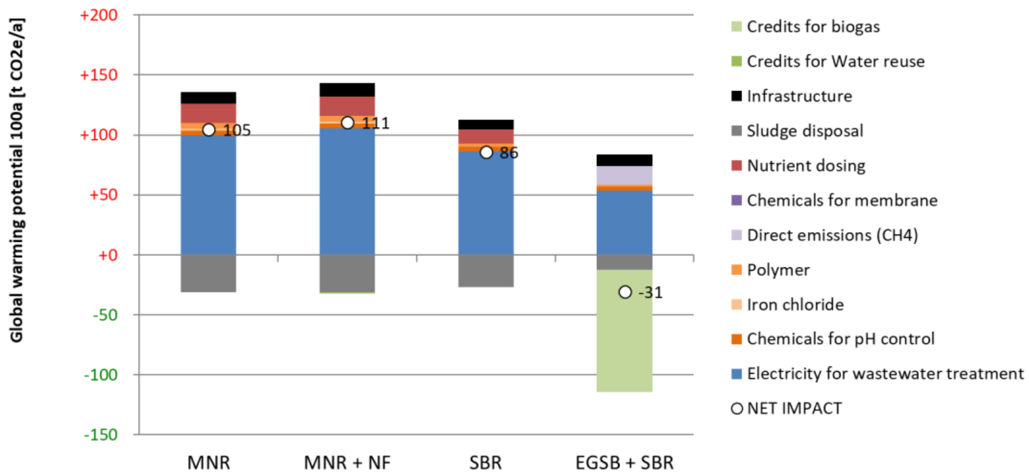

Figure 39: Global warming potential of NEXTGEN scenarios for LaTrappe brewery

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Looking at the individual contributions of GWP changes, water reuse in NF adds GWP for additional electricity and infrastructure, while savings in water production at the brewery can compensate 19% of GWP from NF operation (Figure 7). In analogy to CED, water reuse generates more GHG emissions (552 g CO_2e/m^3) than existing water production in the brewery (102 g CO_2e/m^3).

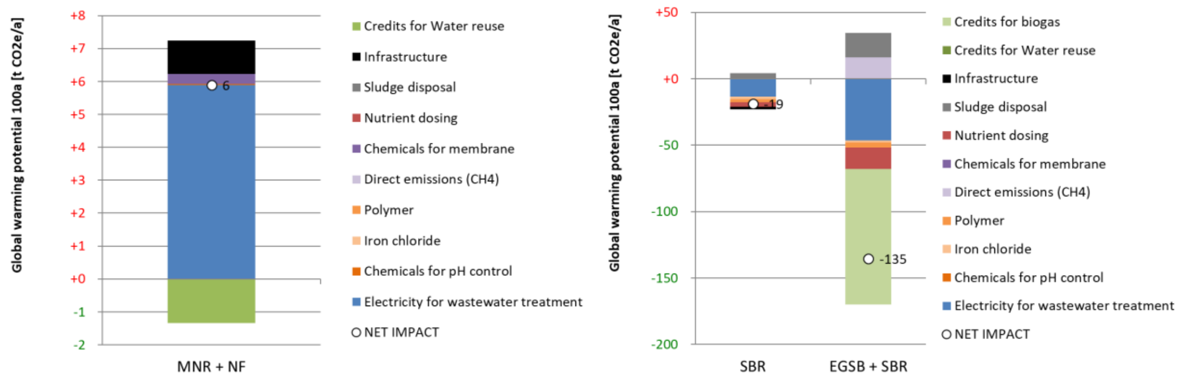

Figure 40: Changes in global warming potential compared to MNR scenario for LaTrappe brewery (left: MNR+NF, right: SBR and EGSB+SBR)

The SBR system has a lower GWP compared to the MNR, mainly due to lower electricity and chemicals demand. Again, the anaerobic EGSB benefits from low electricity demand and high biogas recovery. Losses of methane to the atmosphere with dissolved CH_4 in EGSB effluent (1.75% of produced biogas) contribute to GWP, but are low compared to the overall benefits of the anaerobic system and do not change the net GWP balance of this scheme significantly.

Freshwater eutrophication potential (FEP)

Net FEP of the MNR scenario amounts to 18 kg P-eq/a, which originate from P emissions with MNR effluent (59%), and indirect P emissions in electricity production (21%) and chemicals supply (11%) (Figure 8). The high share of background processes in this indicator illustrates that total P loads in MNR effluent are already very low (0.2 mg/L TP), so that indirect P emissions from the life cycle contribute more significantly to this impact.

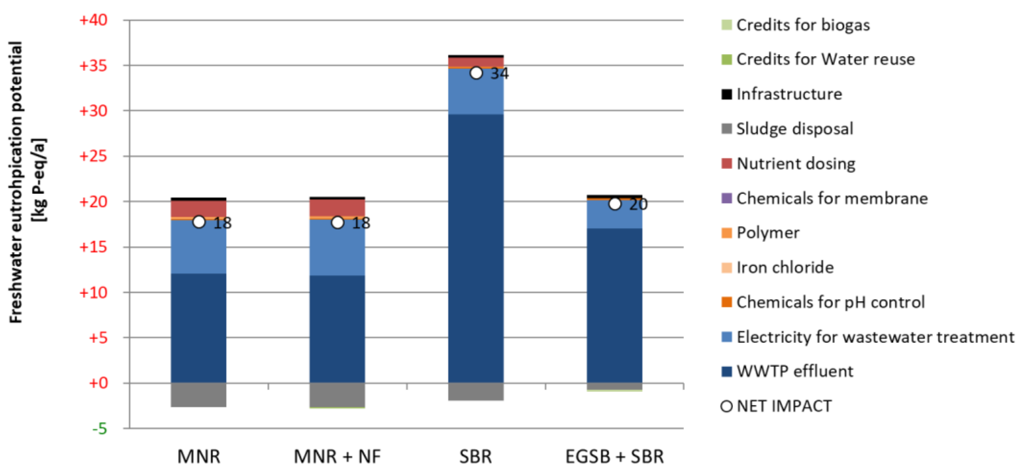

Figure 41: Freshwater eutrophication potential of NEXTGEN scenarios for LaTrappe brewery

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N°776541

Net FEP does not change with water reuse in scenario MNR+NF, as additional electricity, chemicals and infrastructure for NF have a low FEP. In addition, a small fraction of input P ends up in recycled water and thus does not contribute to P loads to the environment any more.

For the SBR scenario, net FEP increases due to a higher effluent concentration of P in this system (0.5 mg/L TP) compared to MNR. It is to be noted that effluent P concentration in the SBR is estimated here from nutrient mass balances and could probably adjusted to lower values in real operation (e.g. optimised P dosing, or addition of $FeCl_3$ for residual P removal). However, as the MNR system uses high amounts of $FeCl_3$ for DAF operation, a lower total P effluent concentration for this system still seems somewhat reasonable compared to an SBR without any Fe dosing. For the EGSB+SBR scenario, P concentration in effluent is also slightly higher (0.3 mg/L TP) compared to MNR: this system operates with a lower Fe dose (mainly for fixing sulphide) than MNR, but also needs no additional P dosing for the biological treatment.

Overall, P effluent concentrations of both SBR and EGSB are estimated here based on mass balances, and could be lower with changes in operational regime (e.g. more Fe dosing). Hence, differences in FEP between the scenarios reported in this study are reflecting design values and operational modes defined here, and not absolute potential of P removal of the different systems in comparison. In addition, the impact of high P dosing for both MNR and SBR (= factor 4-5 compared to P load in brewery wastewater) to cover nutrient demand of the biomass on the final P concentration in the effluent should be investigated with real operational data rather than design calculations.

Marine eutrophication potential (MEP)

Net MEP of the MNR scenario amounts to 99 kg N-eq/a and is dominated by N loads in WWTP effluent (Figure 9). Life-cycle MEP of electricity, chemicals and infrastructure contributes around 25% to the total MEP. With water reuse in scenario MNR+NF, N loads with WWTP effluent are slightly lower: as N rejection of the NF membrane is limited (28%), NF permeate still contains some N which is recycled to the brewery and not discharged to nature.

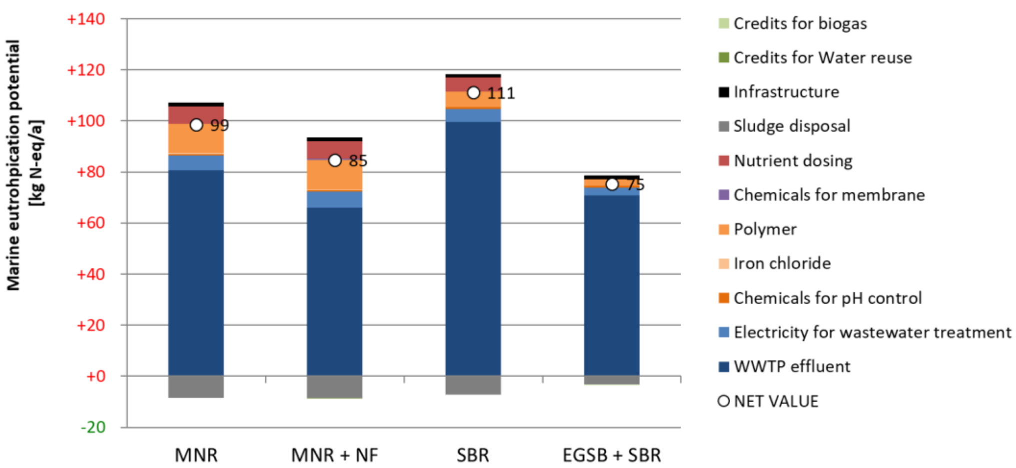

Figure 42: Marine eutrophication potential of NEXTGEN scenarios for LaTrappe brewery

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N effluent concentration in SBR scenario is slightly higher than MNR (cf. Table 5), which results in a higher net MEP of 111 kg N-eq/a. In contrast, the EGSB scenario has the lowest net MEP of 75 kg N-eq/a, with low N effluent concentration and lower MEP from the life cycle of electricity, chemicals and infrastructure. Again, predicted N effluent concentration in all scenarios is based on design assumptions and N mass balances, and may not represent the actual potential of each system to remove N from brewery wastewater. Finally, all scenarios have a low TN concentration in their effluent (< 2 mg/L TN) and thus have a small impact on the local surface water.

Terrestrial acidification potential (TAP)

TAP of the MNR scenario amounts to 221 kg SO_2e/a, mainly due to electricity (38%) and nutrient dosing (37%) followed by other chemicals and infrastructure (Figure 10). Here, credits for sludge disposal are substantial and compensate 46% of total TAP due to energy recovery and N recycling with sludge.

Water reuse in MNR-NF scenario has no large impact on net TAP (+3% to MNR). The SBR scenario has a lower net TAP than MNR (-25%) because of lower electricity demand and also nutrient dosing (31% less P). Net TAP of the EGSB+SBR scenario amounts to 195 kg SO_2-eq/a: while credits from biogas use for heat production are very low, direct emissions of biogas use (e.g. NO_x, SO_2) contribute substantially to TAP for this scenario. Still, it is better than the MNR scenario (-12%) as electricity consumption is lower and no nutrient dosing is required.

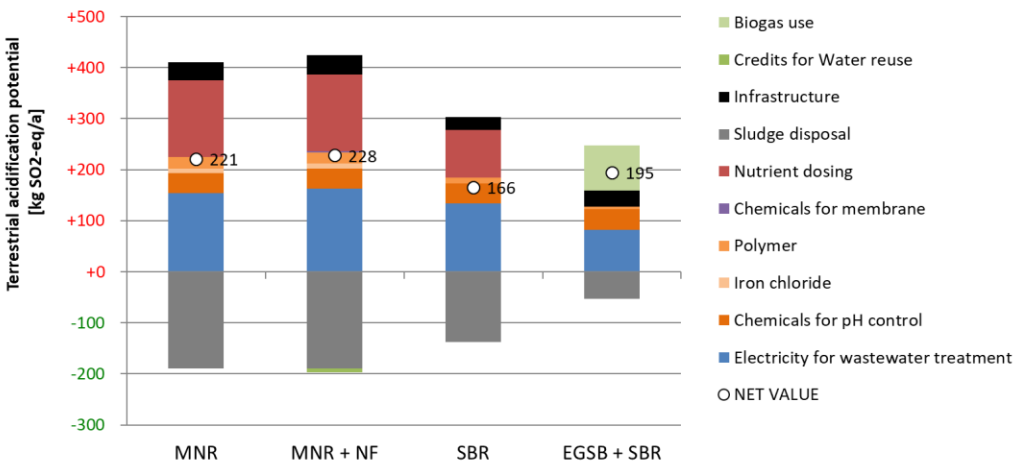

Figure 43: Terrestrial acidification potential of NEXTGEN scenarios for LaTrappe brewery

Interpretation and conclusions

Table 32 gives a summary on the net environmental impacts for all calculated impact categories and scenarios for the La Trappe case study. From the LCA, the following conclusions can be drawn:

- The **MNR system** has a **very good effluent quality** in terms of N and P. **Energy use of the system and corresponding GHG emissions are higher** than for the SBR system as benchmark of aerobic treatment. This is mainly due to less efficient aeration (lower tank depth than SBR), but also due to the energy and chemical-intensive DAF operation to separate the excess biomass. Potential benefits of the nature-based biofilm system such as lower sludge production and efficient aeration could not be confirmed with the results of this study. However, it has to be noted that both MNR and SBR results are based on design assumptions and modelling, and not on real data from full-scale operation.

- **Water reuse with a NF membrane adds 4-6% in energy demand and corresponding GHG emissions** for electricity and infrastructure. Compared to water production from groundwater, recycled water is more energy-intensive (factor 3) and causes higher GHG emissions (factor 5). However, it enables the **supply of process water to the brewery without putting additional pressure on local groundwater resources**. Due to the low water recovery of the membrane process, the remaining concentrate can still be discharged without restrictions to the local surface water.
- **SBR as benchmark for aerobic treatment** of brewery wastewater has a **better energy and GHG profile** than the MNR system due to a higher aeration efficiency. Effluent water quality is slightly inferior to the MNR system in this study, although this estimate mainly relies on design assumptions and operational mode rather than a lower performance of the technical system.
- **Anaerobic treatment of brewery wastewater** in an EGSB has a **significantly better energy and GHG profile** than both MNR and SBR in this study. The system benefits from low energy input, and high energy recovery in form of biogas. Overall, the entire treatment of brewery wastewater can operate with a **net energy output and net savings in GHG emissions**, illustrating the potential of anaerobic treatment for industrial wastewater with high COD. Dissolved methane contributes to GHG emissions, but has a low contribution here with the highly concentrated wastewater and the post-treatment in an aerobic stage.

Table 32: Summary of net environmental impacts for La Trappe brewery for NEXTGEN scenarios

Scenario		MNR	MNR + NF	SBR	EGSB + SBR
Products of NEXTGEN	1/a		13,125 m^3 water		
Cumulative energy demand (non-renewable)	GJ/a	1572	1636 (+4%)	1302 (-17%)	-1290 (-182%)
Global warming	t CO_2-eq/a	105	111 (+6%)	86 (-18%)	-31 (-129%)
Freshwater eutrophication	kg P-eq/a	18	18 (0%)	34 (+92%)	20 (+11%)
Marine eutrophication	kg N-eq/a	99	85 (-14%)	111 (+13%)	75 (-24%)
Terrestrial acidification	kg SO_2-eq/a	221	228 (+3%)	166 (-25%)	195 (-12%)

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Overall, the LCA results show that the treatment of brewery wastewater in aerobic processes such as MNR and SBR is associated with a significant electricity demand (2.8 to 3.3 kWh/m³), which translates into high primary energy demand and related GHG emissions. On top, the unfavourable nutrient balance of the raw wastewater requires the addition of a significant amount of nutrients to compensate the deficit of N and P for biomass growth. However, both systems are able to produce a very good effluent quality and thus have a low impact on the receiving surface water. An anaerobic treatment of brewery wastewater is very beneficial from an environmental point of view, as high COD loads favour the recovery of biogas and enable an energy-positive and carbon-negative operation of such a system. However, the economic and technical feasibility of an anaerobic system with biogas production at a relatively small site such as La Trappe with limited personnel capacity is questionable, and could pose a serious barrier for implementation of such a concept in reality.

Water reuse from MNR effluent with the capillary NF membrane is feasible and produces a suitable quality for process water in the brewery, but comes at a higher energy and GHG impact than water produced from the local groundwater. A low water recovery seems key to a reasonable energy demand of the NF membrane together with a low concentration factor in the concentrate, which can still be discharged without restrictions.

Input data for this LCA is mainly based on design calculations and modelling rather than operational data. Hence, operational results and primary data of larger systems is required to validate the conclusions from this LCA, representing the actual boundary conditions and situation at La Trappe brewery. Important factors for the LCA outcomes are the real electricity demand of each system in long-term operation, the amount of nutrient dosing for the aerobic systems, the chemical needs for DAF operation, and the long-term performance of the NF membrane for water reuse.

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Spernal (UK): energy, nutrient and water recovery in municipal wastewater treatment

In the NEXTGEN project, Severn Trent Water (STW) together with University of Cranfield (UCRAN) evaluates a new concept of anaerobic treatment of municipal wastewater. This concept includes an anaerobic membrane bioreactor (AnMBR) followed by nutrient removal and recovery using an ion exchange process. For anaerobic treatment, the pilot installation at Spernal wastewater treatment plant (WWTP) includes an upflow anaerobic sludge blanket (UASB) reactor in combination with an ultrafiltration (UF) membrane and a degassing unit. The UASB reactor combines two energetic benefits: 1) low energy consumption for chemical and biological oxygen demand (COD/BOD) removal because no aeration is needed and 2) biogas production in the biological stage of the WWTP. The UF is coupled to the UASB and delivers a pathogen and solids free effluent which can be further treated or re-used in a number of applications such as ion exchangers for nutrient recovery, or directly for irrigation or industrial use. To complete the anaerobic treatment, a degasser is located downstream of the UF to recover the dissolved methane.

In the UASB no targeted nutrient removal takes place, so an ion exchange process (IEX) is tested as post-treatment option to remove and recover nitrogen and phosphorus. The IEX is implemented downstream of the AnMBR setup and enables a targeted removal of ammonia (NH_4) and phosphate (PO_4) depending on the type of IEX material. The first IEX stage removes ammonium (N-IEX) using a specific zeolite resin, and the second IEX stage eliminates phosphate (P-IEX) with a hybrid anionic ion exchange resin. Upon saturation of the IEX resin, the IEX is regenerated by backwashing the resin with a 10% KCl solution for the N-IEX or with a 2 % NaOH solution for the P-IEX. Subsequently, the nutrients can be recovered from the regenerant solution by membrane stripping (N) and precipitation of phosphorus as a mineral salt (P). The benefits of IEX processes include their potential to remove these nutrients to very low concentration limits, and also to recover valuable nutrient products from the regenerant in the form of nitrogen or phosphorus intermediates, which can then be directly used as fertiliser or as input material in the chemical industry.

In this study, the new schemes are compared in their environmental impacts to selected reference WWTP schemes with conventional technology to show the benefits and drawbacks of this innovative technology against the current state. To explore different setups of the technologies, several potential scenarios are investigated. As alternative to the energy-intensive membrane degasser, residual methane can also be oxidised again using an membrane-aerated biofilm reactor (MABR). In another scenario the UF effluent is used directly for irrigation in agriculture without removing nutrients. Therefore, both water and also N and P can be directly reused in agriculture (“fertigation”).

The analysis will be done for a typical WWTP of STW treating municipal wastewater of 100,000 pe as benchmark. The focus of this LCA is on comparing efforts for wastewater treatment (primary energy demand, greenhouse gas (GHG) emissions) and impact on water quality (eutrophication), also considering the recovered products of biogas, nutrients, and water for reuse.

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Goal and scope definition

The goal of this LCA is to assess the potential environmental impacts of an anaerobic reactor for carbon removal and biogas production in combination with an ion exchange process for nutrient removal and recovery at a municipal WWTP. The LCA considers all relevant effects on the entire wastewater treatment process including sludge treatment and disposal.

The NEXTGEN schemes are compared to a reference system, which reflects a typical existing WWTP in the United Kingdom (UK) with 100,000 population equivalents (pe). The comparison allows to quantify environmental benefits and impacts or drawbacks of the NEXTGEN scheme. The target group of this study consists primary of stakeholders which are interested in high biogas recovery rates and nutrient recovery in combination with low effluent concentrations. Consequently, this group includes WWTP operators, engineers and scientists working in the wastewater sector.

Function and functional unit

The function of the system studied relates to the treatment of municipal wastewater to comply with defined discharge limits for COD, NH_4-N and P in the WWTP effluent. The primary system function can be formulated as "municipal wastewater treatment to reach a defined effluent quality". The recovery of biogas, nutrients or water for reuse is a secondary function of the system. This secondary function is reflected by crediting the avoided production of equivalent products to the respective scenario.

Based on the primary system function, the functional unit is defined as the impacts of a wastewater treatment process "per population equivalent (pe) and year" [impacts/(pe*a)].

System boundaries

The system boundaries of the LCA include all processes of a WWTP related to wastewater treatment, sludge treatment and disposal (Figure 44).

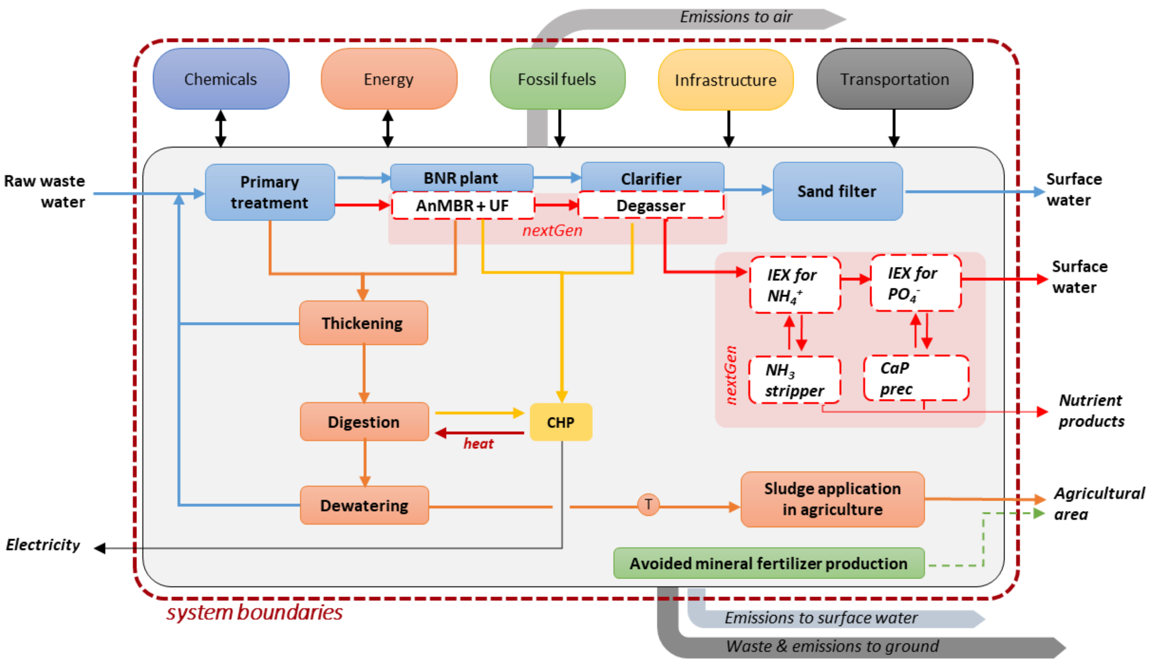

Figure 44: System boundaries of the LCA for conventional and NEXTGEN configurations tested at Spernal

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In particular, the LCA includes:

- Conventional wastewater treatment processes to reach defined effluent quality
- NEXTGEN configurations: UASB, UF, stage for CH_4 removal (degassing unit or MABR) and IEX in combination with nutrient recovery from regenerant
- Sludge thickening, digestion, dewatering, transport and disposal in agriculture
- Biogas valorisation in combined heat and power (CHP) plant
- All major background processes required for production of electricity, chemicals, and fuels
- Infrastructure for conventional WWTP and new scheme with AnMBR are assumed to be equal, therefore only the additional infrastructure of the IEX system is calculated

The geographical and temporal scope of the LCA is defined for the UK in 2020. Background data is related to UK conditions (electricity mix) or EU/world averages (chemicals, transport, infrastructure, mineral fertiliser production). Data for the reference system is assumed to represent mean operating conditions for WWTPs in the UK.

Allocation

All efforts (e.g. energy and chemicals consumption) and benefits (e.g. avoided production of electricity or mineral fertiliser) are related to the function of wastewater treatment. Therefore, no allocation is required. Nutrients delivered to agriculture via sludge or IEX products application are credited with “avoided mineral fertiliser production”. WWTP effluent for irrigation avoids groundwater pumping and are credited with “avoided electricity production”, following an “avoided burden” approach.

Scenarios

For the LCA, a typical WWTP and three NEXTGEN schemes have been designed in cooperation with STW and UCRAN. An overview of these scenarios is given in Table 33.

Table 33: Overview of scenarios for energy, nutrient and water recovery with NEXTGEN schemes for the Spernal LCA

Scenarios	BOD elimination	Methane removal	N removal/ recovery	P removal/ recovery
0. Reference WWTP	Activated sludge	-	Nitrification and denitrification	Biological P removal and tertiary sand filter with Fe dosing
1. UASB + Degasser + IEX	Anaerobic reactor + UF	Membrane degasser	N-IEX removal and recovery	P-IEX removal and recovery
2. UASB + Aerobic stage + IEX	Anaerobic reactor + UF	Aerobic stage (MABR)	N-IEX removal and recovery	P-IEX removal and recovery
3. UASB + Degasser + Irrigation	Anaerobic reactor + UF	Degasser	No targeted nutrient removal/recovery, water with nutrients for direct irrigation	

0. Reference WWTP: This scenario represents a typical biological nutrient removal (BNR) plant of STW with a size of 100,000 pe. After a primary clarifier, the secondary treatment consists of biological P and N removal combined with iron dosing. For tertiary treatment to remove P to very low limits, a second stage of iron dosing in combination with a sand filter is

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applied. Sludge treatment (thickening, digestion, dewatering) takes place on-site at the WWTP, and dewatered sludge is applied in agriculture. The effluent limit values for nutrients are defined as 0.5 mg/L NH_4-N and 0.3 mg/L TP.

1. UASB + Degasser + IEX: After primary treatment, secondary treatment consists of a combination of a UASB and UF membrane system for BOD and total solids (TS) removal but without targeted nutrient removal, i.e. without nitrification/denitrification and without Fe dosing. A membrane degasser recovers the dissolved biogas in the UF effluent. Tertiary treatment consists of a two-stage IEX system for NH_4^+ and PO_4^{3-} removal to reach the defined effluent standards. A large share of the nutrients can be recovered from the regenerant with stripping or precipitation processes. The setup of the sludge line is similar to the reference scenario. This scenario describes the configuration tested in the NEXTGEN pilot trials.

2. UASB + Aerobic stage + IEX: The second scenario is built the same way as the first scenario: it considers a UASB and UF combination for BOD removal and an IEX system for N and P removal/recovery. The only difference is the technology to remove the dissolved methane downstream of the UASB. The energy-intensive membrane degasser is replaced by an aerated stage using a membrane aerated biofilm reactor (MABR). This process converts residual CH_4 into CO_2 to prevent the direct emission of the potential greenhouse gas methane. CO_2 from the aerobic stage is of biogenic origin and therefore not accounted for global warming. The setup of the sludge line is similar to the previous scenario.

3. UASB + Degasser + Irrigation: This scenario considers the UASB configuration and degassing, but without an IEX for nutrient removal. The UF effluent is directly used for irrigation in agriculture, assuming that both nutrients and water can be utilized for the whole year, e.g. in greenhouse farming. Hence, the total amount of recovered water and nutrients are credited in this scenario. Therefore, it should be seen as maximum saving potential for a fertigation concept with the NEXTGEN scheme, while the actual demand for water and/or nutrients could be less in a real-world application.

Data source and quality

Table 34 gives an overview of the data quality used in this LCA study. The input data for the reference scenario is based on a typical WWTP operation at STW. The data quality is estimated as high, because STW operates multiple WWTPs in the respective conventional design. The NEXTGEN scheme is completely different to a conventional WWTP, which has an impact on effluent quality, energy demand for treatment, but also sludge amount and composition. These effects were estimated in close consultation with STW and UCRAN based on experience from pilot trials, and this data quality is assumed to be medium to high.

Data used for operating parameters of UASB and UF are based on pilot trials at Spernal WWTP concerning removal rates, water quality, and biogas yield. Energy demand is calculated based on assumptions for each unit (pumps, membrane etc.) by UCRAN and validated by KWB. Energy demand for the degasser was estimated by UCRAN with some uncertainty, which results in low data quality. Data regarding the aerated stage (MABR) is based on literature and is not verified in the project; consequently, the data quality is assumed to medium. Data regarding the IEX is mainly based on primary data collected from the pilot system operated in NEXTGEN and previous EU projects (SMART-Plant). Data quality regarding the effluent quality, energy and chemical demand is assumed to be medium, because the IEX systems have not been tested in full-scale yet. Hence, upscaling of the

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process data from pilot to full-scale was required and done in close cooperation with UCRAN. Data for the recovery of nutrients from the regenerant with a membrane stripper or through precipitation of calcium phosphate are based on laboratory experiments and were supplemented with literature data. Consequently, the data quality is seen as medium. The effects of direct irrigation of the UF effluent (i.e. avoided groundwater pumping and mineral fertiliser production) are estimated and reflect the maximum potential of reuse.

Table 34: Data sources and quality for the Spernal LCA

Process	Data source	Responsible partner	Data quality
WWTP: influent, effluent, sludge, energy + chemical demand	Full-scale data of operator	STW	High
Operational data of sludge line in NEXTGEN schemes	Estimations	STW, KWB	Medium to high
UASB and UF	Calculation	UCRAN	Medium
Degasser	Estimation	UCRAN	Low
Aerated stage	Literature	UCRAN	Medium
N-IEX and P-IEX layout and operation, including regenerant management	Pilot data	UCRAN	Medium to high
Recovery of NH_4 or calcium phosphate recovery from regenerant	Estimations, laboratory experiments	UCRAN	Low to medium
Irrigation	Estimates to assess maximum potential	KWB	Low
Background data	Ecoinvent v3.8	KWB	Medium to good

Input data for LCA

This chapter serves to present and discuss the used input data for reference WWTP and NEXTGEN schemes as well as background processes.

Water quality

The influent wastewater parameters represent an average wastewater of a 100.000 pe WWTP of STW (see Figure 45). The annual raw wastewater flow amounts to 9,110,400 m^3 (mean of 1,040 m^3/h). The effluent targets are defined as <0.5 mg/L TP and <3 mg/L NH_4-N for direct discharge into surface water. In the third scenario, the effluent is used for irrigation and no targeted nutrient removal takes place.

The return load consists of sludge thickening, sludge dewatering and sand filter backwashing, which is modelled separately for each scenario. For the reference scenario, backwash water of the sand filter of the reference scenarios adds as part of the return load to the WWTP.

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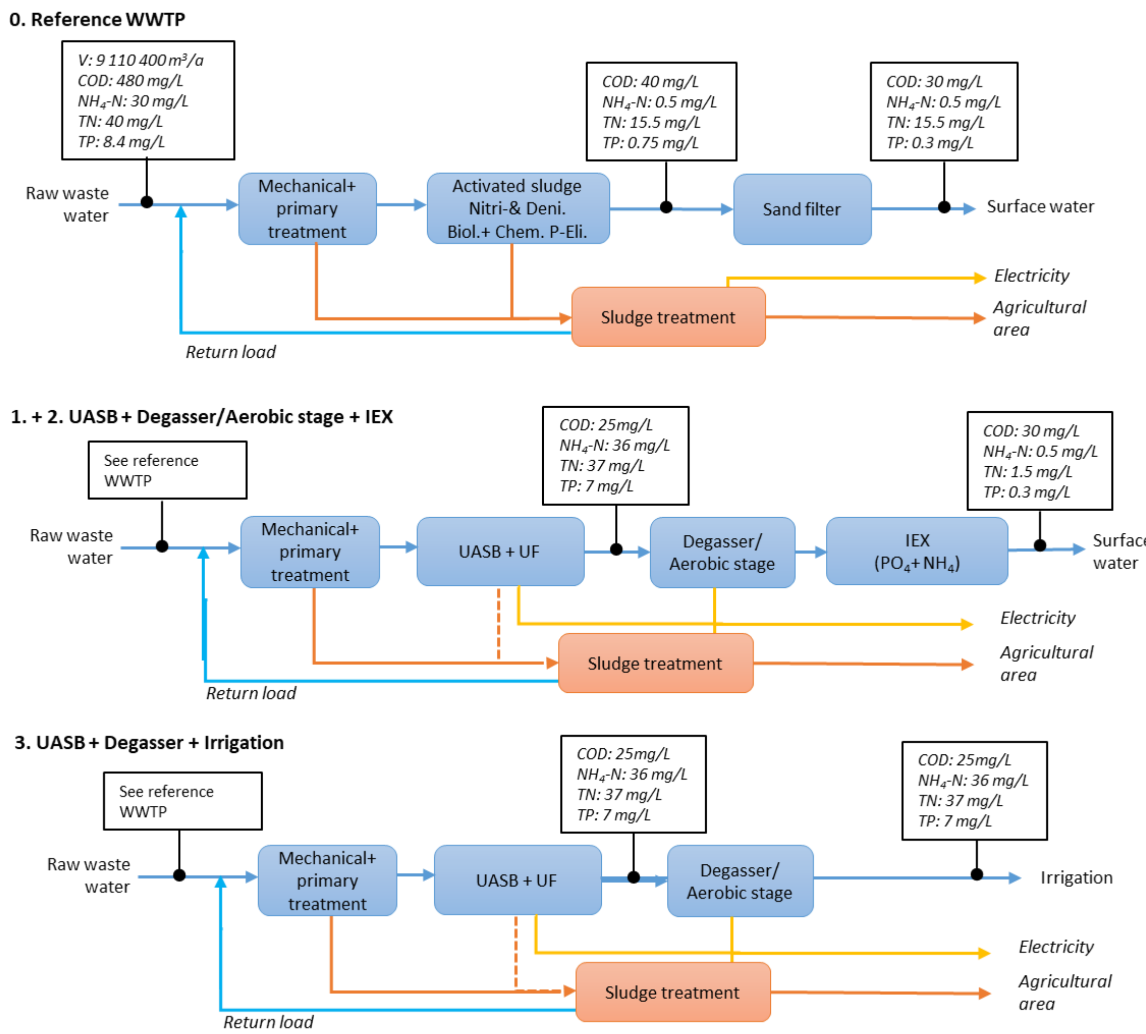

Figure 45: Water quality of the reference WWTP and NEXTGEN schemes

Energy demand

The energy demand for the scenarios is shown in Table 35. For all scenarios the specific electricity demand for primary treatment and sludge treatment (thickening, digestion and dewatering) is estimated to be equal. Electricity demand for the BNR stage in the reference scenario amounts to 0.25 kWh/m³ as a typical value for BNR plants of STW. Electricity demand for the UASB stage is lower by a factor of 5 (0.046 kWh/m³), as no aeration and only pumping is required. However, additional electricity is needed for the ultrafiltration (0.25 kWh/m³ due to high scouring of UF membranes with biogas to avoid fouling) and methane removal (membrane degasser: 0.25 kWh/m³ or aerated stage with MABR: 0.11 kWh/m³). Electricity demand of both UF and degasser are estimated based on pilot trials and expert guess from UCRAN and STW, and should be confirmed with real operational data. For the reference, an electricity consumption of 0.06 kWh/m³ is estimated for the final sand filter. For the IEX scenarios, 0.02 kWh/m³ is assumed for the pumps for the IEX modules. For the digester, the electricity demand amounts to 4.8 kWh/m³ sludge.

Biogas yield from sludge digestion is estimated to 500 Nm³/t oDM for primary sludge and 300 Nm³/t oDM for secondary sludge from BNR. The methane content of the biogas produced in the digester is 60%. In the UASB, 70% of incoming COD load is converted into methane. To calculate the produced methane, a maximum conversion of 350 Nm³ CH_4/t

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COD removed is assumed in this study. Although current pilot results show a methane yield of only 150 Nm³ CH_4/t COD removed, it is expected that this value can be increased with an optimizid operation. The methane content of the UASB biogas is assumed to 80%. Deducting 10% losses with dissolved methane at 6 mg/L, a total volume of 691,300 Nm³ CH_4/a can be recovered in the UASB.

Heat produced at the CHP covers the internal heat demand for digestion and other processes, while excess heat can usually not be used at the site and is therefore not accounted. In the fertigation scenario, the wastewater effluent is used for irrigation and substitutes groundwater. Hence, an electricity credit for avoided groundwater pumping equivalent to the volume of water reused is accounted in this scenario. It is assumed here that the reused effluent can replace groundwater for irrigation during the entire year, which in reality depends on the annual pattern of water demand in agriculture. Therefore, the amount of reused water and the corresponding electricity credit for avoided groundwater pumping should be seen as maximum saving potential if the total annual volume of effluent could be used for irrigation.

Table 35: Energy inventory for Spernal LCA. The values refer to the input volume of the respective treatment step

Process	Unit	0. Reference WWTP	1. UASB + Degasser + IEX	2. UASB + Aerobic stage + IEX	3. UASB + Degasser + Irrigation
Electricity					
Primary treatment	**m³/a**	**9,110,400**	**9,110,400**	**9,110,400**	**9,110,400**
Electricity primary	kWh/m³	0.1	0.1	0.1	0.1
Secondary treatment	**m³/a**	**9,794,000**	**9,175,800**	**9,175,800**	**9,175,800**
BNR plant	kWh/m³	0.25	-	-	-
Sand filter	kWh/m³	0.06	-	-	-
UASB	kWh/m³	-	0.046	0.046	0.046
Ultrafiltration	kWh/m³	-	0.25	0.25	0.25
Degasser	kWh/m³	-	0.25	-	0.25
Aerobic stage	kWh/m³	-	-	0.11	-
IEX	kWh/m³	-	0.02	0.02	-
Nutrient recovery from regenerant	**m³/a**	**-**	**N: 410,000 P: 106,300**	**N: 410,000 P: 106,300**	**-**
Stripping (N) or precipitation (P)	kWh/m³ regenerant	-	N: 0.56 P: 0.37	N: 0.56 P: 0.37	-
Sludge thickening	**m³/a**	**251,200**	**67,300**	**67,300**	**67,300**
Electricity	kWh/m³ sludge	0.06	0.06	0.06	0.06
Sludge digestion	**m³/a**	**44,000**	**25,800**	**25,800**	**25,800**
Digestor	kWh/m³ sludge	4.8	4.8	4.8	4.8
Dewatering of sludge	**m³/a**	**44,000**	**25,800**	**25,800**	**25,800**
Electricity	kWh/m³ sludge	2.00	2.00	2.00	2.00

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Process	Unit	0. Reference WWTP	1. UASB + Degasser + IEX	2. UASB + Aerobic stage + IEX	3. UASB + Degasser + Irrigation
Total electricity demand	MWh/a	4,271	6,569	5,275	5,068
Biogas production					
Methane from digestor	Nm^3 CH_4/a	482,400	302,500	302,500	302,500
Methane recovered from UASB	Nm^3 CH_4/a	-	691,300	691,300	691,300
Dissolved methane in UASB effluent	Nm^3 CH_4/a	-	75,900	75,900	75,900
Methane recovery in degasser	Nm^3 CH_4/a	-	75,100	-	75,100
Total biogas to CHP	Nm^3 CH_4/a	482,400	1,068,900	993,800	1,068,900
Electricity from CHP	MWh/a	1,982	3,837	3,529	3,837
Electrical self-sufficiency	%	46	58	67	76
Other credits					
Substitution of groundwater pumping	MWh/a	-	-	-	911

Chemicals and materials for operation

An overview of the specific chemical consumption is given in Table 36.

In the reference scenario, mainly iron sulphate for chemical P elimination and polymer for sludge dewatering are used. For tertiary treatment iron dosing upstream of the sand filter is applied. No chemical consumption is expected for operating the UASB. UF operation requires regular replacement of membranes, assuming a lifetime of 5.5 years for the modules.

The IEX needs resin, chemicals for regeneration and chemicals for product recovery from the regenerant. The amount of cationic and anionic resin is based on data from the pilot plant at UCRAN operated with effluent wastewater from the Spernal WWTP and considers regular losses with abrasion and full replacement of resin after lifetime.

The amount of potassium chloride required for N-IEX regeneration is calculated by molar ion balancing: each NH_4^+ ion replaces one K^+ ion, which is lost in the effluent and has to be replaced with fresh salt solution. The anionic ion exchanger adsorbs PO_4^{3+}-ions and releases them into the regeneration solution at a high pH value, exchanging with OH^- ions. These ions are "recharged" to the regeneration solution by using caustic lime for P precipitation. Consequently, the sodium hydroxide consumption is comparatively low and covers only the regular losses (2% per regeneration cycle).

For recovering nitrogen from the N-IEX regenerant, sulphuric acid is used to produce ammonium sulphate (21 % N) with membrane stripping. CaP as the product of P-IEX has to

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be treated with sulfuric acid to convert it into a plant-available form of P before it can be accounted to substitute conventional plant-available P fertilizer. Hence, a stoichiometric amount of sulfuric acid is calculated for conversion of CaP into a plant-available form.

Table 36: Chemical demand in Spernal LCA. Unless specified otherwise, data refers to input volume of respective treatment step.

Wastewater line	Unit	0. Reference WWTP	1. UASB + Degasser + IEX	2. UASB + Aerobic stage + IEX	3. UASB + Degasser + Irrigation
Secondary treatment	**m^3/a**	**9,794,000**	**9,175,800**	**9,175,800**	**9,175,800**
Iron sulphate	g Fe/m^3	2	-	-	-
Membrane for UF	m^2/a	12,000	12,000	12,000	12,000
Tertiary treatment (Sand filter/IEX columns)	**m^3/a**	**9,543,000**	**9,108,500**	**9,108,500**	**9,108,500**
Iron sulphate	g Fe/m^3	4	-	-	-
Potassium chloride (100%)[(1)]	kg/kg N_{elim}	-	3.42	3.42	-
Sodium hydroxide (50%)[(2)]	kg/a	-	73	73	-
Cationic resin[(3)]	t/a	-	40.57	40.57	-
Anionic resin[(3)]	t/a	-	12.31	12.31	-
Nutrient recovery					
Sodium hydroxide	kg/kg N	-	1.75	1.75	-
Sulphuric acid (98%) for ammonium sulphate	kg/kg N in product	-	3.57	3.57	-
Hydrated lime ($Ca(OH)_2$ 100%)[(4)]	kg/kg P	-	2.64	2.64	-
Sulphuric acid (98%) for conversion of CaP[(5)]	kg/kg P in product	-	3.22	3.22	-
Thickening	**m^3/a**	**251,200**	**67,300**	**67,300**	**67,300**
Polymer (100% active sub.)	kg/t DS	3.00	3.00	3.00	3.00
Dewatering	**m^3/a**	**44,000**	**25,800**	**25,800**	**25,800**
Polymer (100% active sub.)	kg/t DS	7.00	7.00	7.00	7.00
Credit for avoided mineral fertilizer					
Sludge	t/a	N: -3 P: -95	N: -5 P: -17	N: -5 P: -17	N: -5 P: -17
Irrigation water	t/a	-	-	-	N: -84 P: -145
IEX products	t/a	-	N: -320 P: -61	N: -320 P: -61	-

[(1)] Nutrient recovery takes place at > 800 mg N/L in regenerant. [(2)] Adsorption process, ions are not spent. Regeneration takes place at >600 mg P/L in regenerant. 100 regeneration cycles with the same solution. [(3)]Resin lifetime: 5 years, mechanical abrasion: 4% per year. [(4)] Beta factor for calcium dosing is 1.8 mol Ca/mol P [(5)] calculated stoichiometrically to convert recovered CaP into a plant-available form

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Direct emissions of WWTP

For the reference WWTP, direct N_2O emissions of the WWTP process are estimated to 1% of influent TN at 60% TN removal. This assumption is based on a linear correlation between TN removal and N_2O emission factors (Valkova et al., 2021). Direct ammonia emissions of biological treatment are assumed to be 0.6 % of NH_4-N of the influent (Bardtke et al., 1994). For the NEXTGEN scenarios, no N_2O emissions of the biological stage are assumed because no targeted N elimination takes place in the UASB. Both the amount of N_2O emissions due to biological N removal and the complete absence of N_2O emissions with UASB are only assumptions and must be validated with on-site monitoring.

Sludge treatment and disposal

The setup of the sludge line is similar for each scenario, but the water line configurations has consequences on the amount of secondary sludge and consequently on the biogas production in the digester. The sludge amount of the UASB amounts only to around 6% of the sludge amount from the secondary treatment in the reference WWTP. Therefore, the absolute biogas production in the digester decreases in the UASB scenarios. Electricity demand for sludge dewatering and thickening are shown in Table 35 and polymer demand in Table 36. In all scenarios the digested sludge is transported 15 km and applied in agriculture.

Nutrient credits and emissions

Table 37 gives an overview of nitrogen and phosphate credits in the sewage sludge, in the IEX products and irrigated WWTP effluent. Additionally, the emissions of the nutrient application in agriculture are shown.

Table 37: Efficiency of mineral N/P fertiliser substitution and emissions of nutrient application in agriculture

	Phosphorus	Nitrogen	Source
Efficiency of mineral N/P fertiliser substitution			
Sludge in agriculture	60% (iron dosing) 95% (no iron dosing)	25%	(LWK NS, 2010) and (Remy and Jossa, 2015)
IEX products	100% (CaP treated with sulfuric acid)	100% (ammonia solution)	estimated
WWTP effluent for irrigation	100% (maximum potential)	100% (maximum potential)	estimated
Emissions of nutrient application in % of TN or of P_2O_5 applied			
Direct ammonia emissions	-	13% (sludge/irrigation) 6.2% (mineral fertiliser)	(EEA, 2016; Eionet, 2017a)
Direct emissions dinitrogen monoxide	-	1.6%	(Eionet, 2017a)
Direct nitrogen dioxide emissions	-	4%	(EEA, 2016)
Emissions to groundwater	5.3%	7.3%	(Ecoinvent, 2021)

Infrastructure

Material demand for additional infrastructure is accounted only for the IEX because it is assumed that the reference WWTP and a WWTP with UASB have a comparable impact for infrastructure. A potential new building for the IEX is neglected. A rough estimation of the additional infrastructure for the IEX system was made and includes 5 t of stainless steel, 5 t

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of reinforcing steel, 1,000 m^3 of concrete and 50 t of PE. The corresponding lifetimes of the equipment are estimated to 25 years for concrete, 20 years for steel and 12 years for PE.

LCA results

Cumulative energy demand (CED)

Figure 46 shows that the electricity consumption of wastewater treatment and the CHP credit for biogas production both have a high influence on the results of this indicator in all scenarios. The net CED of the reference scenario accounts for +191 MJ/(pe*a), which results from a gross CED of +387 MJ/(pe*a) for operating the WWTP scheme and credits for biogas and nutrients of -195 MJ/(pe*a). The NEXTGEN scheme of scenario 1 with UASB, degassing and IEX increases the net CED by 6% to +203 MJ/(pe*a). Here, the net credits increase by 300% to -587 MJ/(pe*a) due to more biogas from UASB and credits for nutrient products from IEX. However, at the same time the expenditures for operating the NEXTGEN systems such as chemicals for the IEX (192 MJ/(pe*a)) and electricity (486 MJ/(pe*a)) increase the impacts of WWTP operation by a factor of 2, thus fully off-setting the recovered products of the NEXTGEN scheme and leading to an overall small increase in energy demand. The decisive factors for the inferior energy balance of the NEXTGEN scheme is the high electricity demand of the UF and degassing stage (0.5 kWh/m^3 in total) compared to the BNR process (0.25 kWh/m^3).

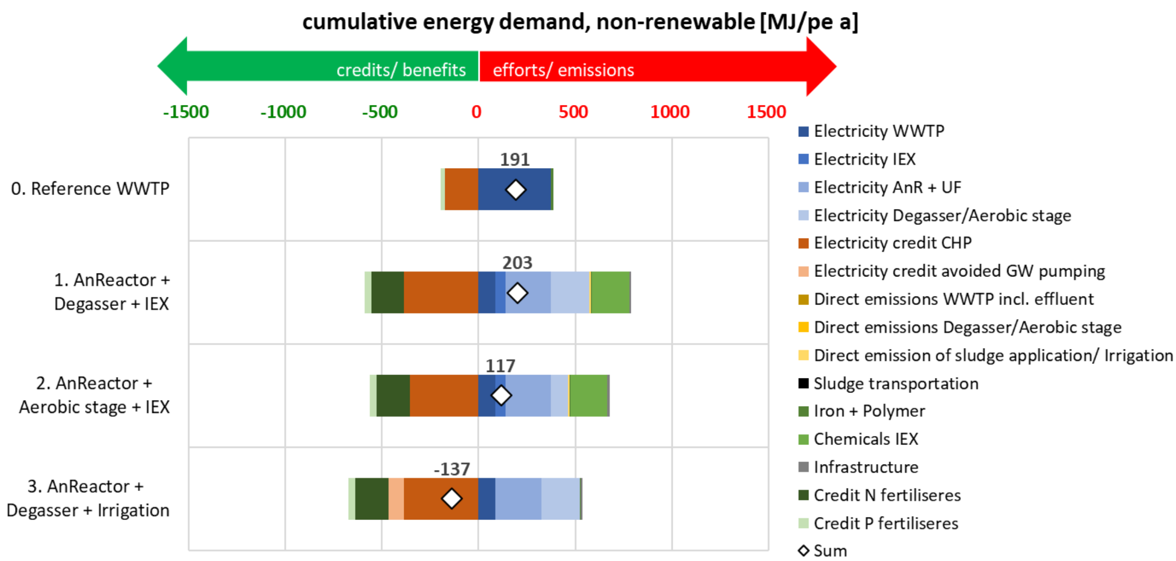

Figure 46: Non-renewable cumulative energy demand for conventional and NEXTGEN scenarios in Spernal LCA

The results show a different picture if the degassing unit is replaced by an aerated stage for methane removal (scenario 2). In this case, the net CED is reduced to +117 MJ/(pe*a), which is -39% compared to the baseline. Now, 10% of the UASB biogas credits are lost (27 MJ/(pe*a)) because the dissolved methane is eliminated and not captured. However, the MABR saves 110 MJ/(pe*a) in electricity demand compared to the energy-intensive degasser. Overall, it is obvious that the additional biogas recovered with degassing does not justify the high electricity expenditure for the membrane degasser.

If targeted nutrient recovery with the IEX is omitted and the UF effluent with N and P is directly applied to agriculture (fertigation scenario 3), the total amount of nutrients can be

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accounted (100% for N and P, cf. Table 37) and significantly less chemicals are consumed. Additionally, some credits for avoided groundwater pumping are gained from water reuse (-80 MJ/(pe*a)). This leads to a decrease of the net CED by nearly 172% to -137 MJ/(pe*a) compared to the reference scenario and results in a net energy-positive WWTP scheme. It is important to note, however, that the nutrient credits and electricity savings shown here reflect the maximum potential of fertigation and do not necessarily reflect avoided water and fertiliser supply in a real case. It is assumed that the WWTP effluent replaces groundwater for irrigation and the nutrients mineral fertiliser year-round, without any losses of water and nutrients in this valorisation route.

Relative changes from reference to NEXTGEN schemes are between +12 MJ/(pe*a) and -328 MJ/(pe*a) depending on methane recovery and nutrient recycling (Figure 47). All NEXTGEN schemes have higher credits for biogas recovery up to -384 MJ/(pe*a) and for substitution of mineral N/P-fertiliser up to -211 MJ/(pe*a). A smaller benefit to the reference is the omission of precipitation agent (-6 MJ/(pe*a)). However, this is countered by increased energy consumption of up to 200 MJ/(pe*a) mainly for UF and methane recovery, and chemical consumption for IEX up to 192 MJ/(pe*a). In particular, the use of a membrane degasser is not beneficial in the overall energy balance, as it has a high electricity demand and only recovers a small amount of dissolved methane (6 mg/L or +10% in biogas yield).

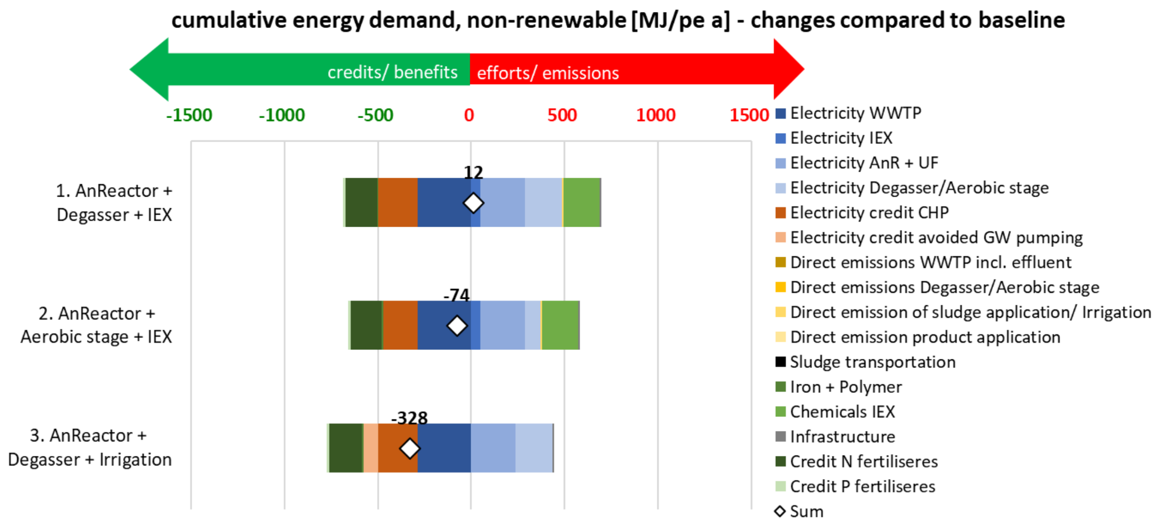

Figure 47: Changes of the cumulative energy demand for conventional and NEXTGEN scenarios in Spernal LCA compared to the reference WWTP

Global warming potential (GWP)

The GWP shows similar results between the scenarios as the CED. The net GWP of the reference WWTP amounts to +23 kg CO_2-eq/(pe*a), which results of +30 kg CO_2-eq/(pe*a) gross impacts and -8 kg CO_2-eq/(pe*a) gross savings. The main drivers are electricity demand (43%) and direct emissions from the WWTP (53%), mainly N_2O emissions from the biological stage. Here, the N_2O emissions are estimated relatively high compared to other BNR WWTPs due to a low total nitrogen elimination (60%) in the biological stage.

The total net GWP for the NEXTGEN schemes is between +12 and -6 kg CO_2-eq/(pe*a). For scenario 1, net GWP decreases by 49% to +12 kg CO_2-eq/(pe*a). Compared to the reference WWTP, the impacts of the NEXTGEN schemes (+35 kg CO_2-eq/(pe*a)) are significantly higher due to a higher electricity and chemical consumption. However, the higher credits for nutrient and biogas recovery (-24 kg CO_2-eq/(pe*a)) and also a complete reduction of N_2O

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emissions from the biological stage fully compensate the additional impact of treatment in NEXTGEN. As for CED, the MABR stage for dissolved methane removal (scenario 2) is superior to the degasser and results in a lower net GWP. For the IEX stage, potassium chloride contributes mainly to the CO_2e-footprint of the IEX chemicals (55% of the total IEX chemicals). If potassium chloride is replaced by sodium chloride, the total GWP impact of IEX chemicals could be reduced by 47%.

The net GWP of the fertigation scenario 3 amounts to -6 kg CO_2-eq/(pe*a) and is the only scenario with a negative carbon footprint. Again, the nutrient credits and energy credits for avoided groundwater pumping reflect the maximum saving potential of fertigation.

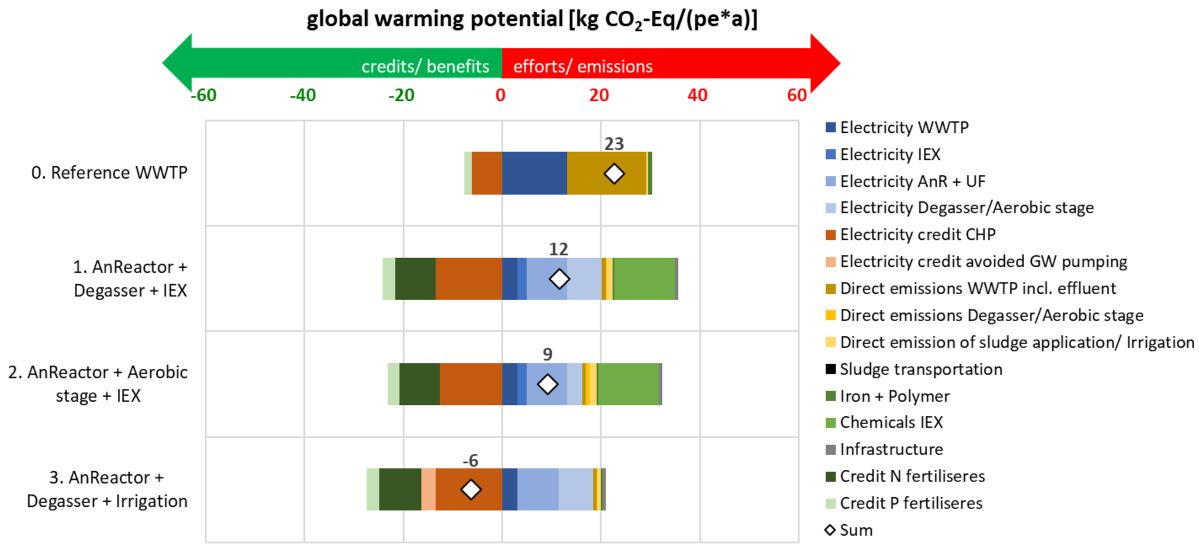

Figure 48: Global warming potential for conventional and NEXTGEN scenarios in Spernal LCA

Overall, switching from the reference WWTP to a NEXTGEN scheme results in a reduction of net GWP of 49-128%. It should be noted, however, that a modern conventional WWTP as benchmark can have a significantly lower GWP if N_2O emissions are lower than in this study (1% of influent N). A decisive factor for the N_2O emissions is the total N removal which corresponds with the N_2O emission factor. Savings of NEXTGEN technologies are less if the reference plant has high TN removal and consequently lower N_2O emissions.

Figure 47 shows the effects on the GWP in relation to the reference. If a NEXTGEN scheme is installed, the increased nutrient credits, avoided direct emission and energy savings at the WWTP off-set the impacts due to additionally required chemicals and energy (-11 to -13 kg CO_2-eq/(pe*a). For this indicator, scenario 3 is the most beneficial NEXTGEN configuration. This is primarily due to the avoided emissions of the IEX process (chemicals: 12 kg CO_2-eq/(pe*a) and electricity 2 kg CO_2-eq/(pe*a). A major advantage of NEXTGEN schemes in all scenarios is the fully avoided N_2O emissions in the biological stage.

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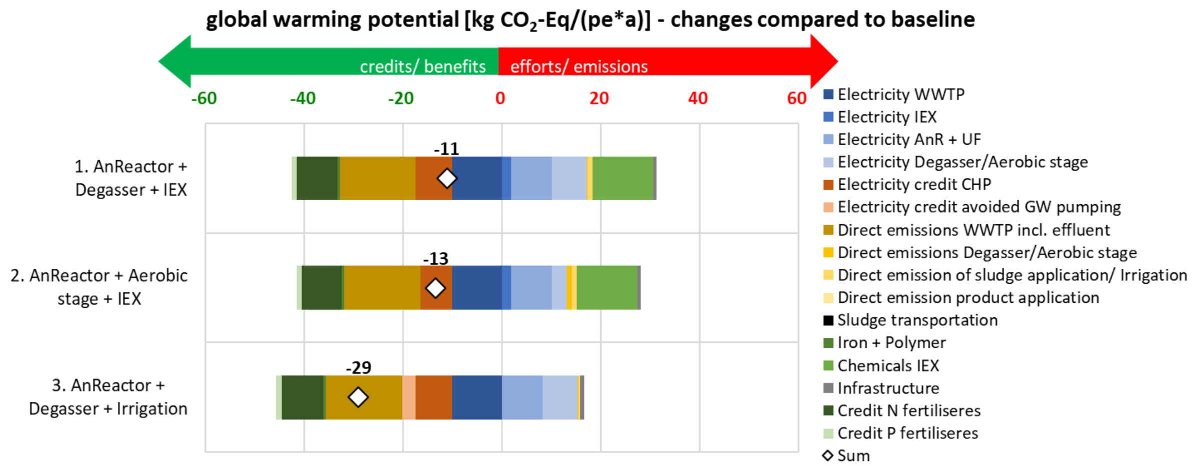

Figure 49: Changes of the global warming potential for conventional and NEXTGEN scenarios in Spernal LCA compared to the reference WWTP

Freshwater eutrophication potential (FEP)

The net FEP of the reference WWTP amounts to +43 g P-eq/(pe*a) and +28 g P-eq/(pe*a) for the scenarios with an IEX (Figure 50). For the reference scenario, the gross impact originates from direct emissions with WWTP effluent (60%) and from sludge application (40%). The latter effect is fully avoided for the scenarios with IEX, since P mainly ends up in the IEX product and not in sludge where the P use efficiency is limited compared to mineral P fertilizer. Both reference and IEX scenarios have the same effluent quality regarding TP, therefore direct WWTP emissions are comparable.

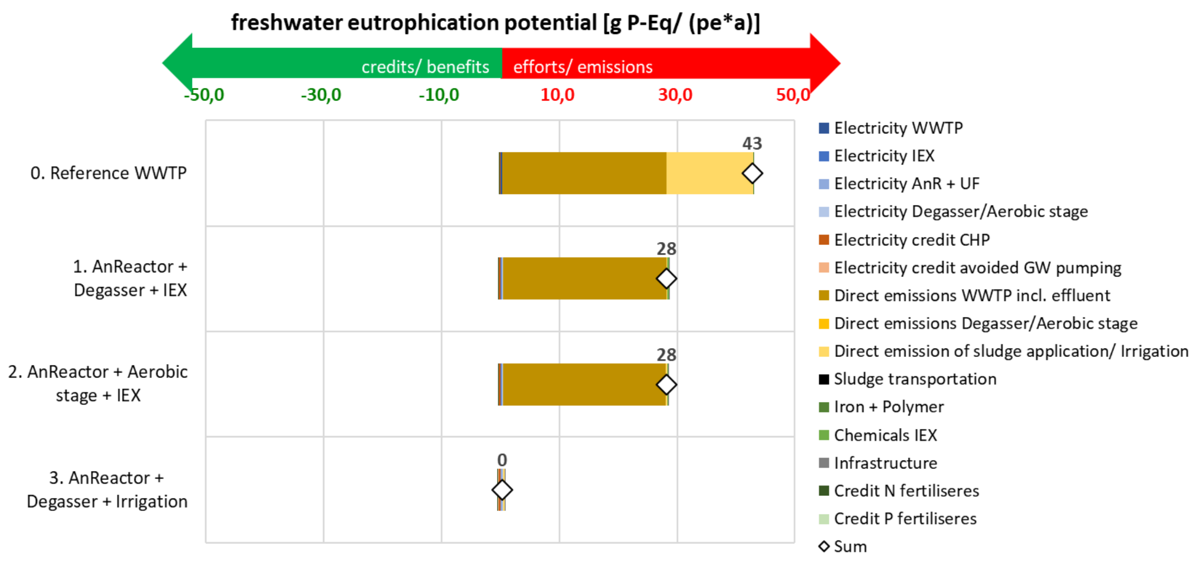

Figure 50: Freshwater eutrophication potential for conventional and NEXTGEN scenarios in Spernal LCA

The fertigation scenario is different, since the WWTP effluent is applied to agriculture and not discharged to a surface water body. This leads to an almost neutral FEP of 0 g P-eq/(pe*a), equivalent to a “full” prevention of P emissions into surface waters if no additional transfer of P losses from soil via groundwater or surface run-off are considered compared to mineral P fertilizer.

Marine eutrophication potential (MEP)

The reference net MEP accounts to +1.5 kg N-eq/(pe*a) (Figure 51). Direct emissions of the WWTP process play a major role for this indicator, which is caused by nitrogen in the WWTP

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effluent. Hence, the implementation of an IEX is beneficial for the MEP, as the WWTP effluent quality is improved from 15.5 mg/L TN (reference) to 1.5 mg/L TN (IEX). This leads to a reduction of nearly 90% to a MEP of kg +N-eq/(pe*a) for the IEX scenarios and 99% for the fertigation scenario.

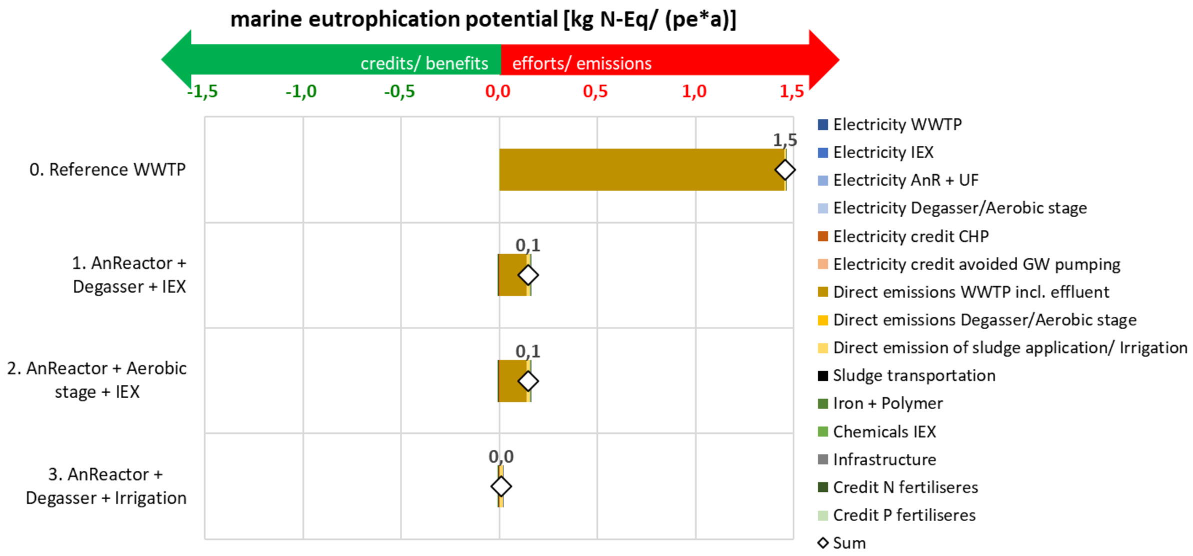

Figure 51: Marine eutrophication potential for conventional and NEXTGEN scenarios in Spernal LCA

Terrestrial acidification potential (TAP)

The reference net TAP accounts to +0.09 kg SO_2-eq/(pe*a) (Figure 52). For the IEX scenarios, the net TAP increases by factor 2 up to +0.19 kg SO_2-eq/(pe*a). The increase is mainly due to the demand for sulfuric acid and the associated indirect emissions in the life cycle of sulfuric acid production. Furthermore, the direct emissions at the WWTP and during nitrogen application with sludge or irrigation water play a major role for this indicator, as TAP is strongly influenced by ammonia emissions. Electricity consumption plays only a minor role.

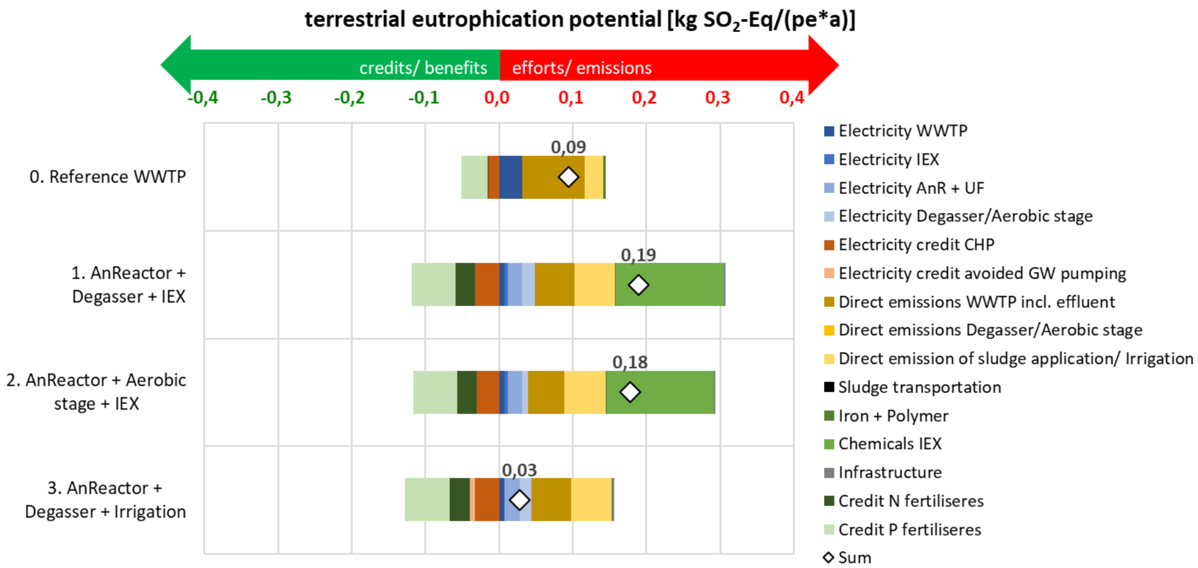

Figure 52: Terrestrial acidification potential for conventional and NEXTGEN scenarios in Spernal LCA

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Interpretation and conclusions

Table 38 gives an overview of the net environmental impacts and benefits for the NEXTGEN schemes for all calculated impact categories. The NEXTGEN schemes are associated with a number of environmental benefits, but can also be associated with some drawbacks depending mainly on a) the system for dissolved methane removal and b) the effective amount of nitrogen recycled with irrigation water and sludge.

Table 38: Summary of net environmental impacts and benefits for all impact categories in Spernal LCA.

Impact category	Unit	0. Reference WWTP	1. UASB + Degasser + IEX	2. UASB + Aerobic stage + IEX	3. UASB + Degasser + Irrigation
Products from NEXTGEN*	1/a		320 t N 61 t P	543 MWh elec 320 t N 61 t P	1058 MWh elec 84 t N 145 t P
Cumulative energy demand	MJ/pe*a	191	203 (+6%)	117 (-39%)	-137 (-172%)
Global warming	kg CO_2-eq/pe*a	23	12 (-49%)	9 (-59%)	-6 (-128%)
Freshwater eutrophication	kg P-eq/pe*a	43	28 (-34%)	28 (-34%)	0.2 (-99%)
Marine eutrophication	kg N-eq/pe*a	1.5	0.1 (-90%)	0.1 (-90%)	0 (-99%)
Terrestrial acidification	kg SO_2-eq/pe*a	0.09	0.19 (+100%)	0.18 (+88%)	0.03 (-70%)

** Electricity represents net gain compared to reference*

The following conclusions can be drawn:

- Replacing the aerated secondary stage of municipal WWTP with an **anaerobic treatment stage and IEX** for nutrient removal has several **benefits for energy and GHG profile**. First, GHG emissions are reduced mainly because **direct N_2O emissions** resulting from N removal in the biological stage are **completely eliminated**. Second, the recovered biogas and thus the amount of **electricity production in the CHP can be increased** by a factor of 2. However, the electricity demand of the secondary stage is comparable between aerobic BNR and anaerobic system in this study (0.25 kWh/m^3 for BNR plant vs. 0.26 kWh/m^3 for UASB + UF). This is mainly due to the high electricity consumption of the UF membrane (high scouring with biogas), which should be optimised in the future.

- With a **membrane degasser** downstream of the UASB, 10% additional methane can be recovered, which leads to **higher energy credits**. However, the high electricity consumption of the degasser (0.25 kWh/m^3 as estimate) **fully off-sets** this advantage in the energy balance in this study. Hence, energy efficiency of the degasser should be improved to make recovery of dissolved methane energetically viable.
- Converting dissolved methane back to CO_2 with an efficient **aerobic stage** (MABR) after UASB shows a **lower electricity consumption than degassing** and is better in

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the overall energy balance, even if a small amount of methane (10% of the UASB biogas) is lost.

- The **IEX system for nutrient recovery** comes with high energy expenditures (mainly for KCl), which is close to the energetic value of recovered nutrient products and thus brings **no substantial energy and GHG benefit** for nutrient recovery with IEX. If KCl could be replaced by NaCl, primary energy demand and GHG profile of the IEX would be reduced by 60%.
- The **fertigation scheme without IEX** has **additional advantages in energy balance and water quality**, as it brings additional water and valuable nutrients to agriculture through irrigation with the WWTP effluent. With fertigation, the **stress on local water resources can be decreased**, and the chemical-intensive nutrient extraction with IEX process can be avoided. This can be a solution for water-scarce regions, which are under rising water stress with impacts of climate change. However, an efficient use of produced irrigation water and contained nutrients is decisive for the environmental benefits of this scheme, and the results presented here **show the maximum potential of fertigation** with high efficiency of water and nutrient application. Whether the effluent quality of the AnMBR scheme is sufficient for agricultural reuse also depends on the upcoming directives at national and EU level.

The input data in this LCA for NEXTGEN schemes is based on large-scale pilot trials at Spernal WWTP (UASB, UF, degasser), but also on smaller pilot plants for IEX. To validate the results of this LCA, more data is required from long-term pilot and full-scale operation. Particular attention should be paid to the following points: N_2O emissions of the BNR plant as benchmark are relatively high compared to other BNR WWTPs due to the low TN removal assumed. This results in a comparatively high carbon footprint of the benchmark, and consequently large savings in NEXTGEN schemes without N_2O emissions. In a BNR plant with higher TN removal, its carbon footprint and therefore the relative savings with NEXTGEN would be lower. Furthermore, the energy demand for operating the UF and also the degasser is decisive for the results and only based on calculations and estimations in this study. Hence, electricity demand of both units should be verified with real data from operation. In addition, the biogas yield from UASB is assumed as the maximum potential and should be further verified in full-scale. Another important factor for the LCA profile of fertigation is the actual use efficiency of nitrogen in the irrigation water in replacing mineral N fertilizer. The full use assumed in this study (100% of N replaces mineral fertilizer) represents the maximum potential of this scheme. For a real fertigation scheme, water and nutrient demand can differ throughout the seasons, and lower nitrogen efficiency would result in lower savings and higher footprints of fertigation.

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Athens (GR): sewer mining at a tree nursery for recovery of water, nutrients, and heat

This case study demonstrates the concept of "sewer mining", i.e. the decentralized treatment of municipal wastewater taken directly from the sewer system at the place of demand to recover water, nutrients and heat. It is located at a tree nursery in the suburban area of Athens, which has a high demand for irrigation water, but also for nutrients to grow the plants. Currently, the water demand is met by using drinking water from the network, while mineral fertilizer is used to provide nutrients to the plants.

The systems tested in NEXTGEN are composed of three major elements (Figure 53):

- A **sewer mining unit** (SMU) with a membrane bioreactor (MBR) treating the wastewater drawn from the local sewer system. It is followed by a UV treatment for water disinfection. The produced irrigation water is then stored and used to irrigate the plants at the tree nursery.
- A **rapid composting plant** where the excess sludge from the MBR system is treated together with shredded pruning waste from the tree nursery to produce a nutrient-rich compost. This compost is used to provide nutrients and organic matter to the plants at the tree nursery.
- A **heat recovery unit** with an in-line heat exchanger and heat pump, which extracts heat from the MBR effluent. This heat is used internally at the composting unit to accelerate the composting process, and surplus heat can be used for other purposes.

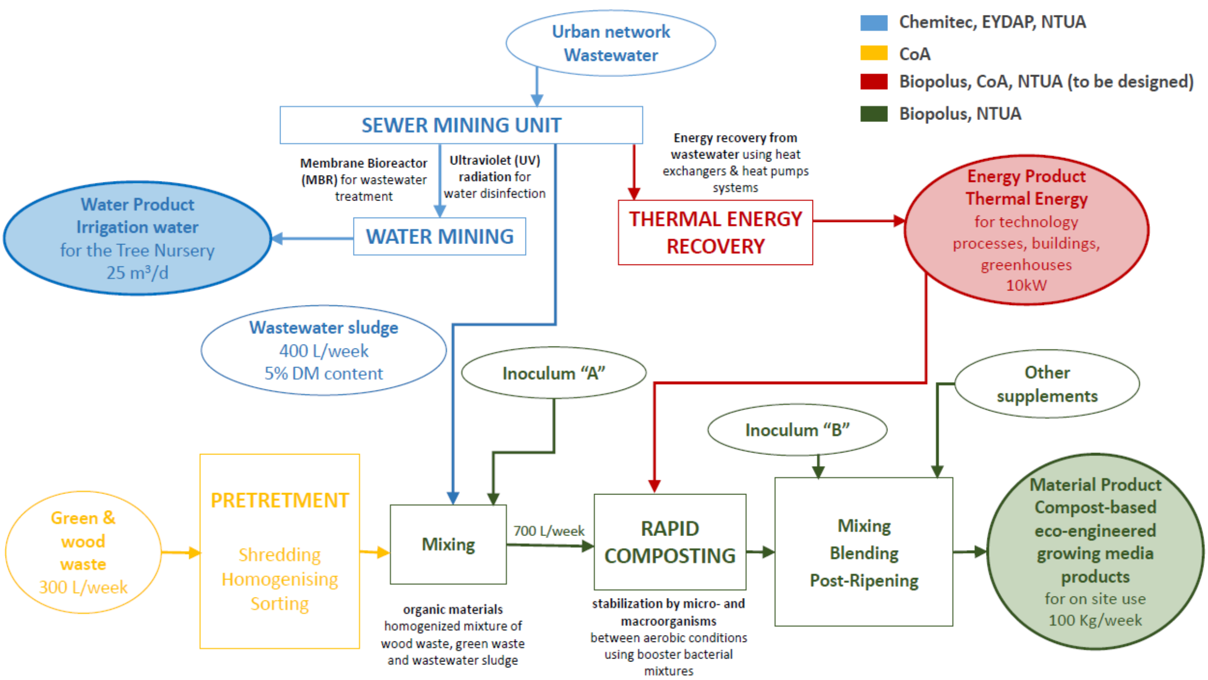

Figure 53: Pilot activities in NEXTGEN for water, nutrient and heat recovery from municipal wastewater at the Athens tree nursery

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The three systems are installed and tested at the tree nursery in pilot scale. Based on the findings in the pilot trials, the system is evaluated in its environmental impacts compared to the status quo ("baseline") of water and nutrient management at the tree nursery. Therefore, the performance and scale of the systems is extrapolated from the pilot trials to a suitable full-scale size for the tree nursery. The driving factor here is the actual water demand of the tree nursery, which defines the required size of the SMU unit and then also the downstream processing of compost and the unit for heat extraction.

Goal and scope definition

The goal of this LCA is to analyse potential environmental impacts of the concept of sewer mining at the Athens tree nursery. It will compare the impacts of the NEXTGEN concept to a baseline which represents the status quo of water and nutrient management at the site. In detail, the following aspects will be analysed in the LCA:

- Impacts of production of drinking water for irrigation, disposal of pruning waste, and treatment of wastewater in a central wastewater treatment plant (WWTP) in the baseline scenario
- Impacts of operation and infrastructure for SMU (MBR + UV), rapid composting plant, and heat exchanger in the NEXTGEN scenario
- Avoided production of mineral and organic fertilizers in the NEXTGEN scenario, and credits for surplus heat from the heat exchanger

This LCA serves as an example for decentralized water, nutrient and heat recovery in an urban context for agricultural or irrigation purposes, compared to the operation of centralized systems for water production and wastewater treatment and conventional fossil-based fertilizer and heat supply. The target group of this study consists primarily of professionals dealing with conceptual planning of water systems (e.g. engineers, researchers), but also for water system operators or end users of water for irrigation (e.g. local administration for urban green spaces).

Function/ Functional Unit

The function of the systems under study is multi-dimensional. It comprises of a) the delivery of irrigation water and nutrients to the tree nursery and b) the disposal of municipal wastewater and pruning waste. The LCA includes all relevant processes related to these two functions. However, it is very difficult to identify a dedicated functional unit, as the system functions cover different input materials and services. Hence, it was decided to define an overarching functional unit as "the operation of the systems fulfilling these functions for a period of one year" ("per a"). The amount of irrigation water and nutrients produced in each system is defined based on information of the local partner NTUA (Table 3).

System boundaries

This LCA includes all relevant processes for water and nutrient management in the two scenarios (see Figure 54). In particular, it includes the demand of electricity and chemicals for operation of central drinking water and wastewater treatment, or the NEXTGEN systems of SMU, rapid composting, and heat exchanger. Major flows of direct emissions into the environment are also accounted, such as effluent water quality of the central WWTP, gaseous emissions of wastewater treatment and composting. The avoided fertilizer production due to recovery of nutrients and organics via compost of SMU sludge and

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pruning waste and the surplus heat are subtracted as "avoided burden" in the NEXTGEN scenario. The additional infrastructure required for the NEXTGEN scenario is also accounted in terms of material demand. For the baseline system, infrastructure already exists and will not change with introduction of the NEXTGEN system.

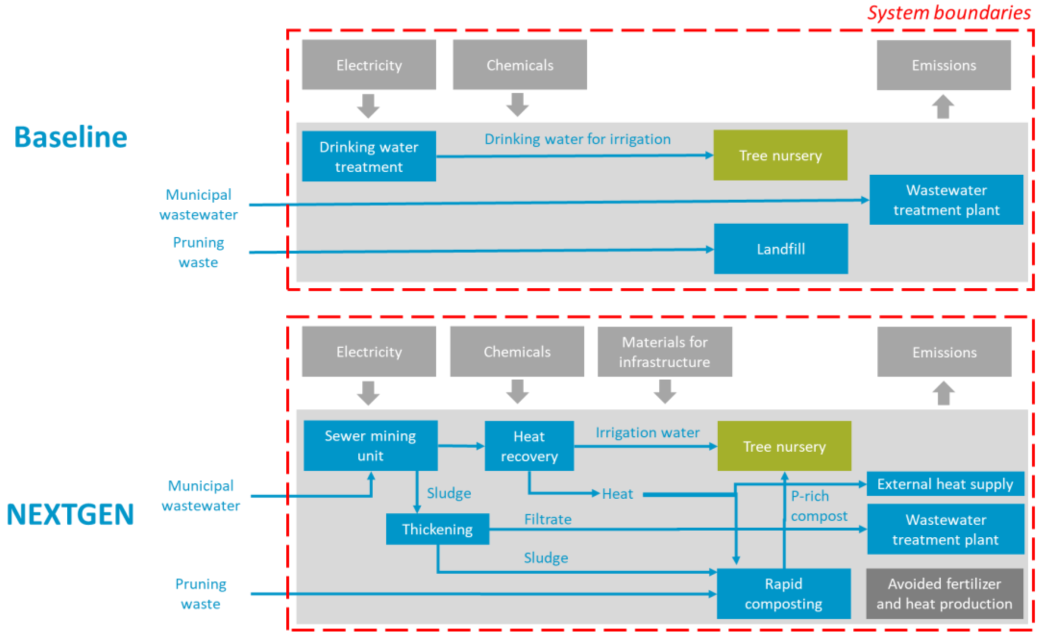

Figure 54: System boundaries of baseline and NEXTGEN scenario for wastewater and biowaste treatment at the Athens tree nursery

Allocation

Due to the multi-dimensional function of the systems under study, allocation of environmental impacts would be required if the functional unit is related to a specific singular product or service. However, the wide functional definition in this study includes all relevant services into one overarching system function. Therefore, allocation is not necessary, and all environmental impacts of the system are related to the operation of the entire system based on the functional unit ("per a").

Scenarios

This LCA compares two major scenarios (Figure 54):

- **Baseline:** provision of drinking water for irrigation at the tree nursery, treatment of municipal wastewater at a central WWTP, and disposal of pruning waste in a landfill
- **NEXTGEN:** extraction of municipal wastewater from the sewer system and treatment in a SMU with MBR and UV, storage of produced water and final irrigation (pumping), thickening of excess sludge from SMU and discharge of filtrate back to the sewer system and treatment in a central WWTP, composting of thickened sludge together with shredded pruning waste, heat extraction from the SMU effluent to supply the composting unit and other external demand, and the avoided production of mineral and organic fertilizers by using compost. The latter aspect is reflected in different ways in two sub-scenarios: **NEXTGEN1 "current nutrient demand"** is related to the actual demand of nutrients at the nursery, which is significantly lower than the maximum amount of nutrients delivered by NEXTGEN compost and irrigation water.

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The full potential of nutrient recycling with NEXTGEN is reflected in sub-scenario **NEXTGEN2 "max nutrient potential"**, which reflects the maximum nutrient amount to be delivered by the NEXTGEN products compost and irrigation water.

The size of the units is related to the projected demand of irrigation water at the tree nursery and available wastewater in the nearby sewer (Table 39). In total, 62,250 m^3 of irrigation water are produced with the SMU per year (250 m^3 per day at 249 days per year), and the equivalent amount of water is delivered in the baseline scenario via drinking water network. Municipal wastewater mined in the NEXTGEN scenario has to be treated in the central WWTP in the baseline. Excess sludge generated in SMU (140 m^3/a with 5% TS) is treated in rapid composting unit together with a suitable amount of pruning waste (105 t/a) to achieve a good composting product. This amount of pruning waste is currently disposed in a landfill in the baseline scenario. Finally, the heat exchanger is sized according to the total effluent volume of the SMU and an extraction of 5°C, resulting in a maximum heat output of 50 kW.

Table 39: Scenarios and size of the units for the Athens tree nursery

Scenario and system	Size	Remarks
Baseline		
Drinking water treatment	62,250 m^3/a	Annual demand for irrigation water to be delivered by SMU
Wastewater treatment plant	62,250 m^3/a	Equivalent to SMU influent
Disposal of pruning waste	105 t/a	Calculated to fit demand for rapid composting unit
NEXTGEN		
SMU (MBR + UV + storage and irrigation)	62,250 m^3/a (250 m^3/d for 249d)	Annual demand for irrigation water to be delivered by SMU
Rapid composting unit	Input: SMU sludge (140 m^3/a at 5% TS) plus 105 t/a pruning waste	Size according to complete processing of SMU sludge and adequate mixing ratio with pruning waste
Heat exchanger	Inflow of 250 m^3/d, max output 50 kW	Size according to effluent water volume of SMU and maximum heat extractable (5°C)

Data quality

Major input parameters for the LCA inventory are discussed below regarding data quality. An overview of data sources and data quality is provided in Table 40.

- Baseline: data for drinking water treatment and central WWTP are based on information from local operator EYDAP with good data quality. Disposal of pruning waste in landfill is modelled with a generic dataset from the LCA database, which may not be fully representative of the actual disposal in Athens (medium data quality).
- NEXTGEN systems: energy demand for SMU, composting and heat exchanger is estimated from design data and supplier information (medium quality). Chemical consumption for MBR and effluent quality is based on results of pilot trials (high quality). Infrastructure data is estimated by KWB. For the composting process, input data for

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energy demand, mass balance and emissions are based on design data of BIOPOLUS and estimates by KWB (medium quality). Performance of heat exchanger is based on design data and typical efficiencies of heat pumps for wastewater (medium to good quality).

- Background data for production of electricity, chemicals, transport, fertilizers, and materials for infrastructure is taken from LCA database ecoinvent v3.8 (Ecoinvent, 2021).

Table 40: Data sources and quality for LCA of Athens tree nursery

Parameter/ Process	Data source	Data quality
Baseline		
Drinking water treatment	NTUA/EYDAP	Good
Wastewater treatment plant	EYDAP (previous study)	Good
Disposal of pruning waste	LCA database (ecoinvent v3.8)	Medium
NEXTGEN		
SMU (MBR + UV + storage and irrigation)	NTUA: pilot trials for water quality and chemicals, up-scaling for electricity demand and infrastructure	Medium to good
Rapid composting unit	BIOPOLUS: estimate from mass balance, emission data: KWB estimate	Medium
Heat exchanger	BIOPOLUS: supplier data	Medium to good
Background data	Ecoinvent database (v3.8)	Medium to good
Electricity	Greek power mix	Good
Chemicals, materials	Europe or world market	Medium to good
Fertilizer production	Greek market mix	Good

Indicators for impact assessment

For the impact assessment, indicators are selected with a focus on four aspects: a) impact on use of local water resources for irrigation b) primary energy demand and greenhouse gas emissions as indicators for impacts from electricity, chemicals, and materials for infrastructure b) water quality parameters for N and P emissions as indicators for impacts from wastewater treatment effluent and c) acidification to account for direct gaseous emissions from wastewater treatment and composting.

In detail, the following indicator models are used for impact assessment:

- Water scarcity footprint (direct) with AWARE factors (Boulay et al., 2018)
- Cumulative energy demand (CED) of fossil and nuclear resources (VDI, 2012)
- Global warming potential (GWP) for a time horizon of 100a (IPCC, 2014)
- Freshwater eutrophication potential (FEP), marine eutrophication potential (MEP) and terrestrial acidification potential (TAP) from the ReCiPe method v1.13 (hierarchist perspective, without long-term emissions) (Huijbregts et al., 2017)

For system modelling and calculation of indicators, the LCA software UMBERTO® LCA+ has been used (IFU, 2018).

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Input data for LCA

Primary data

Inventory data for this study is provided by the partners NTUA and BIOPOLUS based on results from pilot trials or planning data for water quality, compost mass balance, and electricity and chemicals demand of unit operation. Data gaps have been filled with available process data from previous projects and estimates by KWB.

Water quality

Water quality data includes input wastewater flow, effluent from central WWTP or SMU unit, and filtrate from sludge thickening (Table 41). The central WWTP is modelled according to a previous LCA study for the WWTP Psyttalia (Remy et al., 2020). Process data has been recalculated based on the defined wastewater composition in the present study. SMU effluent quality data reflects the mean results during the pilot trials. Thickening of excess sludge from SMU is done by gravity in simple filter bags, and filtrate quality is estimated by KWB.

Table 41: Flow and quality of water for Athens case study: input wastewater, filtrate from thickening, and effluent from WWTP

Parameter	Unit	Raw wastewater	WWTP effluent	SMU effluent to irrigation	Filtrate from thickening	WWTP effluent (treated filtrate)
			Baseline	NEXTGEN	NEXTGEN	NEXTGEN
Volume	[m³/a]	62,250	62,250	62,250	597	597
COD	[g/m³]	410	29	25	690	48
TSS	[g/m³]	183	14	0.1	617	14
Total N	[g/m³]	90	13	73	31	4
Total P	[g/m³]	10.3	6.0	6.0	23	13
Source		NTUA	Based on (Remy et al., 2020)	NTUA	KWB estimate	Based on (Remy et al., 2020)

Biowaste and sludge

For pruning waste, excess sludge from SMU and resulting compost product, data has been collected mainly from BIOPOLUS and NTUA. Amount of pruning waste was adjusted to the amount of produced excess sludge, with a ratio of 6 t DM of pruning waste for each 1 t DM of sludge. Sludge production from SMU has been estimated to 118 g DM/m³ influent by NTUA, and 5% sludge DM is lost into filtrate. Sludge content of N and P is estimated by KWB based on previous studies (N) or mass balance (P). Amount and quality of final compost is calculated based on a preliminary mass balance of the composting process with data of BIOPOLUS (Table 42). The final product is a nutrient-rich compost (60 t/a) with a high content of N (1 t/a) and P (0.34 t/a).

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Table 42: Flow and quality of pruning waste, excess sludge from SMU, and compost in Athens case study

Parameter	Unit	Pruning waste	Thickened excess sludge from SMU	Compost
		Baseline + NEXTGEN	NEXTGEN	NEXTGEN
Mass	[t/a]	105	140	60.4
Dry matter (DM)	[%]	40	5	60
Volatile solids	[% of DM]	60	80	50
Total N	[% of DM]	2	5	2.7
Total P	[% of DM]	0.2	3.7	0.9
Source		BIOPOLUS	NTUA/KWB	NTUA

Nutrient balance

Another source of nutrients is the irrigation water (62.250 m³/a) with a high load of N (4.5 t/a) and P (0.37 t/a). In this study, a utilisation efficiency of 70% for N from irrigation water (mainly as nitrate), 100% of N from compost (slow-release organic N), and 100% for P from both sources is assumed. Finally, the two products compost and irrigation water can substitute an amount of 4.15 t mineral N-fertilizer and 0.7 t mineral P-fertilizer per year in the scenario “max nutrient potential” (Table 43). Regarding the actual nutrient demand at the nursery, a lower amount of 450 kg N and 150 kg P is estimated to be replaced by NEXTGEN fertilizers. This nutrient demand is estimated from the nursery area (3 ha) and a nutrient demand of 150 kg N/(ha*a) and 50 kg P/(ha*a). To account also for the delivery of organic matter with compost, an equivalent amount of peat (60 t/a) is also credited in both scenarios.

Table 43: Nutrient content in compost and irrigation water, and equivalent amount of substituted mineral and organic fertilizers in NEXTGEN for Athens case study

Parameter	Unit	Compost	Irrigation water	Substituted fertilizer in NEXTGEN scenarios	
		NEXTGEN	NEXTGEN	NEXTGEN1 “Current demand”	NEXTGEN2 “Max potential”
Mass	[t/a]	60	62.250	60 (peat)	60 (peat)
Total N	[t/a]	1	4.5	0.45 (mineral)	4.15 (mineral)
Total P	[t/a]	0.34	0.37	0.15 (mineral)	0.71 (mineral)
Source		BIOPOLUS	NTUA/KWB	BIOPOLUS	KWB

Direct emissions of processes

Direct emissions are accounted for the SMU, central WWTP and the composting process. For the SMU and central WWTP, emission factors are estimated to 0.6% of influent N as N_2O and 0.6% as NH_3 (Remy et al., 2020). For the composting process, direct gaseous emissions are estimated to 10% of TN_{in} as NH_3, 0.04% of TN_{in} as N_2O, and 0.05% of TOC_{in} as CH_4. A downstream biofilter for waste air reduces emissions of NH_3 by 90% and CH_4 by 10%.

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Electricity, chemicals and material for infrastructure

Inventory data for electricity and chemical demand for operation of major processes is listed below (Table 44). Input data for drinking water production and central WWTP is collected from partners NTUA and EYDAP. WWTP data is adapted from a previous study (Remy et al., 2020) and recalculated based on actual wastewater composition. Sludge from WWTP is dried on-site and disposed in cement kiln, which is credited according to sludge heating value. Disposal of pruning waste in baseline scenario is modelled with a dataset for landfilling from ecoinvent.

Table 44: Inventory data for baseline and NEXTGEN scenario for electricity and chemicals demand in Athens case study

Process	Value	Unit	Source and remarks
Drinking water treatment			
Electricity demand	0.5	kWh/m³	NTUA/EYDAP for drinking water in Athens
Wastewater treatment plant			
Electricity demand	0.31	kWh/m³ influent	Data of WWTP Psyttalia as compiled in (Remy et al., 2020), recalculated based on wastewater composition, electricity for sewer pumping included (0.03 kWh/m³)
Polymer demand	7.4	g/m³ influent	
Sludge production	110	g DM/m³ influent	
Disposal of pruning waste in landfill	105	t/a	Calculated with dataset from ecoinvent
Sewer mining unit			
Electricity for MBR	2.5	kWh/m³	NTUA (estimate)
Electricity for UV	0.04	kWh/m³	NTUA (estimate)
Electricity for storage tank	0.012	kWh/m³	NTUA (pumping)
Electricity for irrigation	0.06	kWh/m³	Estimate KWB (pumping, 1.2 bar)
NaOCl (15%)	0.04	L/m³	NTUA, for periodical membrane cleaning
Citric acid (50%)	0.01	L/m³	NTUA, for periodical membrane cleaning
Rapid composting unit			
Electricity for shredding	10	kWh/t input	KWB (estimate), for pruning waste
Electricity for composting	410	kWh/t output	BIOPOLUS
Heat for composting	750	kWh/t output	BIOPOLUS, total annual value for 3 months of heat supply per year
Heat exchanger			
Electricity for heat pump	0.22	kWh_{el}/kWh_{heat}	KWB, COP = 4.5
Heat extractable	4.7	kWh/m³ effluent	Estimate (5°C, 80% efficiency of extraction)
Surplus heat	244	MWh/a	Credited for substituting fossil-based heat

For the SMU, electricity demand for MBR and UV has been estimated by NTUA based on pilot trials and previous experience with this process. Pumping from storage tank and to irrigation is calculated based on required pumping height or pressure. Chemical demand for periodical membrane cleaning is adapted from pilot trials of NTUA. For the rapid composting

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unit, data for electricity and heat demand are delivered by BIOPOLUS based on design of the process. For the heat exchanger, it is assumed that a mean coefficient of performance (COP) of 4.5 can be expected in regular operation, meaning that 1 kWh of heat can be extracted using 0.22 kWh electricity. The amount of extractable heat from MBR effluent (Vol = 62250 m^3/a, 5°C temperature difference) is around 290 MWh/a, assuming a heat exchanger efficiency of 80%. As the composting process requires only 45 MWh/a in heat for operation (heat boost required for 3 months per year), the heat exchanger operation generates excess heat (244 MWh/a) which is credited here with substitution of natural-gas based heat for district heating.

Required infrastructure is roughly estimated to 500 m^3 concrete, 90 t reinforcing steel, and 20 t HDPE for the entire NEXTGEN installation (SMU including sewer extraction pump, rapid composting, heat exchanger, and foundation and building for SMU). Lifetime of the infrastructure is estimated to 15a.

Background data

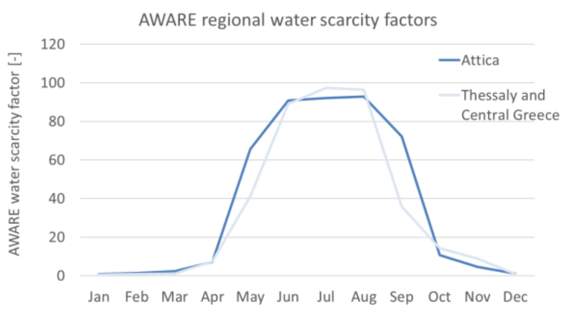
Background processes for production of electricity, chemicals, materials, transport, and fertilizer production are modelled with datasets from LCA database ecoinvent v3.8 (Ecoinvent, 2021). A full list of processes and related models is available in the annex (Table 57). Transport of materials is estimated by truck for chemicals (600 km), sludge of central WWTP to co-incineration (250 km), and materials for infrastructure (200 km).

LCA results

This chapter presents results of impact assessment, comparing the baseline situation with the NEXTGEN scenario. Indicators are discussed separately and analyzed towards major contributors, important input parameters, and respective conclusions for the analysis.

Water footprint

Direct water footprint of providing drinking water for irrigation at the tree nursery is depending on local water scarcity factors. For the Athens region and central Greece where the drinking water of Athens is sourced, regional water scarcity is high during the summer months (May-Sept) (Figure 55). Consequently, the related water scarcity footprint of supplying 170 m^3/d of drinking water is highest in summer, and relatively low in winter months.



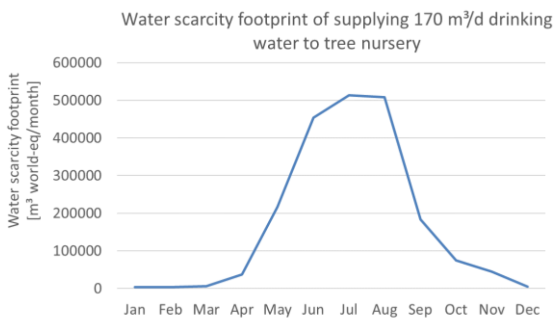


Figure 55: Monthly regional water scarcity factors (left) and resulting water scarcity footprint (right) of irrigation water supply at Athens tree nursery using drinking water from the network (Boulay et al., 2018)

In total, the provision of 62.250 m^3/a of drinking water for irrigation generates a water scarcity footprint of more than 2 Mio m^3 world-eq/a (Figure 56). This illustrates that the

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pressure on local water resources is significantly higher than typical water scarcity on a world average. With the SMU concept, this entire volume of drinking water can be substituted with purified municipal wastewater. For the water scarcity footprint, the NEXTGEN scenario has zero impact, meaning that no natural water resources are exploited for irrigation (Figure 56). Although quite intuitive in its result, the water scarcity footprint clearly quantifies the lower pressure on local water resources when irrigation water is produced with sewer mining.

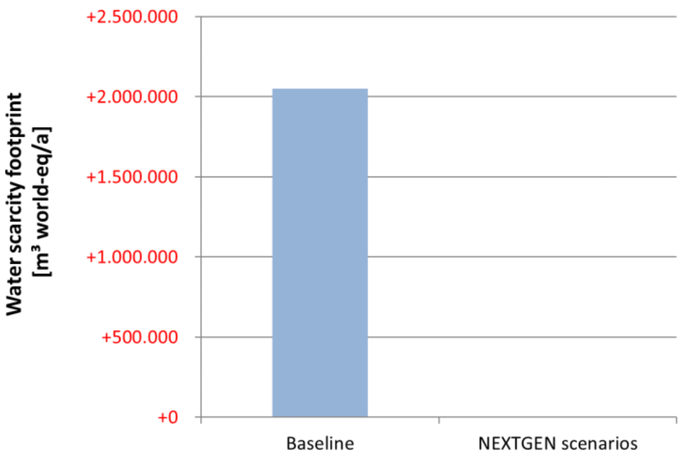

Figure 56: Water scarcity footprint (direct) for baseline and NEXTGEN scenario for the Athens tree nursery

Cumulative energy demand (CED)

Total net CED of the baseline amounts to 578 GJ/a (Figure 57). Drinking water treatment has the highest share with 65%, followed by regular treatment of wastewater in the central WWTP (29%). Landfilling of pruning waste adds another 6% to total CED. For the NEXTGEN scenario “current nutrient demand”, net CED amounts to 1672 GJ/a, which is 189% higher than the baseline. If the maximum nutrient potential in NEXTGEN products can be utilised, the total CED still amounts to 1227 MJ/a for this scenario (+112% to the baseline).

The high energy demand of the NEXTGEN scenarios is due mainly to the high energy demand for SMU operation (electricity of the MBR), but also due to electricity for heat pump operation and composting unit. The high gross CED of more than 3000 GJ/a is partially off-set by products from the system, which are substituted fertilizer and surplus heat. Overall, it is obvious that the SMU concept requires more electricity for operation than the central drinking and wastewater treatment in Athens. In fact, the sum of electricity demand for drinking water production (0.5 kWh/m^3) and wastewater treatment (0.31 kWh/m^3) is significantly lower than electricity demand for MBR operation (2.5 kWh/m^3). For the Athens location, the SMU concept is thus more energy-intensive than the central water systems, which finally leads to a higher CED for the NEXTGEN scenarios. The composting process is energy-positive, meaning that it needs less energy input than the products can substitute. The heat exchanger itself also requires some electricity to operate, but this is more than neutralized by credits from the surplus heat. Overall, composting and heat recovery both generate a net energy surplus with their products, while the water recovery with SMU has a high additional energy need compared to the central water system of Athens.

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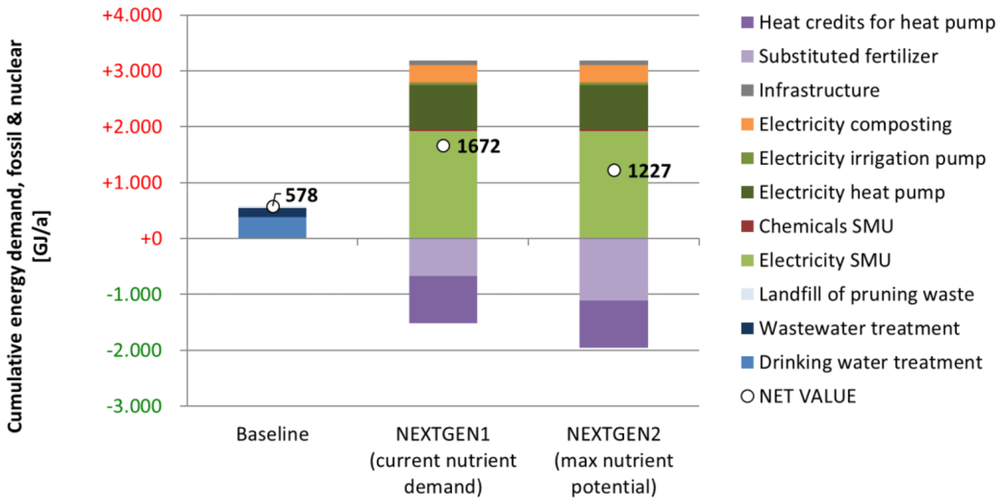

Figure 57: Cumulative energy demand of baseline and NEXTGEN scenarios for the Athens tree nursery

Global warming potential (GWP)

For GWP, results are comparable to CED as both indicators are impacted by fossil fuels for energy production. The baseline scenario has a total GWP of 55 t CO_2e/a from drinking water production and wastewater treatment (Figure 58). Here, wastewater treatment has a higher share of total GWP due to some emissions of N_2O from nitrogen removal in the central WWTP. The NEXTGEN1 scenario "current nutrient demand" has a total net GWP of 177 t CO_2e/a, which is a +221% increase compared to the baseline. With maximum nutrient recycling, GWP of the NEXTGEN2 scenario is still at 151 t CO_2e/a (+175% to the baseline).

Again, the higher demand for electricity and the relatively high CO_2e-footprint of the Greek power mix (794 g CO_2e/kWh) lead to a higher impact for the SMU concept compared to a central water system. The large difference in GWP between partial and maximum nutrient recycling originates mainly from the high GWP of mineral N fertilizer: if this product can be substituted in large quantities, it can off-set some of the energy-related drawbacks of the total GWP in NEXTGEN scenarios.

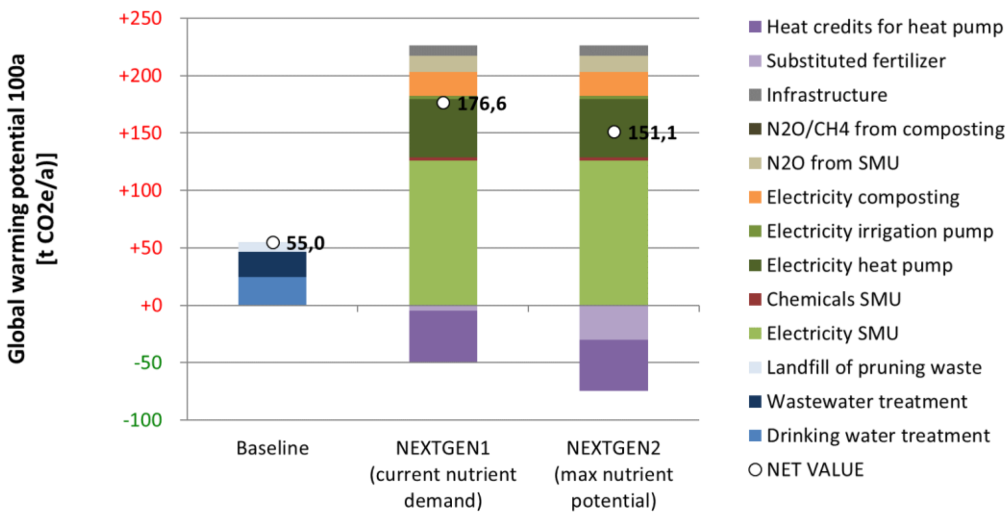

Figure 58: Global warming potential of baseline and NEXTGEN scenarios for the Athens tree nursery

However, the power mix in Greece is expected to change towards more renewable sources with low CO_2e footprint in the future. Assuming 100% electricity from on-shore wind mills

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(14 g CO_2e/kWh), GWP of both baseline and NEXTGEN scenarios is drastically reduced (Figure 59). In fact, the SMU concept now has a negative net GWP of -20 t CO_2e/a with current nutrient demand and -46 t CO_2e/a with maximum nutrient potential, mainly due to the high value of recycled nutrients and renewable heat delivered by the system. This analysis exemplifies that the power mix has a decisive impact on the GWP, and that higher electricity demand of the SMU concept does not automatically mean a higher environmental footprint in the future. Indeed, when using green electricity in the future, the circular concept of NEXTGEN with reuse of water, nutrients and heat from wastewater is superior to the baseline and can contribute to the mitigation of GHG emissions from fossil-based fertilizer and heat production.

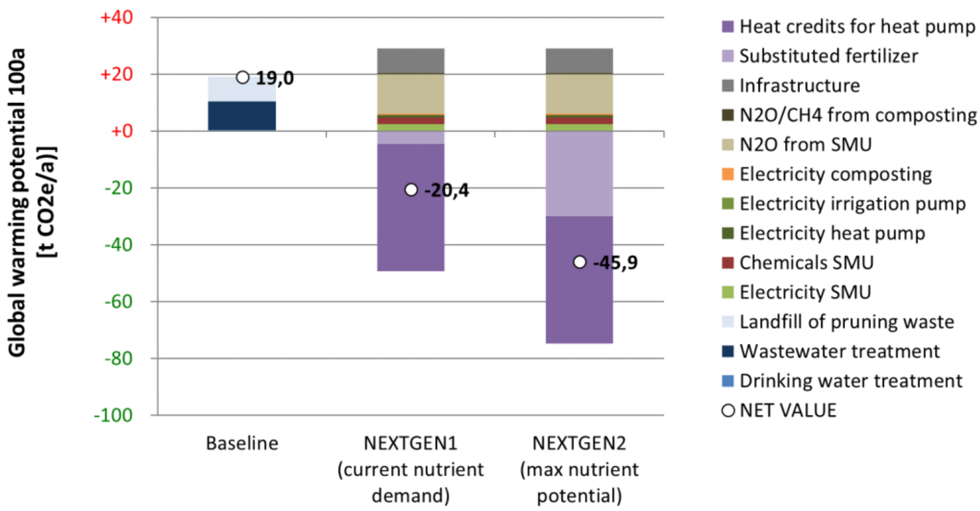

Figure 59: Global warming potential of baseline and NEXTGEN scenarios for the Athens tree nursery using 100% electricity from wind

Freshwater eutrophication potential (FEP)

FEP of the baseline scenario amounts to 385 kg P-eq/a, which almost completely originate from P emissions from wastewater treatment at the central WWTP (Figure 60). With the NEXTGEN scenarios, total FEP is reduced to 52-54 kg P-eq/a. Whereas the emissions at the central WWTP are completely prevented by redirecting the wastewater to the SMU, some P emissions come from the life-cycle of power production in Greece (mostly related to coal mining). Overall, this indicator shows that local water quality can be improved with the SMU concept, as nutrients are redirected from the water towards land application as compost or irrigation water. In this study, no transfer of P from irrigation water or compost to groundwater or surface water is assumed, so recycled P applied in the tree nursery has no impact in FEP. This assumption has to be validated in future studies to explore the fate of P loads in irrigation water and compost after application.

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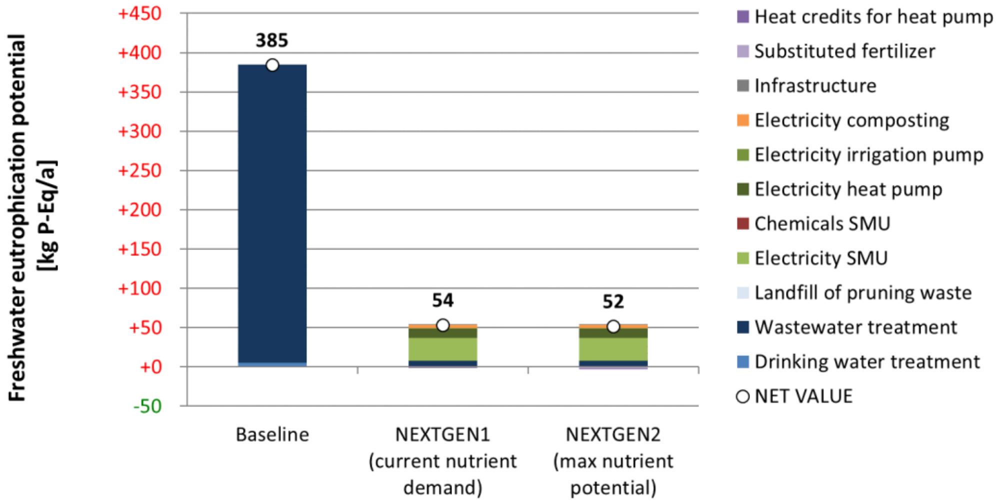

Figure 60: Freshwater eutrophication potential for baseline and NEXTGEN scenarios for the Athens tree nursery

Marine eutrophication potential (MEP)

MEP shows comparable results to FEP (Figure 61): again, baseline emissions originating from N emissions at the central wastewater treatment (837 kg N-eq/a) are mitigated with NEXTGEN by redirecting the nitrogen to the tree nursery via irrigation water and compost. Here, too, the fate of recycled nitrogen and its potential emission into atmosphere or groundwater is not included, and should be further investigated in future studies.

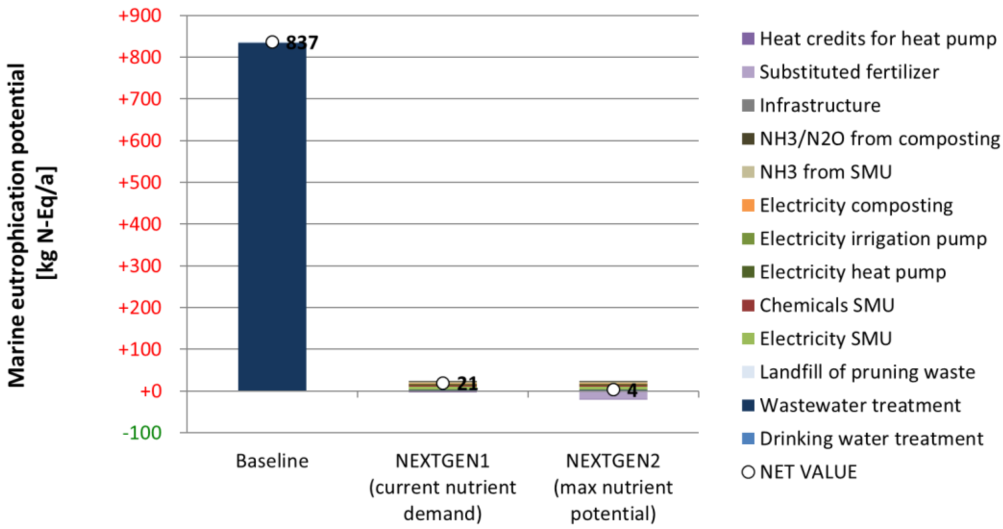

Figure 61: Marine eutrophication potential for baseline and NEXTGEN scenario for the Athens tree nursery

Terrestrial acidification potential (TAP)

TAP of the baseline scenario amounts to 256 kg SO_2e/a, whereas the NEXTGEN scenarios have a net impact of 824-1065 kg SO_2e/a (Figure 62). The TAP impact is dominated for all scenarios by the impact of electricity production, so that the large increase with NEXTGEN is mainly contributed by the higher electricity consumption, as already discussed above for CED and GWP. Some emissions of acidifying substances originate from the SMU and rapid composting, where NH_4-N is stripped from wastewater or during the conversion of sludge nitrogen in the composting process. While emissions from composting are mitigated by the biofilter (-90% NH_3), off-gas air from the SMU is not cleaned and thus contributes more to TAP. However, the most important option to reduce TAP would be to reduce electricity

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demand for the NEXTGEN concept, or changing to an electricity mix with less acidifying gases (i.e. less coal for power generation).

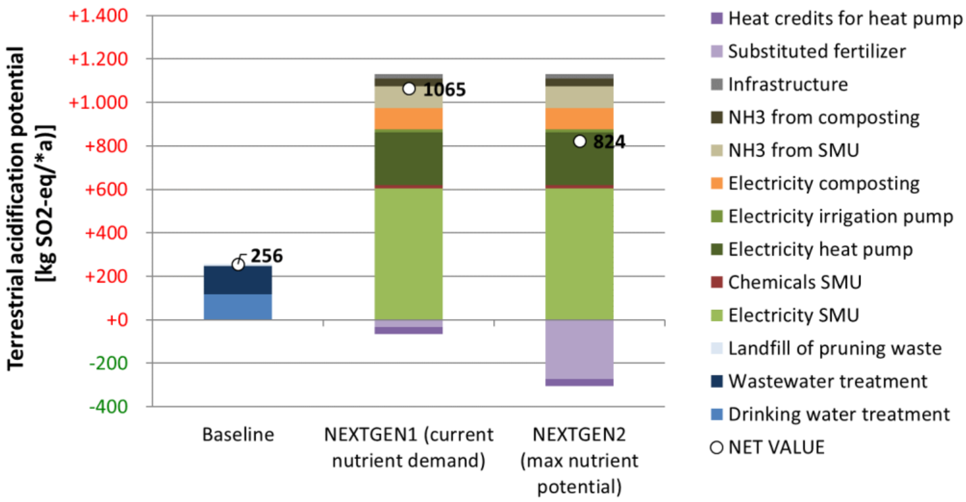

Figure 62: Terrestrial acidification potential for baseline and NEXTGEN scenario for the Athens tree nursery

Interpretation and conclusions

Table 10 gives a summary on the net environmental impacts for all calculated impact categories and scenarios. From the LCA, the following conclusions can be drawn:

- **Water reuse by sewer mining can help to reduce the pressure on local water resources,** which is especially relevant for areas and in periods of high water scarcity such as the summer period in Athens.
- **Energy demand and related GHG emissions are higher for the decentralized SMU**. This is mainly due to the **high electricity demand of the MBR**, which is significantly higher than for central water and wastewater treatment in Athens. However, if green electricity is used **in the future, the NEXTGEN concept will be able to reduce net GHG emissions**, mainly by substituting fossil-based mineral fertilizer and heat.
- The tree nursery has a significantly lower annual nutrient demand than what can actually be recycled by compost and irrigation water with NEXTGEN. Thus, the environmental profile of the NEXTGEN system at this site could be further improved by **redistributing the recycled nutrients to other places** of nutrient demand nearby. This approach is however limited by the irrigation water demand, which supplies water and contained nutrients together at one place and time. Finally, a more optimised “fertigation” concept using irrigation water with high nutrient content seems useful to maximise the benefits of both water and nutrient recycling with the SMU concept.
- Another benefit of the SMU concept is the **reduction of nutrient input into surface water by redirecting wastewater from the central WWTP to a local reuse**. Thus, the nutrients remaining in treated wastewater are not emitted with the WWTP effluent, but are recycled and used to support plant growth.

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Table 45: Summary of net environmental impacts for the tree nursery in Athens: baseline and NEXTGEN scenario

Impact category	Unit	Baseline	NEXTGEN: sewer mining, rapid composting, and heat exchanger	
Scenario			"Current nutrient demand"	"Maximum nutrient potential"
Products from NEXTGEN	1/a		62,250 m^3 water 0.45 t N 0.15 t P 244 MWh heat	62,250 m^3 water 4.15 t N 0.71 t P 244 MWh heat
Water scarcity footprint (direct)	m^3 world-eq/a	2,050,000	0 (-100%)	0 (-100%)
Cumulative energy demand (non-renewable)	GJ/a	578	1672 (+189%)	1227 (+112%)
Global warming	t CO_2-eq/a	55 19*	177 (+221%) -20* (-305%)	151 (+175%) -46* (-342%)
Freshwater eutrophication	kg P-eq/a	385	54 (-86%)	52 (-86%)
Marine eutrophication	kg N-eq/a	837	21 (-97%)	4 (-99%)
Terrestrial acidification	kg SO_2-eq/a	256	1065 (+316%)	824 (+222%)

** using 100% green electricity from wind mills*

Overall, the LCA results show that using a decentralized SMU concept combined with composting and heat exchanger can lead to a lower environmental impact of operation at the tree nursery. However, this decentralized CE solution requires more electricity than the centralized water and wastewater system in Athens, with related GHG emissions using the actual fossil-based power mix in Greece. Therefore, it is highly recommended to use green electricity with low GHG footprint for operating this type of NEXTGEN system. Otherwise, this CE solution could increase the impact on global warming. Minimizing electricity demand of MBR operation should also be targeted to reduce energy demand of the SMU concept.

In general, the concept of sewer mining for reuse of water, nutrients and heat is particularly suitable for regions with high water scarcity to promote local recycling of water and can be operated with lower environmental footprint than the central provision of water services. The burden on local drinking water resources and surface waters receiving the central WWTP effluent can be reduced, but at the price of higher electricity consumption as shown for the Athens case. With power generation getting greener in the near future, the latter aspect will be no obstacle any longer for an environmentally friendly operation of an SMU concept. The substitution of fossil-based products such as mineral fertilizer and heat with recovered products from wastewater is in any case beneficial to reduce GHG emissions.

Input data for this LCA is mostly based on estimates regarding electricity consumption of the units, quality of composting products, and efficiency of the heat exchanger. More practical results and long-term data of larger systems is required to validate the conclusions from this LCA. For this task, decisive parameters for the environmental profile of the NEXTGEN system should be monitored regularly, e.g. electricity demand for MBR operation, nutrient content in compost and its effective substitution potential of mineral fertilizer (i.e. plant-available fraction), and also the coefficient of performance for the heat exchanger under real operating conditions.

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Conclusions on environmental impacts of NEXTGEN systems

The six case studies have shown in their LCA results that CE concepts and technologies can lead to a lower environmental footprint of wastewater treatment, considering the value of recovered products and the substitution of conventional alternatives from the linear economy. However, it depends on the specific situation at the site of these potentials can actually be realized, or if CE leads to a higher environmental footprint at least in some areas of environmental concern. A summary of all LCA results of each case study is presented below (Table 46).

Table 46: Overview of LCA results for all case studies

Case study	CE product	CED	GWP	FEP	MEP	TAP	Other
Altenrhein	Nitrogen Phosphorus Activated carbon	0 ++ -	++ ++ -	0 + 0	+ 0 0	- -- -	
Braunschweig	Energy + nutrients	+	+	-	+	+	Human tox: ++
Tossa de Mar	Water for irrigation	+	+	-	++	-	
LaTrappe	Water for industry	-	-	0	+	0	
Spernal	Energy + nutrients	++	++	++	++	++/--	
Athens	Water + nutrients + heat	--	--	++	++	--	Water footprint: ++

CED: cumulative energy demand, GWP: global warming potential, FEP: freshwater eutrophication potential, MEP: marine eutrophication potential, TAP: terrestrial acidification potential
Scale: ++ is large reduction, + is small reduction, 0 is no effect (<3%), - is small increase, -- is large increase

For the different CE concepts, the following conclusions can be drawn from LCA:

- For **water reuse**, it was shown that the use of reclaimed water is feasible for irrigation ("non-potable reuse"), but also for aquifer recharge with a more advanced treatment. While the positive impact of water reuse for the local environmental water balance is logical, the impact of water reuse on the energy and GHG emissions of water supply depends on the local situation. If water reuse is an alternative to other energy-intensive options for water supply such as seawater desalination or water import over long distance, water reuse can lead to overall savings in energy demand and related GHG emissions (Tossa de Mar). However, if local drinking water supply is energy-efficient and production of reclaimed water is more energy-

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intensive, water reuse can also increase energy and GHG impact of water supply (Athens, LaTrappe). This potential trade-off between water recycling and energy demand should be closely investigated and assessed for each site, and potential drawbacks of water reuse schemes could be mitigated by using renewable energy and optimizing water reclamation plants in energy demand.

- For **energy recovery from wastewater or sludge**, it is important to assess the holistic energy balance of the systems rather than focusing only on the additional biogas or heat recovered. In principle, anaerobic treatment of wastewater yields the potential for energy-neutral or even energy-positive wastewater schemes. However, it was shown that energy-intensive degassing of treated effluent can deteriorate the energy balance of anaerobic wastewater treatment and results in an overall increase in energy demand (Spernal). Biogas recovery from sludge can also be enhanced by thermal treatment, but use of additional biogas to cover the additional heat demand should be minimized to end up with an overall benefit in the energy balance (Braunschweig). It should also be noted that energy from organic matter in sludge can only be valorized once: either as biogas, or in final incineration of sludge. Heat recovery from wastewater is feasible, but GHG benefits can only be realized if used electricity for heat pumps has a lower GHG footprint than fossil heat, also considering the conversion efficiency from electricity to heat in the heat pump (Athens).
- **Nutrient recovery** is possible through a variety of options to recover nitrogen or phosphorus from wastewater, sludge water, or sludge. Often, chemical and heat consumption for nitrogen recovery as a pure N fertilizer off-sets a major part of the benefits from substituting mineral N fertilizer (Braunschweig, Altenrhein, Spernal), so that N recovery comes more or less neutral in energy demand and GHG impact. Compared to N recovery, P recovery is often less intensive in chemical and energy demand if extracted from wastewater, sludge water, used in compost, or valorized by converting sludge ash into a fertilizer (Spernal, Braunschweig, Athens, Altenrhein). However, reaching good plant availability of recovered P products is a challenge, and can require additional efforts in chemicals. Overall, nutrient recovery from wastewater is affected by trade-offs between chemical and energy intensive “high-tech” processes and the need for pure and high-quality products. “Low tech” nutrient recovery with sludge or compost yields more benefits in energy and GHG balance, but product quality can be minor. Low efficiency of recycled nutrients in agriculture or with fertigation concepts can also lead to excessive nutrient losses compared to highly efficient application of mineral N/P products.

Finally, the environmental benefits of CE concepts have to be assessed with regards to the specific situation in which they are implemented. It has been shown that the comparison between linear and CE concepts depends also on the benchmark of the linear system (i.e. how optimized this concept is in terms of environmental impact). **CE concepts should target to operate their systems efficiently and make use of synergies with good system**

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integration (e.g. use excess heat for thermal steps, use improved water quality of membranes for water recycling). In addition, existing challenges at a site such as an overloaded WWTP or an energy-intensive water supply can help to implement CE solutions, which can recover valuable resources and improve the overall situation in the system simultaneously.

In any case, it is advisable to **check a potential implementation of CE systems beforehand with life-cycle based tools** such as LCA to identify hot-spots of environmental concern and allow for proper integration and optimization of CE concepts. Otherwise, implementing a CE approach can also lead to negative impacts on the environment, especially regarding energy demand and related GHG emissions from wastewater treatment.

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Risk assessment

Assessment of microbial risk of water reuse

Introduction and objectives

In the NEXTGEN project, water reuse and recycling is one of the key resource streams for which the project seeks to find more sustainable solutions by closing existing cycles.

Water reuse in particular is implemented/considered in various case studies, namely Athens, Filton, Tossa del Mar, and Timisoara. The degree of implementation varies from a conceptual feasibility study (Timisoara) to an already existing full-scale water reuse site (Tossa del Mar). While water reuse is considered a suitable solution to cope with increasing problems of water scarcity due to climate change and associated water scarcity, it comes with specific risks which have to be analyzed, assessed, and managed.

Microbial safety is one of these risks and demonstrating that microbial risks can be managed effectively is key to gaining and maintaining trust for water reuse projects. Therefore, it is one of the objectives of the NEXTGEN project to conduct and illustrate approaches to microbial risk assessments in the various case studies.

To this end, a web-based tool, previously developed in the research project AQUANES, was used to conduct a first stage risk assessment in the various case studies. The AQUANES tool consists of a freely available database, an R package used as a calculation engine, as well as a Java based front end, guiding the user through the various steps of quantitative microbial risk assessment (QMRA). These steps include:

a. the selection of the source water used for water use (e.g. treated wastewater, surface water, groundwater),
b. the definition of the intended water use (e.g. drinking, agricultural and urban irrigation, toilet flushing), as well as
c. the definition of the existing or planned treatment scheme.

The database of the tool provides default values for the expected concentrations of viral, bacterial and protozoan reference pathogens in the source water, the treatment performance of the selected treatment scheme for these pathogens, and predefined exposure scenarios consisting of the number of exposure events per year and the volume per exposure events. The database furthermore includes published dose-response relationships for the individual reference pathogens, which are used to calculate the microbial risk, both in terms of risk of infection per year and in disability adjusted life years (DALYs) per person per year (pppy). The tool uses rotavirus, *Campylobacter jejuni* and *Cryptosporidium parvum* as reference pathogens for viral, bacterial, and protozoan pathogens.

In the NEXTGEN project, the QMRA activities were done in two phases. The first phase focused on optimization (speed) and extension of the existing functionalities of the AQUANES QMRA tool. The second phase consisted of applying and troubleshooting the updated tool in the case studies which performed water treatment with the purpose of closing water cycles (i.e. water reuse).

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The extension of functionalities of the updated tool include:

- extended opportunities to customize risk assessment by letting users create user-specific treatments and exposure scenarios
- long-term storage of multiple risk assessment configurations
- ability to perform side-by-side comparisons of different risk scenarios (e.g. for different treatment configurations)

Background

Microbial risk assessment aims to systematically analyze and prioritize existing microbial risks with the goal of supporting risk-based decision making to ensure microbial safety of products. According to WHO (2016), microbial risk assessment can be structured into four steps (see Table 47). Microbial risk assessment and management are incremental approaches that assess the existing risk against the background of the existing information and uncertainty. Therefore, it is perfectly feasible to conduct a first stage risk assessment during the planning phase (conceptual study) of a new project, based on information collected from existing norms, standards, a literature review, or expert knowledge. Usually, first stage risk assessments are able to identify how existing knowledge gaps affect predefined health targets, and thus support decision making in regards to allocating existing resources towards closing the most relevant knowledge gaps first.

In general, the QMRA approach consists of estimating a dose of pathogenic microorganisms, identifying a specific population group exposed per exposure event, identifying the annual frequency of exposure events (exposure scenario), and identifying the related annual risk. Risk is commonly expressed either in terms of tolerable risk of infection, i.e. the probability that a pathogenic microorganism starts multiplying/replicating inside the human body, or disability adjusted life years (DALYs). In contrast to the risk of infection, the DALY indicator additionally accounts for the probability of illness given infection, as well as the severity of the illness caused by a specific pathogen.

Due to the large number of pathogens in wastewater and to the limited number of existing dose-response relationships, water related QMRAs are usually conducted only for selected reference pathogens. These are selected from amongst the most frequently occurring and most infective pathogens within their specific group (viruses, bacteria, protozoa). Therefore, it is assumed that controlling these references pathogens simultaneously covers other pathogens in the specific group. Reference pathogens in water related QMRA focus on gastroenteritis, as it is a major consequence for human health. In the World Health Organization's (WHO) Guidelines for Drinking Water Quality, rotavirus, *Campylobacter jejuni* and *Cryptosporidium parvum* are identified as reference pathogens for viral, bacterial, and protozoan pathogens (WHO, 2011). More recently, norovirus is recommended instead of rotavirus as the reference pathogen for viral indicators in the WHO's Potable reuse: Guidance for producing safe drinking-water (WHO, 2017). However, this has been criticized, as norovirus is not readily cultivable from environmental samples (Nappier et al., 2018). In the Netherlands, where QMRA is routinely applied for drinking water system risk estimations, enterovirus is used as the reference viral indicator. The variability of reference pathogens therefore demonstrates that the multiple simultaneously existing approaches to conducting QMRA can be considered suitable.

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Estimating the exposure dose per exposure event requires an estimation of both the pathogen concentration in the water to which the population is exposed (e.g. drinking water, irrigation water) as well as the ingested water volume per exposure event. For the ingested volume per exposure event, standardized assumptions have been published by various guidance documents, such as the Australian Guidelines for Water recycling (NRMMC-EPHC-AHMC, 2006).

For estimating pathogen concentrations in treated water, QMRA generally prefers a process-based approach over end product quality testing, as pathogen concentrations in the final product waters are usually very low and thus hard to detect. Moreover, if pathogens are detected in the final product water, the water from which the compliance samples were taken is likely to have been already distributed and used. By focusing on a process-based approach, QMRA inherently supports the development and implementation of risk-based water management strategies like Water (Reuse) Safety Plans. The latter aims to reduce the uncertainty, i.e. increase the *knowledge*, about the system's capability of fulfilling predefined process performance targets to such a degree that compliance of the final product water with existing water quality standards can be taken as given, i.e. *is known*.

Therefore, quantifying the uncertainty, i.e. lack of knowledge, is at the center of any risk assessment study. To address these uncertainties, the current state of the art is to use probabilistic approaches. In probabilistic QMRA, uncertain model inputs are defined as random variables and a Monte Carlo simulation (MCS) is used to simulate and evaluate distributions of potential risk outcomes (WHO, 2016). MSC refers to a simulation technique where probability distributions, which represent the individual model inputs, e.g. source water pathogen concentrations, are approximated by sampling a high number of pseudo-random samples from a predefined distribution. Thus, highly complicated probability calculus can be replaced by straightforward simulation. MCS can be conducted by many of the common existing data-related software tools and programming languages like Excel, R, Python, MATLAB or Julia. However, conducting and evaluating a probabilistic QMRA using MCS is still a barrier towards the broader adoption of QMRA in practice. In the Netherlands, where QMRA is mandatory, *QMRAspot (Schijven et al., 2011)* has been developed as a practical tool to ease and standardize data evaluation and MCS for drinking water systems. In the AQUANES project, a database and simulation model was developed to ease and lower the barrier of entry for conducting QMRA using MCS. The AQUANES tool was then further developed through application in NEXTGEN's water reuse case study sites.

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Table 47: Steps of QMRA and support provided by NEXTGEN web-based QMRA software

QMRA Step	Content	Support from the QMRA tool
Problem formulation (Scope and purpose)	• System description • Definition of relevant exposure pathways and groups of people • Hazard identification	• WHO reference pathogens for hazard identification • System specifics and definition of relevant exposure routes must be provided by the user
Exposure assessment	• Source water concentrations • Removal efficiency of treatment processes • Magnitude and frequency of exposure	• Database of guideline values for source water concentrations, log reduction values (LRV), and exposure scenarios • Customization options for user-specific treatments and exposure scenarios
Health effects assessment	• Dose-response relationships • Secondary transmissions and immunity	• Tool includes dose-response relationships of WHO's reference pathogens (rotavirus, *Campylobacter* and *Cryptosporidium*
Risk characterization	• Risk quantification • Assessment of uncertainty • Sensitivity analysis	• Supports all risk characterization tasks by implementing Monte Carlo simulation, enables comparison of risk scenarios

Method

Description of the open-source QMRA software

To enable the local case studies to conduct a QMRA, the open-source software developed in NEXTGEN implementing major steps of the QMRA approach, was used.

The software builds upon a freely available database developed in AQUANES, where information from scientific literature and international guidance documents was collected and summarized into a database. The database and its content can be found at: https://kwb-r.github.io/qmra.db/. NEXTGEN QMRA software enables a first-stage QMRA to be conducted in the absence of locally collected data by supplying default values from literature. Since published information on log reduction values (LRV) usually shows a high degree of variability between sites, first-stage risk assessments reflect this uncertainty by calculating wide ranges of plausible outcomes.

In most cases, reducing the uncertainty of risk outcomes requires updating risk estimations with locally collected, site specific data. To this end, the software provides users with the option to tailor the risk assessment to their specific needs by including local information on removal efficiencies for viruses, bacteria, and protozoa as well as for site-specific exposure scenarios. Furthermore, the software allows direct comparison of risk scenarios for different

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groups of people and system configurations. By implementing these features, the software can be used at any stage of a system life cycle, meaning that it can be used to:

1. assess the microbial risk of an existing system against existing benchmarks;
2. assess the suitability of different system configurations at the planning stage;
3. derive the required log reduction for a specific water reuse application; and
4. assess, compare and prioritize the most vulnerable groups of people at the specific water reuse site.

In NEXTGEN, the tool was mainly used for purposes 1 and 2. The level of flexibility makes the software very suitable for conducting QMRAs at the different case studies in NEXTGEN, because the degree of implementation varies widely between case studies. The version of the tool used for the NEXTGEN project was deployed at https://www.qmra.org. The documentation of the software can be found at https://qmra.readthedocs.io/en/latest/.

QMRA workshop and individual follow up meetings

To support the application of NEXTGEN QMRA software in the various case studies, a workshop was conducted with the local project partners on November 25th, 2021. During the workshop, the partners were given an overview of the implemented functionality of the tool as well as specific guidance on how to apply the tool at their local sites.

Based on the specific applications of the partners, individual follow up meetings were conducted between KWB and the local partners. These follow up meetings were intended to guarantee the correct application of the tool and provided an additional opportunity to ask remaining questions related to the application of the tool at the local sites.

The QMRA results, which are based on the case study specific application of the tool, were presented at the practitioners' workshop in June 2022 and are summarized in the following sections. The selection of exposure scenarios and water treatment technologies was done by the case study owners.

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Results

Athens

Problem formulation

At the case study in Athens, an innovative approach to water reuse was applied by extracting urban wastewater with a sewer mining (SM) unit to produce safe urban green irrigation water at the point of demand. Additionally, a high-quality fertilizer was produced onsite by mixing pruning waste with the produced sludge from the SM unit after its thickening. Finally, energy recovery schemes were tested to recover thermal energy for the configuration needs of the composting unit. In Athens, QMRA was used to address and quantify potential health risks resulting from the exposure of people to irrigation water produced by the SM unit.

Exposure assessment

For the exposure assessment, the scenario “garden irrigation” was used as a default exposure scenario in the QMRA. In this irrigation scenario, an exposure volume of 1 mL with an annual frequency of 90 times per year was assumed. This scenario can be considered a conservative estimate for regular exposures. The scenario did not include any accidental exposures due to unintended spills of irrigation water.

The selected treatment train, including the applied LRVs of the assessed treatment scheme, is shown in Figure 63. The LRVs were based on the default values provided by the AQUANES database. The values indicated a wide range of expected log reduction, especially for viruses (3.5-9) and bacteria (5.5-10). With a minimum LRV of 5.5 for bacteria, the proposed treated scheme was expected to be in line with the “class A” quality standard of the new European water reuse regulation, which requires 5 LRVs for bacteria. For viruses, however, compliance with the regulations’ requirements of 6 LRVs for viruses remains uncertain, as the default values indicate a high variability between treatment units.

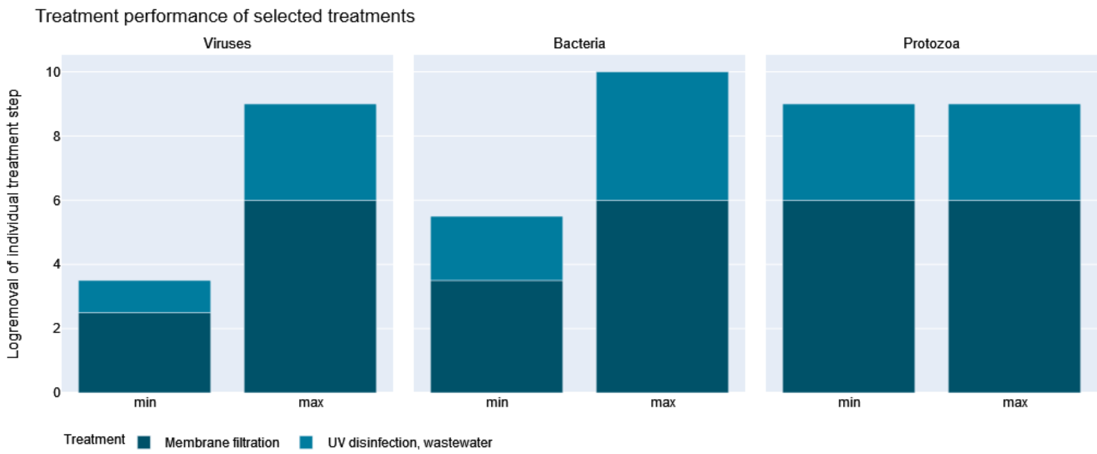

Figure 63: Treatment scheme at the sewer mining case study in Athens.

Risk characterization

The results of risk simulations are shown in Figure 64 and Figure 65. Risk is expressed as probability of infection (PI) and disability adjusted life years (DALY) per person per year

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(pppy). Risk is calculated separately under the assumption of minimum and maximum LRVs, i.e. treatment performance.

Results indicate that under optimal treatment conditions, the calculated risk remains well below the applied health benchmarks of 1/10.000 infections and 1 µDALYs pppy, respectively. However, results also indicate that under poor or unfavorable operating conditions, tolerable risk benchmarks may not be achieved.

If DALYs are used as the health indicator, this conclusion holds true for viruses, but if the PI is used as the health indicator, then this is also true for bacteria. Thus, if DALYs are used as the health benchmark, QMRA results agree with the conclusions draw from comparing applied LRVs to the reuse regulation requirements, where achieving the required 6 LRVs was uncertain. In contrast, if PI is used, risk simulations indicate an increased risk for bacteria although the reuse regulation requirements are achieved. Results indicate that additional validation monitoring should focus on the treatment performance for viral pathogens, as they are considered the major driver of risk, caused by uncertain removal efficiency, in this particular case.

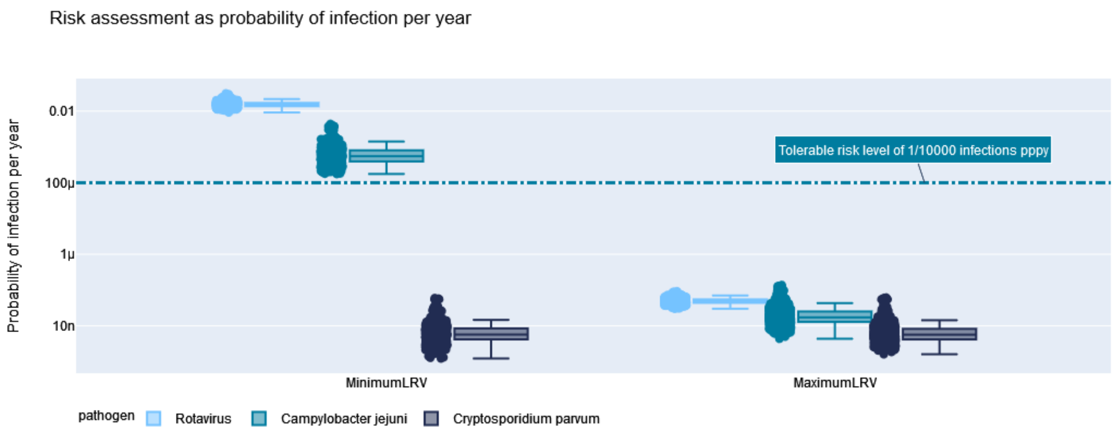

Figure 64: Risk characterization expressed as probability of infection per person per year (pppy). Points next to individual boxplots refer to individual simulation results of the Monte-Carlo-Simulation.

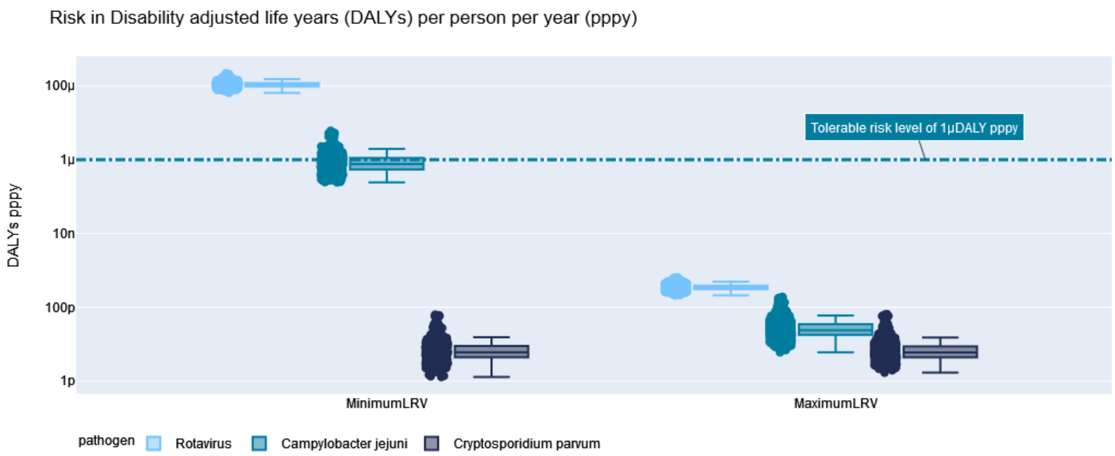

Figure 65: Risk characterization expressed as disability adjusted life years pppy). Points next to individual boxplots refer to individual simulation results of the Monte-Carlo-Simulation.

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Gotland

Problem formulation

At the case study in Gotland, the QMRA tool was used the explore the opportunity of implementing direct potable reuse from raw wastewater, meaning that wastewater is treated to the extent that it is suitable for human consumption in the absence of an additional environmental buffer.

Exposure assessment

For the exposure assessment, the scenario “drinking” was used as a default exposure scenario in the QMRA tool. In this scenario, an exposure volume of 1L with an annual frequency of 365 times per year was assumed. In the absence of local consumption data, this can be considered a realistic worst-case scenario.

The selected treatment train, including the applied LRVs, is shown in Figure 66. The LRVs are based on the default values provided by the AQUANES database. The treatment train consists of primary and secondary wastewater treatment followed by a double membrane system consisting of an ultrafiltration unit and reverse osmosis. This treatment setup leads to LRVs between 9-15 for viruses, bacteria and protozoa. However, the upper limit of achievable log reduction is set to 6 LRVs. Thus, even if reverse osmosis may be considered a complete barrier against pathogens, no more than 6 LRVs are credited to it in the risk calculations.

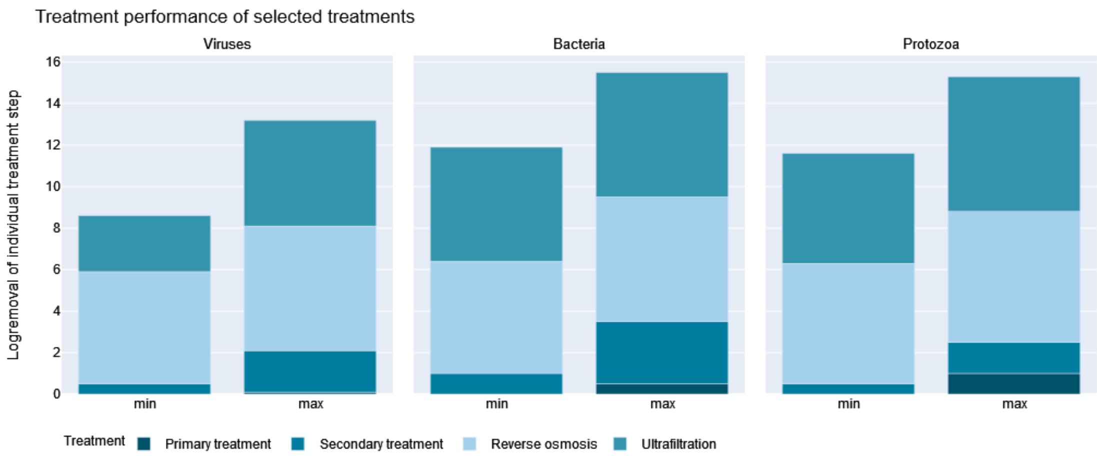

Figure 66: Treatment scheme at the case study in Gotland.

Risk characterization

The results of risk simulations are shown in Figure 67 and Figure 68. Risk is expressed as probability of infection (PI) and disability adjusted life years (DALY) per person per year (pppy). Risk is calculated separately under the assumption of minimum and maximum LRVs, i.e. treatment performance.

Both the PI and DALY risk indicators demonstrate that under maximum LRVs and given the default assumptions, water quality benchmarks for bacteria and protozoa are likely to be achieved. Under minimum LRVs, uncertainties regarding the achievement of health

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benchmarks for viral infections remain. A potential reason for this might be the upper limit of 6 LRVs for reverse osmosis, which if operated well, can be regarded as a complete barrier against virus particles. The upper limit of 6 LRVs for a single treatment step is a measure to ensure that drinking water treatment plants implement enough treatment redundancy in their systems and do not simply rely on a single treatment step to achieve acceptable water quality. Even if health-based targets are likely to be achieved with local measurement validation, providing enough redundancies is essential for increasing the resilience of the system and for ensuring the permanent and sustainable supply of safe drinking water.

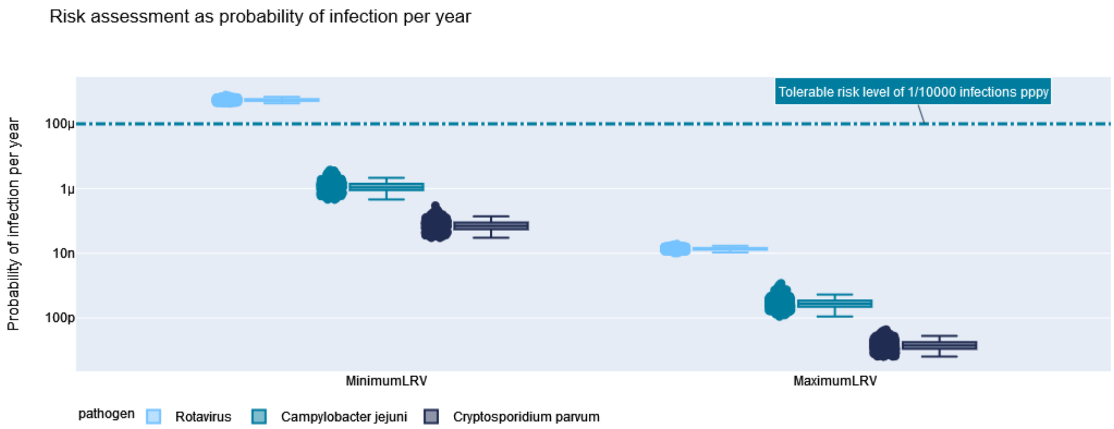

Figure 67: Risk characterization expressed as probability of infection per person per year (pppy). Points next to individual boxplots refer to individual simulation results of the Monte-Carlo-Simulation.

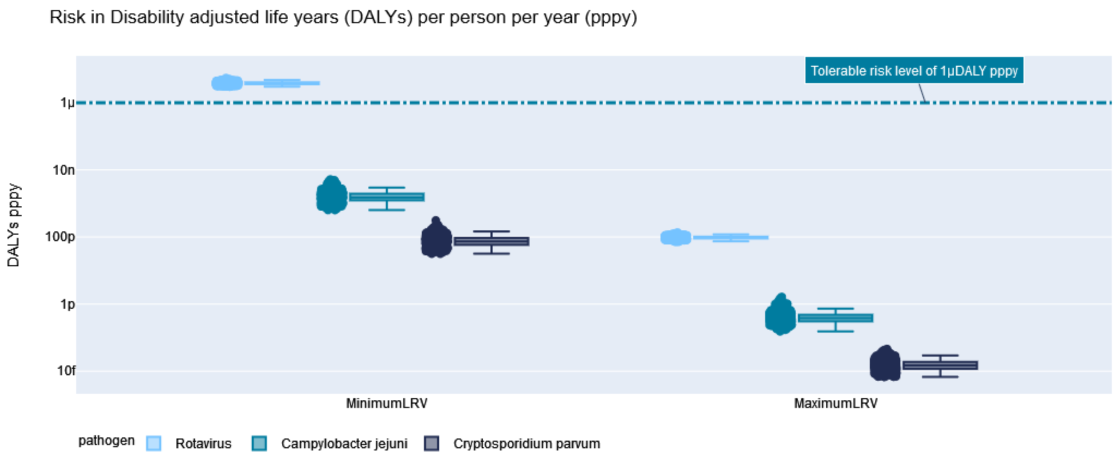

Figure 68: Risk characterization expressed as disability adjusted life years pppy. Points next to individual boxplots refer to individual simulation results of the Monte-Carlo-Simulation.

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Filton

Problem formulation

At the case study in Filton Airfield, QMRA was used to explore the possibility of reusing water collected from rooftops for local toilet flushing.

Exposure assessment

For the exposure assessment, the scenario “toilet flushing” was used. The scenario was provided by the default AQUANES database of the QMRA tool. In this scenario, an exposure volume of 0.00001 L is assumed with an annual frequency of 1.100 times per year. Membrane filtration was considered the only relevant barrier against pathogens. This leads to 2.5-6 LRVs for viruses and 3.5-6 LRVs for bacteria, and 6 LRVs for protozoa. All LRVs were taken from the default values provided by the AQUANES database.

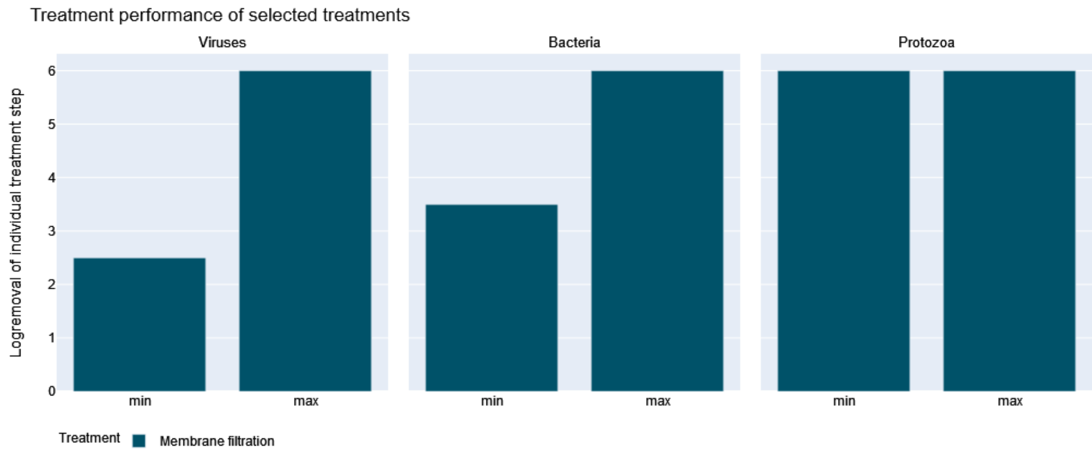

Figure 69: Overview of applied LRV in Filton

Risk characterization

The results of risk simulations are shown Figure 70 and Figure 71. Risk is expressed as probability of infection (PI) and disability adjusted life years (DALY) per person per year (pppy). Risk is calculated separately under the assumption of minimum and maximum LRV values, i.e. treatment performance.

Both the PI and DALY risk indicators show that under both the minimum and maximum LRV conditions, water quality benchmarks are likely to be achieved given the default assumptions. Thus, health-based targets are likely to be achieved if validated with local measurements. The low risk results from the combination of a low concentration of pathogens in the collected rooftop water, the small exposure volumes assumed for toilet flushing, and the additional membrane treatment. In contrast to other risk assessments, in which viruses usually present the highest infection risk, *Campylobacter jejuni* was identified as the pathogen with the highest risk in this case study. This is plausible, as *Campylobacter* often comes from the feces of birds, which in the context of rooftop harvesting of rainwater becomes more relevant than in cases where the source water for risk assessment is municipal wastewater or surface water. The assessment indicates that reusing collected rainwater for toilet flushing can be considered a safe option for reuse at the former airfield.

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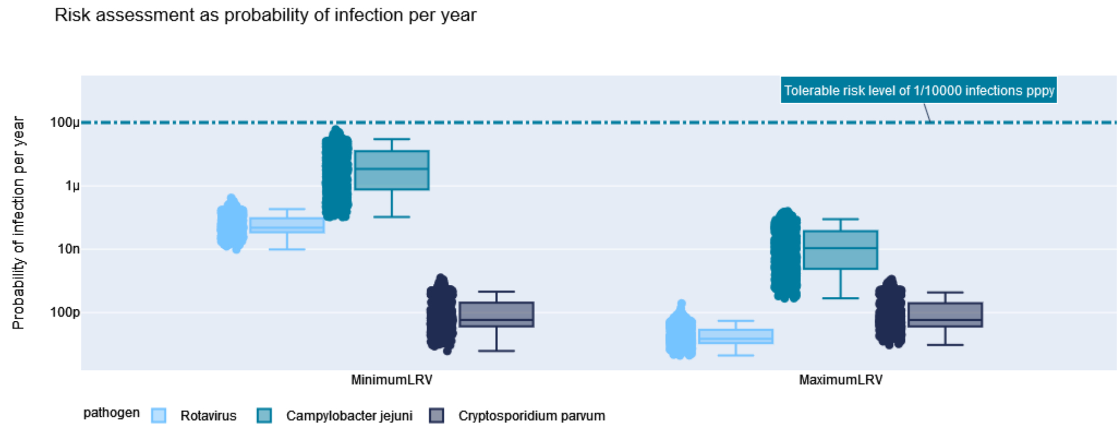

Figure 70: Risk characterization expressed as probability of infection per person per year at Filton Airfield (pppy). Points next to individual boxplots refer to individual simulation results of the Monte-Carlo-Simulation.

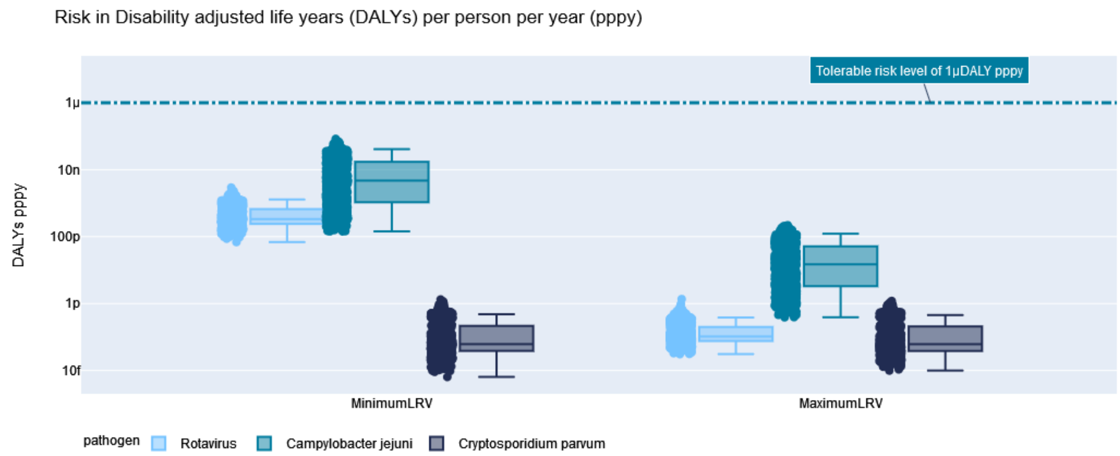

Figure 71: Risk characterization expressed as disability adjusted life years pppy at Filton Airfield. Points next to individual boxplots refer to individual simulation results of the Monte-Carlo-Simulation.

Tossa del Mar

Problem formulation

Tossa del Mar is a water reuse case study in Catalonia (Spain). The NEXTGEN project investigated whether previously used reverse osmosis (RO) membranes can be recycled and reused as UF-NF membranes. The produced water should be used for public irrigation. The QMRA tool was used to explore and compare different treatment configurations and especially the NEXTGEN configuration in regards to their ability to achieve predefined health targets.

Exposure assessment

For the exposure scenario of public irrigation, a predefined exposure scenario already existed in the AQUANES database. The exposure scenario was based on information provided in the Australian Guidelines for Water Recycling and assumes 50 exposure events per person per year and a volume of 1 mL of irrigation water ingested per exposure event.

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For Tossa del Mar, an existing baseline scenario was defined and compared to the proposed NEXTGEN configuration.

The LRVs for the treatment scheme are shown in Figure 72 and Figure 73. For viruses, the figures indicate 3.5-7 LRVs for the baseline scenario, and between 6-12 LRVs for the NEXTGEN configuration. For bacteria and protozoa, ranges lie between 5-9.5 (bacteria) and 5.5-7.5 (protozoa) for the baseline scenario, and 11-15 (bacteria) and 11-14 (protozoa) for the NEXTGEN configuration. The assumptions indicate a substantially higher treatment performance of the NEXTGEN configuration. Most interestingly, the NEXTGEN configuration is expected to be in line with EU reuse regulation (6 LRVs required for viruses) over the complete range of plausible LRV values, whereas under baseline conditions, minimum LRV conditions do not achieve the required 6 LRVs for irrigation. Thus, if risk calculations of the NEXTGEN QMRA tool indicate acceptable risk levels for the NEXTGEN configuration and unacceptable risk levels for baseline conditions, the QMRA results agree the health targets of EU reuse regulation, and indicate that risk simulations provided by the NEXTGEN tool lead to a realistic basis for decision making.

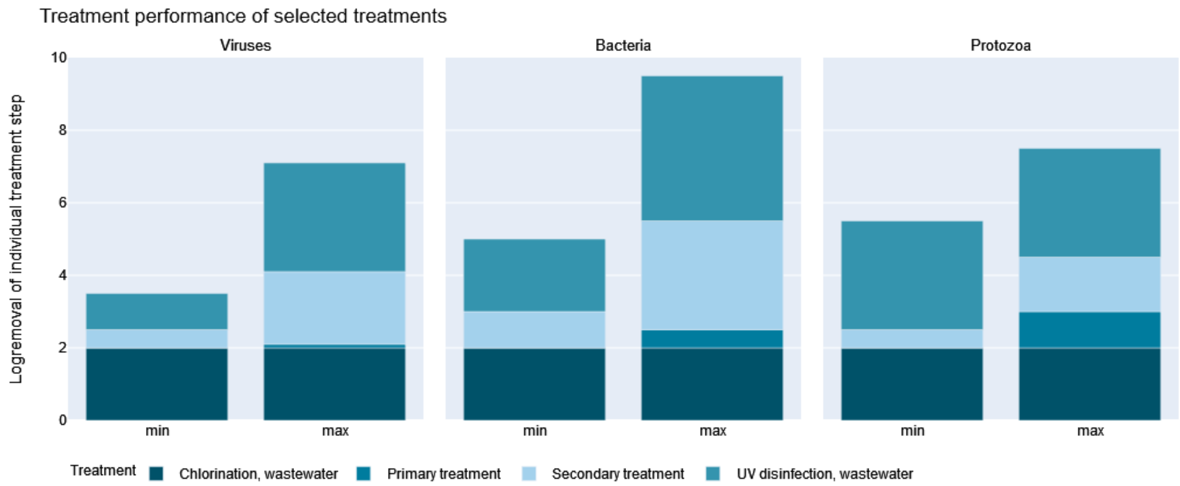

Figure 72: Overview of applied LRVs in the baseline scenario

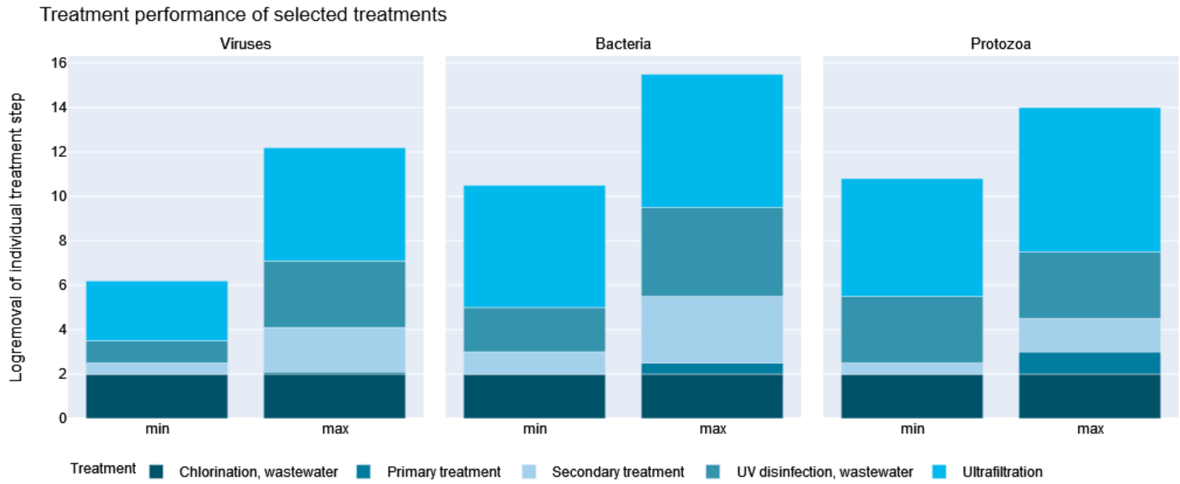

Figure 73: Overview of applied LRVs in the NEXTGEN scenario

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Risk characterization

The QMRA conducted for Tossa del Mar was the only one which made use of the tool's capability to compare different system configurations. The results of the comparison are illustrated in Figure 74. As expected from the assumed treatment performance, the NEXTGEN configuration shows substantially lower risk levels than the baseline configuration. For the NEXTGEN configuration, risk simulations fall completely below tolerable risk levels, indicating good agreement with estimates based on the comparison between assumed LRVs and the LRVs required by the EU water reuse regulation. The results indicate that water treated by the NEXTGEN configuration can be considered suitable for public irrigation use.

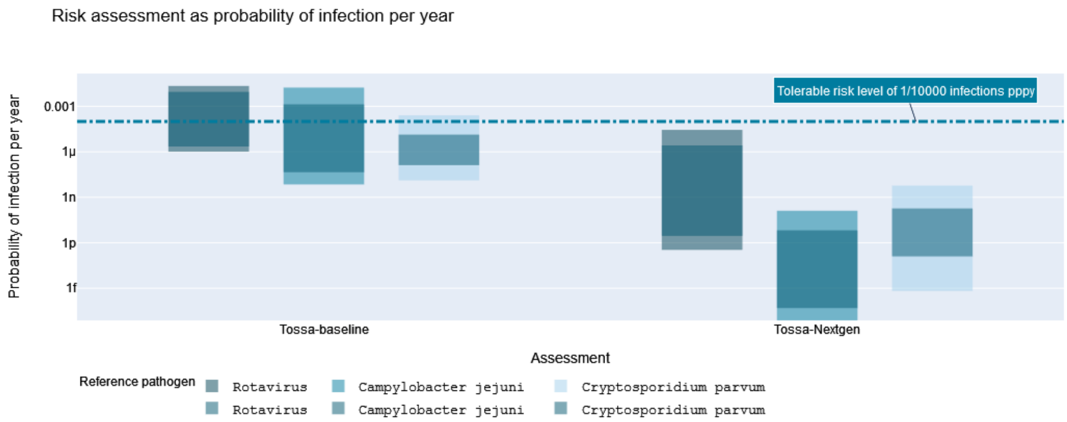

Figure 74: Comparison results between scenarios "baseline" and "NEXTGEN". For each pathogen, the outer boundaries of each bar plot refer to the range between the maximum of the maximum LRV scenario and the minimum of the minimum risk scenario (maximal range). The inner range refers to the range between the mean of the maximum and the mean of the minimum risk scenario (difference in means).

Timisoara

Problem formulation

At the case study in Timissoara, QMRA was used to test the reuse of treated wastewater for agricultural irrigation. To this end, default values provided in the AQUANES database were used.

Exposure assessment

Treated effluent was selected as the source water, followed by UV disinfection as a singular additional treatment step. This treatment step assumed 1-3 LRVs for viruses, 2-4 LRVs for bacteria, and 3 LRVs for protozoa (Figure 75). The unrestricted irrigation exposure scenario assumed that in the worst case (immediately post watering), 100 g of lettuce leaves would hold 10.8 mL water, and cucumbers would hold 0.4 mL of water. A serving of lettuce (40 g) was assumed to hold 5 mL of recycled water and other produce was assumed to hold up to 1 mL per serving.

The scenario of unrestricted irrigation can be directly compared to the class A requirements of the EU water reuse regulation. According to the regulation, unrestricted irrigation requires a minimum 6 LRVs for viruses and 5 LRVs for bacterial and protozoan indicators, respectively. The LRVs provided in Figure 75 cannot be directly compared to these

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requirements, as the regulation requirements include the complete treatment process, whereas Figure 75 only shows LRVs of the additional treatment after primary and secondary wastewater treatment. To be able to compare them, 0.5-2.1 (viruses), 1-3.5 (bacteria) and 0.5-2.5 (protozoa) LRVs for combined primary and secondary treatment should be additionally added to results in Figure 75. Under these assumptions, even under maximum LRV conditions, the defined treatment scheme would only achieve 5.5 LRVs for viruses and would therefore not comply with the regulation requirements. For bacteria and protozoa, the LRV requirements would be achieved under maximum LRV conditions but not under minimum LRV conditions.

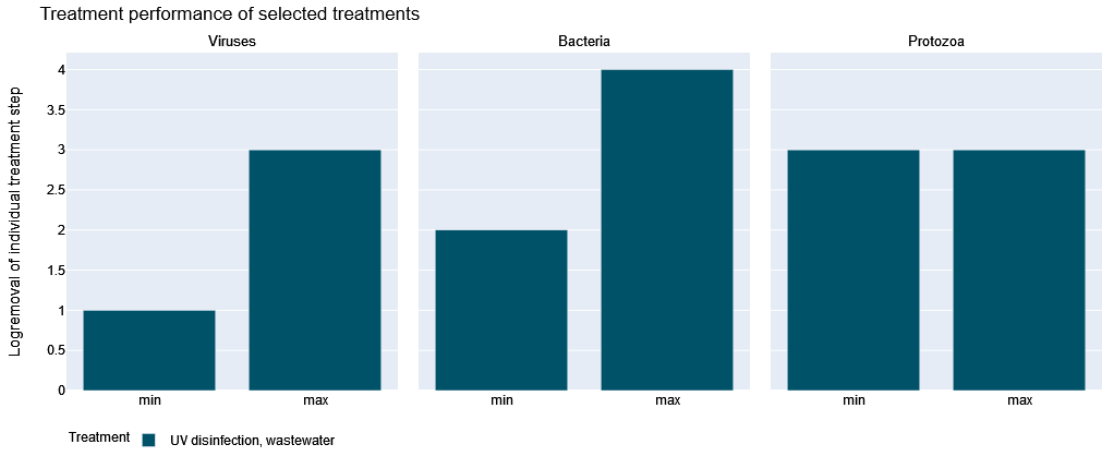

Figure 75: Overview of the applied LRV value for the case study in Timisoara

Risk characterization

The results of the risk simulation are shown in Figure 76. As expected, the results indicate that under minimum LRV conditions, the health objective in terms of DALYs pppy are not achieved. The results agree with expectations deduced from comparing the assumed installed LRV performance to the reuse regulation's LRV requirements. Under maximum LRV conditions, the comparison between assumed and required LRVs for viruses and bacteria also agree, as the health objective was only achieved for bacteria. For protozoa, the health objective was expected to be achieved, as the installed LRV performance was expected to achieve the reuse regulation's required LRVs. However, the risk simulation results still indicate an elevated risk for this scenario. In general, it can be concluded that to achieve required LRVs and reduce risk to below acceptable levels, an additional pre-filtration seems necessary if treated wastewater will be used for unrestricted irrigation. Additionally, validation monitoring to validate LRVs of the primary and secondary treatment steps may be considered to support further planning steps with information about the performance of the existing system.

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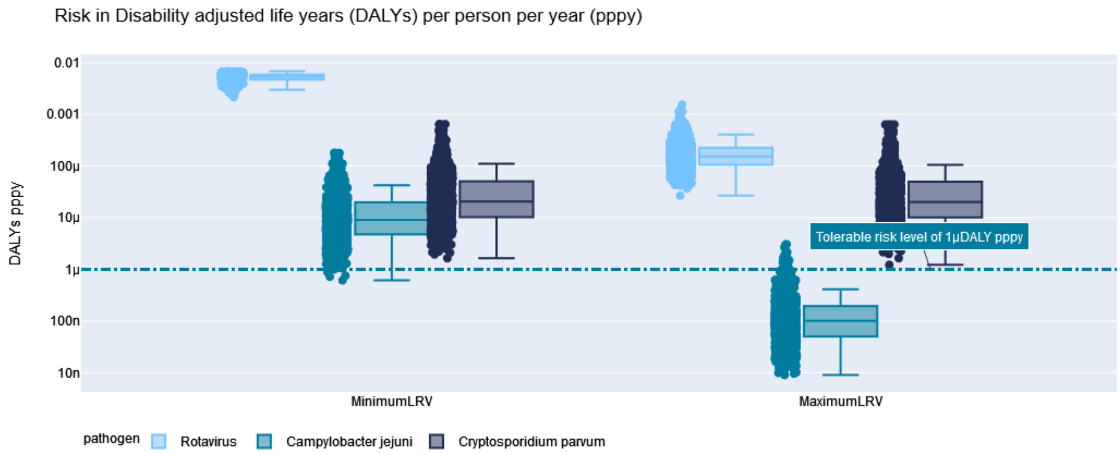

Figure 76: Risk assessment result as disability adjusted life years (pppy). Points next to individual boxplots refer to individual simulation results of the Monte-Carlo-Simulation.

User feedback

An additional objective of applying NEXTGEN QMRA tool to the various case studies was to receive feedback which would further improve it. To this end, users were asked to provide feedback on ease of application, clarity of results and relevance for operators via a poll, the results of which are shown in Figure 77. Overall, the user feedback indicated that the tool had a high relevance for operators, which supports the need for a lower barrier to entry for performing quantitative risk simulations. Regarding the clarity of result, the feedback depended on the level of experience of the user. While experienced QMRA practitioners found it relatively intuitive and easy to apply, they also identified some missing pieces of information which are needed for correctly interpreting the returned results. The constructive and honest feedback will help further improve the upcoming releases of the NEXTGEN QMRA tool.

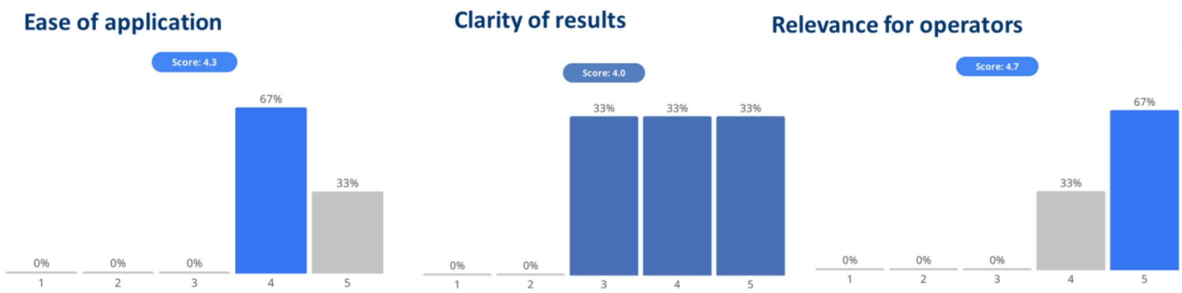

Figure 77: Overview of the poll result received from the individual case studies.

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Conclusions

In the NEXTGEN project, an updated version of the QMRA tool originally developed in the AQUANES project, was applied to various reuse site.

All studies relied on the default values provided by the developed tool. Our results indicate that under two configurations (Filton, Gotland) risk is expected to fall below acceptable limits even under unfavorable LRV assumptions. In Filton, the low source water pathogen concentration (rooftop harvesting) is the major driver for the low risk outcomes, while in Gotland the double UF/RO combination membrane configuration provides confidence in achieving predefined health targets.

In general, our study demonstrates the potential for safe implementation of water reuse applications using almost all tested treatment configurations. However, our results also identify the need for local validation monitoring, as in the absence of additional local information, default values generally result in wide ranges of potential LRVs, which are less informative. The results are thus consistent with the approach proposed by the new EU water reuse regulation.

The new features of the updated QMRA tool now provide users with the opportunity to directly create and configure custom treatments, and thus easily include local validation data. The application of a tool for conducting QMRA can be seen as a benefit to visualize and communicate existing and potential health risk.

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Assessment of chemical risks from recovered nutrient products

Introduction

The recovery of nutrients is one part of the circular economy solutions in NEXTGEN. At the NEXTGEN case studies Braunschweig, Spernal and Athens nutrients are recovered to fertilize agricultural or horticultural areas. As nutrients are recovered from the wastewater stream, they can potentially be contaminated with a variety of pollutants. In contrast to LCA, which describes the impacts of the entire product life cycle on a global scale, the environmental risk assessment focuses on the local risk posed by the products application. It is the first part of a risk management and aims at identification and characterisation of risks.

The identification of hazards was done in a close cooperation with the local partners who have the best knowledge of the production process and the input material. Further stakeholders like farmers or local authorities were included in discussions in the Communities of Practice. As a result, a list of hazards was generated for each case study (Table 48). In Braunschweig, several per- and polyfluoroalkyl substance (PFASs) as emerging contaminants were measured along the treatment train. Although concentrations were consistently below the limit of detection, Perfluorooctansulfonic acid (PFOS) and Perfluorooctanoic acid (PFOA) were included in the risk assessment to characterise a potential risk even at low concentrations.

Table 48: Hazard identification per case study and recovered product for QCRA

Braunschweig Struvite	Braunschweig Ammonia sulphate Solution	Spernal Hydroxyapatite	Athens Compost
Arsenic	Cadmium	Arsenic	Cadmium
Cadmium	Chromium	Cadmium	Chromium
Chromium	Copper	Chromium	Copper
Copper	Mercury	Copper	Mercury
Mercury	Nickel	Mercury	Nickel
Nickel	Lead	Nickel	Lead
Lead	Zinc	Lead	Zinc
Zinc		Zinc	
Benzo(a)pyrene		Benzo(a)pyrene	
PCDD/F + dl-PCB			
PFOS			
PFOA			

Predicted no-effect concentrations (PNECs) were collected for the soil and groundwater ecosystems for all substances considered. To characterise the risk, PNEC values were compared to predicted environmental concentrations (PECs) obtained by exposure modelling of soil after 100 years of fertilization with the recovered products. The exposure model is based on PART II of the Technical Guidance Document on Risk Assessment by the European Commission (IHCP, 2003a),which is actually aimed on assessing the risk caused by organic pollutants. It was extended by the output path “plant uptake” and by the option to

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link substance sorption behaviour to pH value, organic carbon and soil concentration to enable the assessment of heavy metals.

The most relevant variables of the exposure model were described by probability distributions. This probabilistic approach allows the integration of environmental variability and uncertainty. The algorithm distinguishes between spatial and temporal variability. Both variability types are implemented using a Monte-Carlo approach to draw values from predefined distributions. The Monte-Carlo simulation leads to multiple PEC values and thus to multiple risk characterisations. The information of the results was aggregated into simple and clear statements about the risk posed by fertilization. To achieve this, the risk after 100 years of fertilization was compared to a risk after 100 years without fertilization. The results are interpreted with a risk matrix that takes into account the average increase of risk and the dispersion of results. The risk matrix groups the result in 4 categories from negligible to unacceptable risk.

Method

The risk to the soil ecosystem is determined by pollutant input via fertilization and atmospheric deposition and pollutant output via leaching, plant uptake, volatilization, and biodegradation (Figure 78). The output pathways depend on environmental conditions and pollutant characteristics. The most relevant substance properties are Henry constant (K_H), sorption coefficient (K_d), biological half-life (DT50) and bio concentration factor (BCF) from soil to plant for volatilization, leaching, degradation and output via plant harvesting, respectively. Furthermore, the amount of precipitation influences the water balance of the soil.

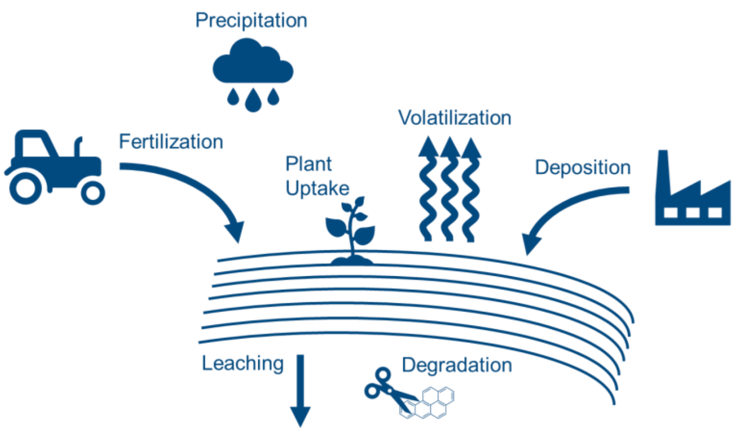

Figure 78: Pathways of the exposure model

Algorithm

The exposure model is based on an annual fertilizer application at the beginning of the growing period. Output is described by the output rate k, which is the sum of all output paths considered. In the period after fertilizer application, this includes plant uptake until the plants are harvested. After this period, it is assumed that the plants are ploughed under and no longer contribute to pollutant removal.

Equation 1 $$k = k_{leach} + k_{volat} + k_{plant} + k_{bio}$$ with $k_{plant} = 0$ after growing period.

$k, k_{leach}, k_{volat}, k_{plant}, k_{bio}$: Overall output rate, leaching rate, volatilization rate, plant uptake rate and biodegradation rate in 1/d.

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The timing of harvesting can be determined individually. For the NEXTGEN risk assessment of agricultural sites the growing period was set at 180 days. After fertilization further input of pollutants only occurs via atmospheric deposition. The pollutant content in soil within one year after fertilization at time t is defined by

Equation 2

$$c(t) = \frac{D_{Air}}{k} - \left(\frac{D_{Air}}{k} - c_0\right) e^{-k\,t}$$

$c(t)$: Concentration in top soil at time t in mg/kg
D_{Air}: Daily soil mass specific atmospheric deposition in mg/(kg d)
c_0: Concentration in soil at time t = 0 after fertilization in mg/kg
t: Time in days

The concentration in soil at t = 0 is the sum of the initial concentration before fertilization and the increase of concentration due to fertilization. To obtain the increase of concentration, the fertilizer amount is referred to the weight of the top soil layer.

Equation 3

$$c_0 = c_i + \frac{c_{fert}\, M_{fert}}{10000\, \rho_{soil}\, d}$$

c_i: Initial concentration in top soil before fertilization in mg/kg
c_{fert}: Pollutant concentration in fertilizer in mg/kg
M_{fert}: Fertilizer application in kg/ha
ρ_{soil}: Top soil bulk density kg/m³
d: Top soil depths in m

While the calculation of leaching, volatilization and biodegradation rate can be found in the TGD, the plant uptake was added subsequently. It depends mainly on the BCF, which is the concentration in a plant divided by the concentration in soil, and the yield of the harvest.

Equation 4

$$k_{plant} = \frac{DM_{plant}\, Y\, BCF}{t_{growth}\, d\, \rho_{soil}}$$

DM_{plant}: Plant dry matter in %
Y: Yield in kg/m²
BCF: Bioconcentration factor from soil to plant (referred to plant dry matter)
t_{growth}: Growing period in days

The sorption coefficient (K_d) affecting the leaching rate, and the BCF affecting plant uptake often depend on pH and soil organic carbon content. The pH value is particularly important for the mobility of heavy metals. To take this into account, a linear regression on a logarithmic scale was implemented in the exposure model for both substance properties.

Equation 5

$$\log_{10} K_d = \beta_1 pH + \beta_2 \log_{10} c_{org} + \beta_3 \log_{10} c_{soil} + C$$

K_d: Sorption coefficient as concentrion in soil devided by concentration in pore water in L/kg
β_1, β_2, β_3: Regression coefficients
pH: Soil pH value
c_{org}: Soil organic carbon content
c_{soil}: Pollutant concentration in soil in mg/kg

The predicted environmental concentration (PEC) is a simulated concentration that is used to describe the future risk. It is calculated for the soil compartment and is defined as the average concentration over 30 days after fertilizer application. The PEC for groundwater is derived by the PEC soil and is described by

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Equation 6

$$PEC_{groundwater} = \frac{PEC_{soil}\, \rho_{soil}}{K_d}$$

$PEC_{groundwater}$, PEC_{soil}: Predicted environmental concentration in mg/L and mg/kg for the groundwater and soil compartment, respectively.
ρ_{soil}: Bulk density of the soil in kg/m³
K_d: Sorption coefficient as concentrion in soil devided by concentration in pore water in L/kg

Thus, the groundwater concentration is actually a predicted porewater concentration. A mixing-factor with unpolluted groundwater, and the time period of leaching including further potential degradation, plant uptake or volatilization processes are not included. The groundwater risk assessment can thus be considered as conservative. Especially for readily degradable organic compounds, the exposure model may lead to an overestimation of the PEC of groundwater.

For risk assessment, the PEC is divided by the predicted no-effect concentration (PNEC) to obtain the risk quotient (RQ). An RQ greater than 1 indicates an unacceptable risk since negative effects cannot be excluded if the PNEC is exceeded.

Equation 7

$$RQ = \frac{PEC}{PNEC}$$

RQ: Risk quotient
PEC: Predicted environmental concentration in mg/L and mg/kg for the groundwater and soil compartment, respectively.
$PNEC$: Predicted no-effect concentration in the same unit as PEC

Data input

The exposure model algorithm is written in the R programming language and part of the open source R-Package “kwb.fcr”, which stands for “fertilizer chemical risk” and is downloadable from the KWB github account (https://github.com/KWB-R/kwb.fcr). Data entry is done through three different Excel spreadsheets that contain information on 1) a pollutant, 2) a fertilizer, and 3) environmental conditions and soil properties.

Pollutants, fertilizers and the environmental properties can be used in any combination. This allows the risk assessment to be easily expanded by adding a fertilizer at multiple sites or to include a new substance. For each model variable, a distribution, a shift of distribution, and information on the type of variability can be entered.

The selection of possible distributions is shown in Table 49. In order to compare the shape of distributions, the density plots show distributions where 95% of all data are between 10 and 100.

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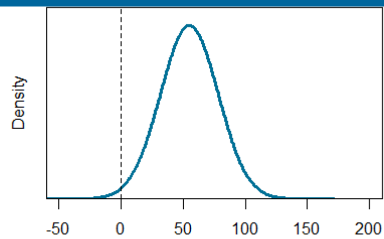
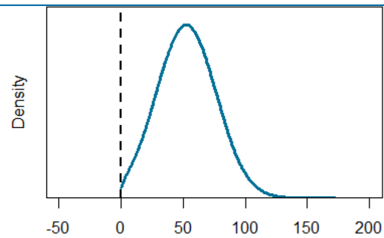
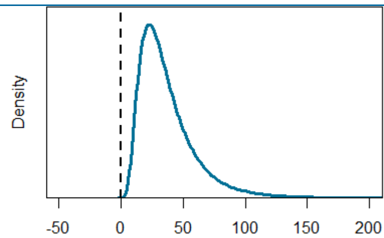
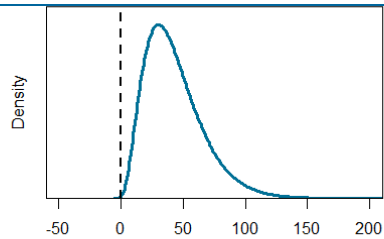
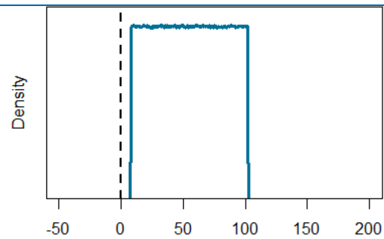
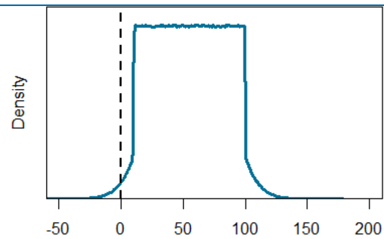
Table 49: Probability distributions that are part of the exposure model for the QCRA

Distribution	Description and Parameters	
Normal distribution	Mean and standard deviation	
Normal distribution truncated at zero	Mean and standard deviation	
Log-normal distribution	Mean and standard deviation both in natural logarithm	
Gamma distribution	Shape and rate	
Uniform distribution	Minimum and maximum	
Extended uniform distribution	A uniform distribution; defined by minimum and maximum values, that represents the inner 95% of the total distribution. It is complimented by two tails of a normal distribution on each side. The mean value of the normal distribution is the mean value of minimum and maximum, the standard deviation is the the distance between maximum of the uniform distribution and mean value of the normal distribution divided by 1.96.	

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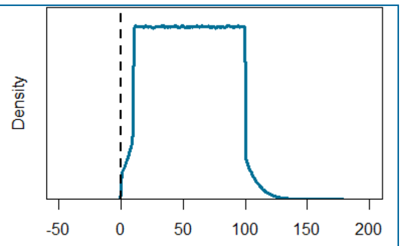
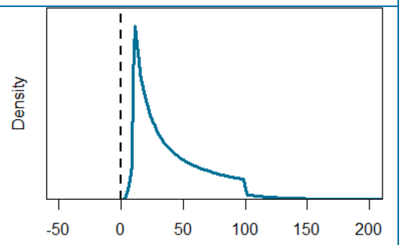
Extended uniform distribution truncated at 0	The same as the extended uniform distribution, but the lower tail of the normal distribution is truncated at 0. Thus, the lower 2.5 % are distributed between 0 and the minimum of the uniform distribution.	
Extended logarithmic uniform distribution	A uniform distribution defined by logarithmic minimum and maximum values (common logarithm), that represents the inner 95% of the total distribution. It is complimented by two tails of a normal distribution on each side. The mean value of the normal distribution is the mean value of minimum and maximum, the standard deviation is the the distance between maximum of the uniform distribution and mean value of the normal distribution divided by 1.96.	

A normal distribution should be used to describe the uncertainty of a particular characteristic (e.g., the concentration of nutrient in fertilizer) or the variation over time (e.g., the amount of fertilizer applied at one site). Furthermore, for spatial variability (i.e., the average amount of precipitation or substance properties that depend mainly on environmental conditions), the normal distribution can be truncated at zero, a log-normal or a gamma distribution with or without shift can be specified. The uniform distribution is to be used only when there is no additional information about the probability of values. The extended uniform distributions are intended for situations where a new situation is described by combined data that are not part of a single population. This may be the case when the behaviour of a substance is described by literature data from very different soils to predict the behaviour in a new, unknown soil, or when data from known substances are used to predict the behaviour of a new comparable substance. The main disadvantage of uniform distributions is the abrupt drop in density at minimum and maximum. If the defined range does not include all possible values, these values can in no case be part of an MCS. This is especially dangerous when the simulation is used to predict unknown situations. To address this drawback, the uniform distribution has been extended by the tails of a normal distribution. This allows for extreme values with low probability. The implementation of a logarithmic uniform distribution is intended for distributions over several orders of magnitude. In this case, low values would be underrepresented in an MCS by a uniform distribution with respect to the relative distance to the defined distribution limits. For example, if the sorption coefficient of a substance is not precisely known and is estimated to be between 1 and 1000 L/kg, an MCS would be equally likely to miss the defined minimum and maximum by 10. However, 10 is a relative distance of 1000% from the minimum, while 990 is only a relative distance of 1% from the maximum. This effect can be avoided by using a logarithmic uniform distribution.

The type of variability refers to the difference between spatial and temporal variability. While for spatial variability the algorithm draws from the defined distribution only once at the beginning of the simulation, for temporal variability a random draw is made every year. The temporal variability and variable uncertainty are treated equally in the exposure model.

Background concentration

The background concentration for the PEC_{soil} simulation was set to corresponding $PNEC_{soil}$ of the substance to enable a normed procedure for risk interpretation. Thus, the soil is already

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contaminated in a relevant way and the initial RQ is 1. A simulation over 100 years leading to a RQ < 1 indicates a higher pollutant output compared to the input. In other words, the equilibrium soil concentration is below the PNEC value under the defined environmental conditions and substance properties. While a RQ > 1 indicates a potential increase of pollutant content above the PNEC.

The starting concentration for the risk assessment of the groundwater compartment is more complex, since the initial concentration depends on the several environmental und substance-specific assumptions, such as the sorption coefficient or the soil bulk density (see Equation 6).

To have the risk quotient for groundwater equal to 1 at the beginning of the simulation, the initial concentration must be back-calculated from the $PNEC_{groundwater}$.

Figure 79 shows an example of the cadmium initial concentration for PEC_{soil} (green line) and $PEC_{groundwater}$ (blue bars) simulation. The background concentration that is used for $PEC_{groundwater}$ ranges from 0.008 to 2.7 mg Cd/kg soil. For each of these concentrations the RQ for the groundwater compartment is 1. Despite the low contamination of some soils, there may be a higher risk for the groundwater compartment, due to low sorption capacity of the soil combined with other unfavourable environmental conditions. This implicates a large pollutant output via leaching. For other soils, sorption is high, so groundwater is at less risk if pollutant levels are low in the soil, however pollutant accumulation is favoured.

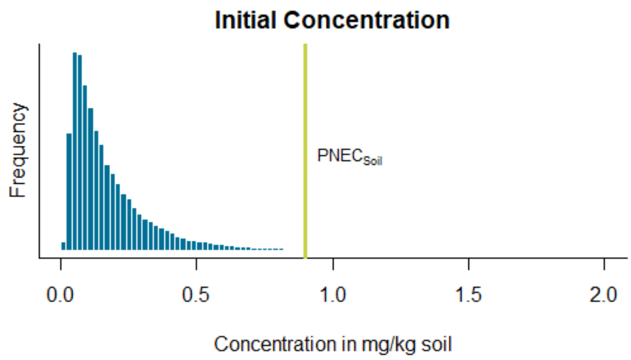

Figure 79: Initial concentration for PEC_{soil} and $PEC_{groundwater}$ simulation (example for cadmium)

Risk characterisation approach

The algorithm calculates multiple PEC values according to the number of defined runs. For NEXTGEN the number of runs was set to 100 000 leading to 100 000 different random combinations of environmental conditions and substance specific properties. It must be noted that some of the random combinations are not likely to represent the agricultural reality. Thus, the resulting probability distribution of RQs does not reflect the true probability. It cannot be used to estimate the likelihood of a critical situation. For risk characterisation either every single result indicating a high risk would have to be checked and evaluated towards its likelihood to occur or the results would have to be aggregated and interpreted. The second approach is more convenient since it can be automated. Furthermore, it is a more objective way if clear indicators can be defined.

Risk is defined as a combination of severity and likelihood. The indicators must assure that a high risk will be ascertained if the product of both is high. On the other side, a lack of knowledge leads to an increase of risk what the indicators need to account for as well. In

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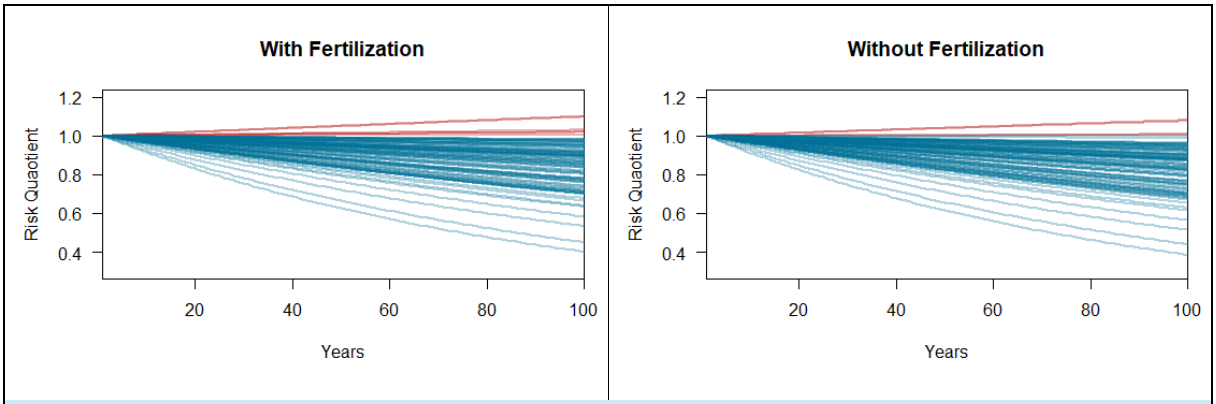
order to quantify the risk caused by fertilization, all runs are simulated twice, with and without fertilization. For the interpretation of increase of risk caused by fertilization only high-risk results are statistically analysed. High-risk results are defined by a RQ greater than 1 at the end of the simulation with fertilization. The indicators used for risk characterisation are

1. Increase of risk caused by fertilization (ΔRQ)
2. Maximum risk of simulations with fertilization (RQ_{max})

and are explained within the following example. Initially the pollutant concentration equals the PNEC, leading to a RQ of 1. In this hypothetical example a Monte-Carlo-Simulation (MCS) with 100 runs was performed. After 100 years of fertilization, 6 runs ended up as high-risk results at a RQ higher than 1. Apparently, the combination of environmental conditions and further assumptions leads to an equilibrium concentration between input and output, at which a negative effect on the environment cannot be excluded. The RQs of all high-risk results are shown in Figure 80.



RQ of high-risk results with fertilization (and corresponding RQ without fertilization)

1.02 (1.002) , 1.03 (1.008) , 1.018 (0.997) , 1.005 (0.988), 1.097 (1.081), 1.101 (1.075)

Figure 80: Example of "high risk" results after soil exposure modelling for 100 years.

The risk increase is defined as the mean increase in high-risk results from simulation without fertilization to those with fertilization (0.02 in the example). The maximum of risk is the average of the upper 5% of all results obtained in the simulation with fertilization. In case of 100 runs, this equals the five highest values. The average RQ of the five highest values is 1.05.

In environmental chemical risk assessments, the final RQ is mostly used to determine the overall risk. RQs greater than 1 are usually interpreted as "unacceptable", RQ between 0.1 and 1 as "acceptable" and RQ smaller than 0.1 as "negligible" van Leeuwen and Vermeire (2007). The logarithmic interpretation scale was adapted to the risk-increase approach of this study. However, the categories "acceptable" and "negligible" were shifted one log-unit lower, since the assessment refers to only high-risk situations. A fourth category "increasing concern" was implemented between "acceptable" and "unacceptable" to emphasize the need for an examination of the causes.

The maximum risk, on the other side, is used to include outliers, which play an important role in every risk assessment considering unlikely but severe events. It was decided to use the average of the top 5% of all results instead of the maximum only. In this way the entire

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upper tail of the probability distribution is part of the evaluation. A high maximum risk can have several reasons. Besides a large input via deposition or fertilization, broad ranges of substance and soil properties can lead to long tails of the probability distribution. Particularly in the case of emerging contaminants, consideration of knowledge about the substance behaviour in the environment is important and must be integrated into the risk assessment. Therefore, both indicators were combined in a risk matrix (Figure 81). If ΔRQ and R_{max} are low, the risk will be described as negligible or acceptable. The "risk of increasing concern" (orange colour) can be interpreted as recommendation for a closer examination, while the unacceptable risk is issued if there is both, a high fertilizer related increase of risk and a high maximum risk of all results.

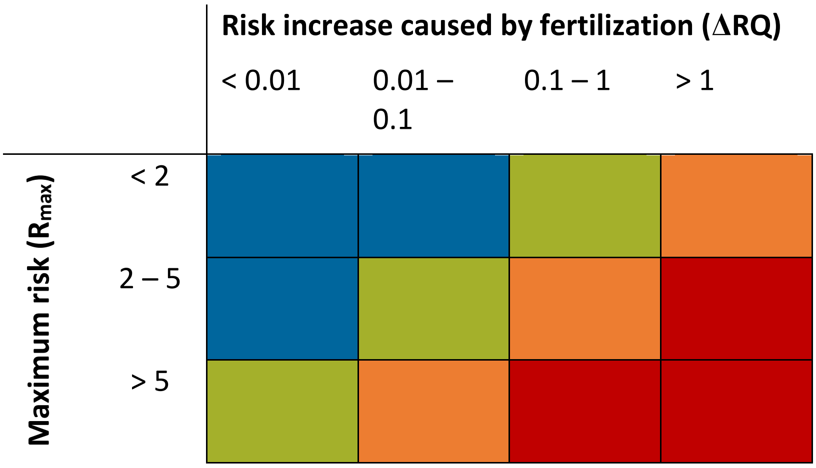

Figure 81: Risk matrix (blue: negligible risk, green: acceptable risk, orange: risk of increasing concern, red: unacceptable risk)

Input data

Data is supplied by three different Excel sheets for the environmental conditions, for substance properties and for fertilizer data. In the following chapters the employed data is described, while the exact data input for simulation is listed in the supplementary information.

Environmental Data

The environmental data is based on the standard soil as described in the technical guidance document (IHCP, 2003a). This is a sandy to loamy soil with 20%, 20% and 60% of air capacity, field capacity and solids fraction, respectively. The average water content is assumed to be equal to the field capacity. Over a whole year 25% of the precipitated water is assumed to infiltrate the soil and leach into the groundwater. The predicted soil concentration is calculated for the topsoil. That is, by definition, the first 20 cm of an agricultural soil. The soil is assumed to be aerated all the time. Furthermore, the average density of solids of 2500 kg/m³ was used.

Pollutant environmental behaviour depends on the soil characteristics. While mostly the relation between substance coefficients and chemical of physical conditions is not mathematically described, for some substance regressions against pH and organic carbon content are available. Thus, both variables are fit into distributions. The pH can vary over a large range in soil, however, in agricultural soil, a slightly acidic to neutral pH is common. An extended uniform distribution between pH 5 and 7 was used to describe the pH variation (Figure 82). The organic carbon content is derived from an exhaustive study of organic

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matter classes (Germany classification) from more the 14 000 top soils in Germany (Düwel et al., 2007). The data was filtered for sandy, agricultural soils. The classes were transformed into organic carbon fractions using the boundaries of the organic matter classes. Finally, a log-normal distribution appeared to be the best fit for the data. The distribution of precipitation was created by long-term data series between 1993 and 2016 at 193 sites in Germany. Per site the data was averaged to get a distribution about the means. The best fit was a gamma distribution that was shifted by 455 mm per year, which becomes the minimum of the distribution. The median yearly rain is 720 mm, while much higher precipitation rates are possible (95th quantile is 1250 mm).

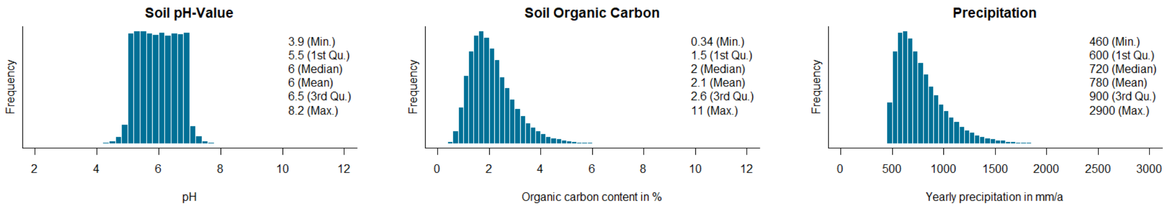

Figure 82: Distributions used for pH, organic carbon content and yearly precipitation

Since wheat is one of most commonly grown plants in Europe it was used to estimate the pollutant output by plant uptake. Wheat yield in European countries was between 3 and 8 t/ha in 2020 according to the FAOSTAT – Database provided by the Food and Agricultural Organization of the United Nations (FAO). To cover this range, a normal distribution with a mean value of 6 t/ha and a standard deviation of 1.5 t/ha was used. The average dry mass of wheat was assumed to be 86% (LVLF, 2008).

The compost from Athens is applied at a tree nursery. At this site the yield was set to zero, since no plants are harvested. Furthermore, the precipitation was changed to a uniform distribution between 400 and 1000 mm/year. Although, the average yearly rain amount in Athens is below 400 mm the horticultural area is expected to be irrigated.

All distributions described in this chapter are based on environmental variability, and thus, spatial variability was used within the MCS.

Pollutant data

In the following subchapters, the properties of each pollutant are briefly introduced as well as their references. The exact data input for the exposure model can be found in the supplementary information.

Arsenic

The soil and groundwater PNECs of Arsenic are based on sensitivity distributions. Since there are many studies on the toxic effect on organisms, assessment factors of 3 and 2 are used for aquatic and terrestrial, respectively, leading to PNECs of 5.6 µg/L and 2.9 mg/kg (ECHA, 2022a). The sorption of Arsenic to soil is very complex. In contrast to most metals, Arsenic does not show an increasing mobility with lower pH. It is especially mobile at pH > 7 (Tyler and Olsson, 2001). Instead of linking the sorption coefficient to soil parameters, a lognormal probability distribution was derived by Allison and Allison (2005) based on 21 data points. For the transfer to plants a review by Wang et al. (2017) was used. All field experiment studies with common arsenic contents in soil (< 20 mg/kg) were used. The so filtered four studies contained 132 data points. In each study a BCF range was quoted. Minimum and

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Maximum of those four studies, being 0.0036 and 0.023, were used to set up an extended uniform distribution truncated at 0.

While biodegradation was set to 0, there is volatilisation if arsenic is transformed to arsine, as a result of biological activity. Mestrot et al. (2011) described a mean arsenic volatilization from two low-contaminated soils in microcosms of 0.011 % and 0.052 %, which correspond to a volatilization rate of 3 x 10^{-7} and 1.4 x 10^{-6} 1/d, respectively, based on a first order kinetic. Those rates are expected to be 1 to 2 magnitudes lower for field conditions (Punshon et al., 2017). For the exposure model a range from 3 x 10^{--9} to 1.4 x 10^{-6} 1/d was used for a logarithmic extended uniform distribution.

Figure 83 shows the final distribution of the logarithmic K_d, BCF, atmospheric Deposition and volatilization rate of arsenic. 50% of the K_d values lie between 2.7 and 3.7, while there is a broad range between minimum and maximum value used for the exposure model. For the BCF the addition of tails to the uniform distribution leads to an increase of maximum from 0.023 used for the uniform distribution to 0.035. Overall the plant uptake of arsenic is comparatively low. The Median and 95th Quantile of the atmospheric deposition are 1.5 and 3.6 g per hectare and year, respectively.

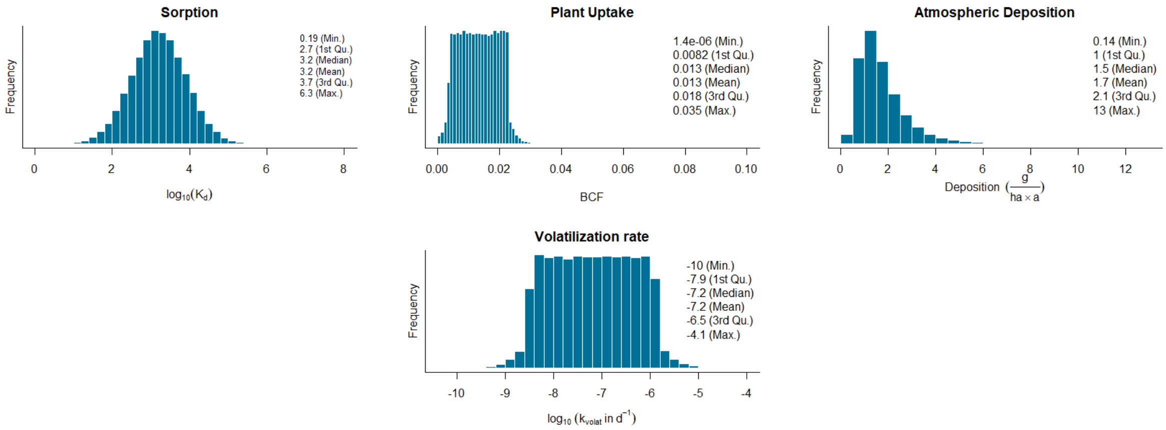

Figure 83: Distribution of sorption coefficient, bioconcentration factor and atmospheric deposition used to predict the environmental arsenic concentration.

Cadmium

Cadmium is a well-studied terrestrial and aquatic pollutant. As PNECs 0.19 µg/L and 0.9 mg/kg were used for groundwater and soil, respectively. Both coming from the the REACH registration dossiers by the European Chemicals Agency (ECHA) for longterm toxicity (ECHA, 2022b).

The atmospheric deposition is based on measurements of 245 different sites all over Germany between 2000 and 2015. The output paths volatilization and biodegradation were set to zero. The sorption to soil is well studied in several studies. Sauvé et. al (2000) used data from 751 measurements in a review to set up a logarithmic linear regression of the dissolved cadmium concentration against pH, organic matter content and total cadmium content in soil. For each coefficient a standard error was provided by Sauvé, which was used in the NEXTGEN risk assessment to form a normal distribution.

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Equation 8 $$\log_{10} c_{diss} = -0.47\, pH + 1.08 \log_{10} c_t - 0.81\, \log_{10} f_{om} + 3.42$$

c_{diss}: Cadmium concentration in porewater in mg/L
c_t: Cadmium content in soil in mg/kg
f_{om}: Organic matter content in %

The concentration in porewater increases with lower pH, lower organic matter content and higher cadmium content in the soil. Since the exposure model uses organic carbon instead of organic matter, Equation 8 had to be transformed to

Equation 9 $$\log_{10} c_{diss} = -0.47\, pH + 1.08 \log_{10} c_t - 0.81\, \log_{10} f_{oc} + 3.42 - \log_{10} 1.72$$

f_{oc}: Organic carbon content in %

using 1.72 as factor between organic carbon and organic matter as suggested by the TGD (IHCP, 2003b). In 2002, an expert meeting on critical limits for heavy metals were held and a relation between the BCF of different plant types and soil properties were described in the meeting report (Schütze, 2003). For NEXTGEN the regression for wheat was used since it is frequently cultivated and the regression showed the best R-square of all considered plants. Once more, the organic matter needed to be transformed to organic carbon content.

Equation 10 $$\log_{10} c_{plant} = -0.15\, pH + 0.76 \log_{10} c_t - 0.39\, \log_{10} f_{oc} + 0.35 - \log_{10} 1.72$$

c_{plant}: Cadmium content in plants in mg/kg dry weight

Figure 84 shows the final distributions of the logarithmic K_d and the BCF using the soil properties as described in chapter about environmental data. 50 % of log K_d and BCF are within the range between 2.6 and 3.1 and between 0.11 and 0.16, respectively. Atmospheric deposition is mostly below 2.5 g per hectare and year (95th quantile) but can be significantly higher at some sites.

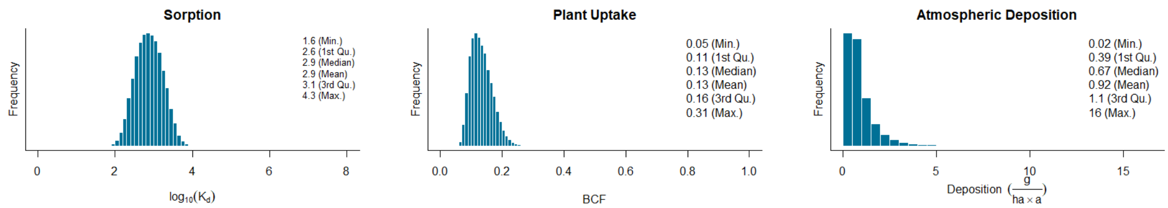

Figure 84: Distribution of sorption coefficient, bioconcentration factor and atmospheric deposition used to predict the environmental cadmium concentration.

Chromium

According to the REACH registration dossier the chromium PNECs for freshwater and soil organisms are 6.5 µg/L and 21.1 mg/kg with assessment factors of 2 and 1, respectively (ECHA, 2022c).

Janssen et al. (1997) found a relation between chromium sorption to soil and soil pH amongst others. Regressions considering Al-Oxide concentration of soil had better R-square, however, Al-Oxide is not part of the exposure model. Thus, the simple pH regression was used for K_d estimation

Equation 11 $$\log_{10} K_d = 0.21\, pH + 2.64$$

K_d: Sorption coefficient in L/kg

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Increasing pH values lead to higher sorption. To account for the relatively high uncertainty of this relation (adjusted $R^2 = 0.54$), the coefficients were described with a normal distribution. The standard deviation was assumed to be 30 % of the coefficient. Kühnen and Goldbach (2004) analysed soil and plant samples of eleven farms. The chromium concentration measured in wheat was used to derive BCF in a range between 0.001 and 0.015. The atmospheric deposition is based on measurements of 84 different sites all over Germany between 2000 and 2015 from the German environmental agency Umweltbundesamt. A normal distribution that was truncated at 0 was the best fit for the deposition data.

Figure 85 shows the final distribution of the logarithmic K_d, BCF and atmospheric deposition. For the pH dependent K_d value the soil properties as described in chapter about environmental data was used.

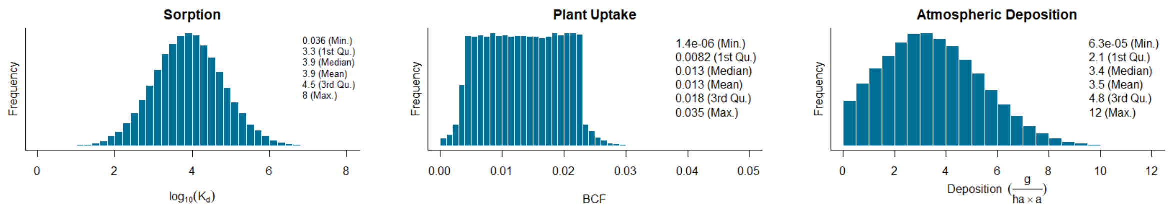

Figure 85: Distribution of sorption coefficient, bioconcentration factor and atmospheric deposition used to predict the environmental chromium concentration.

Copper

Soil and freshwater PNECs used for copper are 65 mg/kg and 7.8 µg/L, respectively (ECHA, 2022d). For both PNECs an assessment factor of 1 is the basis, since copper is a very well-studied hazard.

Sauvé et al. (2000) set up a logarithmic linear regression of the dissolved copper concentration against pH, organic matter content and total cadmium content in soil. They used 351 data points within their review study. For each coefficient a standard error was provided, which was used in the NEXTGEN risk assessment to form a normal distribution.

Equation 12 $$\log_{10} c_{diss} = -0.21\, pH + 0.93 \log_{10} c_t - 0.21\, \log_{10} f_{om} + 1.37$$

c_{diss}: Cadmium concentration in porewater in mg/L
c_t: Cadmium content in soil in mg/kg
f_{om}: Organic matter content in %

The concentration in porewater increases with lower pH, lower organic matter content and higher copper content in the soil. Similar to the calculation of dissolved cadmium Equation 8 had to be transformed to

Equation 13 $$\log_{10} c_{diss} = -0.21\, pH + 0.93 \log_{10} c_t - 0.21\, \log_{10} f_{oc} + 1.37 - \log_{10} 1.72$$

f_{oc}: Organic carbon content in %

using 1.72 as factor between organic carbon and organic matter as suggested by the TGD (IHCP, 2003b). The BCF used for exposure modelling ranged from 0.05 to 0.6 as minimum and maximum values for an extended uniform distribution. The data comes from Kühnen and Goldbach (2004), reviewing literature values complemented by samples from 11 different farms in Germany. The atmospheric deposition is derived by continuous sampling of the German Environmental Agency at 134 sites in Germany from 2005 to 2015. Biodegradation and volatilization rate were set to 0.

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Figure 86 shows the final distributions of the logarithmic K_d, BCF and atmospheric deposition. For the pH and organic content dependent K_d value the soil properties as described in chapter about environmental data were used in. The sorption coefficient distribution is quite narrow. The strongest influence on the porewater concentration is copper content in soil, which is a fixed value at the beginning of the NEXTGEN exposure assessment, being the soil PNEC. The plant uptake is comparatively high with BCF values of 0.33 in average, as copper is a micro nutrient for plants. The 75th percentile of the atmospheric deposition is 39 g per hectare and year, however extreme outliers up to 670 g per hectare and year are possible.

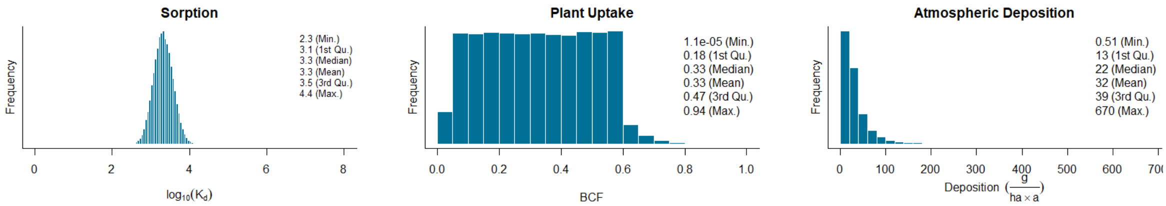

Figure 86: Distribution of sorption coefficient, bioconcentration factor and atmospheric deposition used to predict the environmental chromium concentration.

Mercury

Mercury is a very toxic pollutant leading to negative impacts on the ecosystems in freshwater and soil at low concentrations. The ECHA PNECs are 0.057 µg/L and 0.022 mg/kg, respectively (ECHA, 2022f). Especially for the soil PNEC only few long-term toxicity studies are available. Furthermore, the transformation of inorganic mercury into more toxic organometallic forms has to be addressed. This results in a high assessment factor of 50 to derive the PNEC from toxicological data.

While there is no biodegradation of mercury, the volatilization rate is complex, since it depends on soil temperature and soil moisture amongst others (Beckers and Rinklebe, 2017). Ericksen et al. (2006) have measured mercury emissions from eleven locations in the United States with Hg concentration below 0.1 mg/kg. The emission of mean values was 0.9 ng per m² and hour. Assuming the soil concentration equals the PNEC (0.022 mg/kg) and the emissions come from the topsoil being the top 30 cm with a bulk density of 1700 kg/m³, the volatilization rate would be

Equation 14

$$\frac{0.9\frac{ng}{m^2h} * 24\frac{h}{d}}{0.022\frac{mg}{kg} * 0.3m * 1700\frac{kg}{m^3} * 1000000\frac{ng}{mg}} = 1.925 * 10^{-6}\frac{1}{d}$$

The BCF from soil to plants is relatively low. In the review by Wang et al. (2017), three studies conducted by Zhu (2013), Kang (2011) and Yang (2005) described BCF values between 0.008 and 0.064 in wheat and and corn grains. This range was used to derive an extended uniform destribution, truncated at 0 (see Distribution details). For the sorption coefficient K_d, a lognormal probability distribution was derived by Allison and Allison (2005) based on 17 data points. The logarithmic mean value and standard deviation with base 10 ($\log_{10} K_d = 3.6 \pm 0.7$) had to be converted into natural logarithmic scale prior to exposure modelling.

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The atmospheric deposition is derived by continuous sampling of the German environmental Agency at 74 sites in Germany from 2005 to 2015.

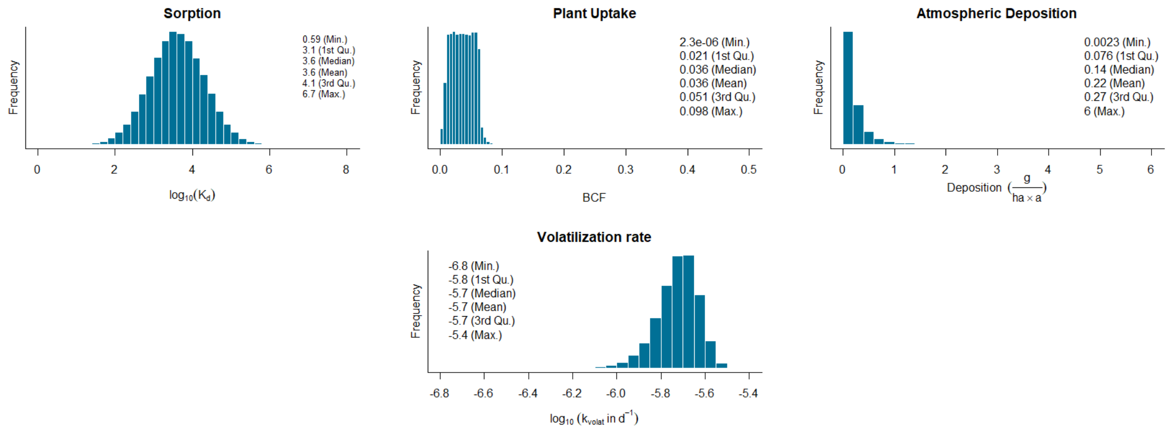

Figure 87: Distribution of sorption coefficient, bioconcentration factor, atmospheric deposition and volatilization rate used to predict the environmental mercury concentration.

Nickel

The PNECs for freshwater and soil ecosystems were calculated by ECHA based on a sensitivity distribution of the available toxicity data. After applying assessment factors of 2 and 1 for freshwater and soil, the resulting PNECs were 7.1 µg/L and 29.9 mg/kg, respectively (ECHA, 2022g).

The sorption of Nickel to soil mainly depends on pH and organic matter content. Sauvé et al. (2000) described a logarithmic linear relationship between those variables and the concentration of nickel in porewater, using 69 data points. Furthermore, standard errors are given for the regression coefficients to account for the uncertainty. Since the organic content must be entered as organic carbon content in the NEXTGEN exposure model instead of organic matter, the equation of Sauvé et al. had to be adapted. This was done with a conversion factor of 1.72 as suggested by the TGD (IHCP, 2003b).

Equation 15 $$\log_{10} K_d = 1.02\, pH + 0.8\, \log_{10} f_{oc} - 4.16 - \log_{10} 1.72$$

K_d: Nickel sorption coefficient in L/kg
f_{oc}: Organic carbon content in %

The sorption in soil increases with pH and organic carbon. A relation between soil properties and plant uptake could not be found. Instead, sample data from Kühnen and Goldbach (2004) was used to build a logarithmic linear regression of BCF against the nickel soil concentration. All 8 measurements of nickel concentration in wheat and maize were considered and combined with the nickel soil concentration.

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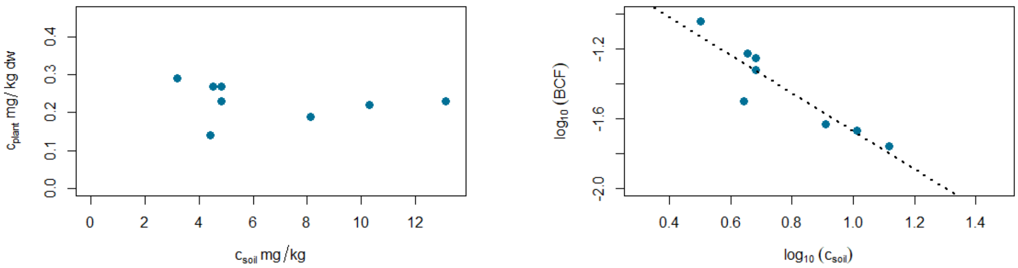

Figure 88: Nickel plant uptake and BCF regression

The concentration range in soil and in the plants was between 3.18 and 13.1 mg/kg and 0.14 and 0.29 mg/kg dry weight, respectively. While the nickel concentration in the plants was quite similar independent of the soil concentration, the BCF declines with increasing concentration in soil.

Equation 16 $$\log_{10} BCF = -1.095 \ \log_{10} c_t - 0.575$$

BCF: Bioconcentration factor from soil to plant of Nickel
c_t: Nickel concentration in soil in mg/kg

The adjusted R^2 of the regression was 0.82 and standard errors for the coefficients were 0.19 and 0.16 for the slope and intercept, respectively.

To get an impression of the range of BCF for different nickel concentrations in soil if Equation 16 is applied, a uniform distribution for nickel soil concentration ranging from 1 to 30 mg/kg is used for Figure 89. The mean 75 % of the BCF are below 0.033, indicating that nickel is taken up easily by plants. This agrees with literature data gathered by Kühne and Goldbach (2004) ranging from 0.01 to 0.05. Only if nickel is very low concentrated in soils, the BCF can be significantly higher. The mean sorption coefficient lies around 100 L/kg. Compared to other metals Nickel is quite mobile, especially if pH is close to 5 and organic carbon content is low, the log K_d can be below 0. The distribution shown in Figure 89 is built with the soil properties as described in chapter about environmental data. The 75th percentile of the atmospheric deposition is 11 g per hectare and year, however extreme outliers up to 120 g per hectare and year are possible. The distribution is derived from 174 different sites in Germany measured from 2005 to 2015 by the German Environmental Agency.

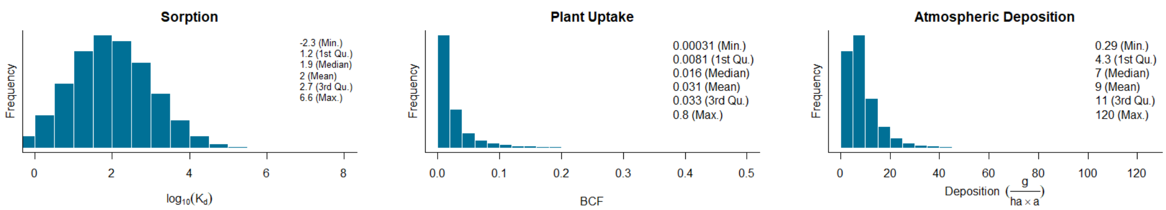

Figure 89: Distribution of sorption coefficient, bioconcentration factor and atmospheric deposition used to predict the environmental chromium concentration.

Lead

The PNEC for lead in freshwater is 2.4 µg/L low while the PNEC for soil ecosystems is comparatively high, being 212 mg/kg (ECHA, 2022e). One reason for this discrepancy is the strong sorption of lead in soil. Sauvé et al. (2000) found a logarithmic linear relation between the sorption coefficient, the pH value and the lead concentration in soil, based on 204 data points from a literature review. For every coefficient a standard error is also provided.

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Equation 17 $\log_{10} K_d = 0.37\,pH + 0.44\,\log_{10} c_t + 1.19$

K_d: Nickel sorption coefficient in L/kg
c_t: Total nickel content in soil in mg/kg

The high sorption is also responsible for the low BCF. Sample data and gathered literature by Kühnen and Goldbach (2004) was used for defining a range of BCF, since no correlation between soil properties and BCF could be found. For wheat and maize there were 8 data pairs of lead concentration in plants and soil available, all lying between 0.002 and 0.009 while the literature data range is from 0.001 to 0.005. For the NEXTGEN risk assessment an extended uniform distribution, truncated at 0 was derived with 0.001 and 0.009 as minimum and maximum, respectively. Biodegradation and volatilization rate were set to 0.

Figure 90 shows the final distribution of the logarithmic K_d, BCF and atmospheric deposition. For the pH dependent K_d value the soil properties as described in the chapter about environmental data was used. The lead concentration in soil was set to the soil PNEC. Thus, the variability of sorption originates solely from the soil pH. The mean logarithmic sorption coefficient of 4.4 is high compared to other metals. The BCF maximum lies around 0.014 which is the lowest of all considered metals. whereas the atmospheric deposition distribution is relatively broad. While the median value is 13 g per hectare and year, the 3rd quantile is significantly higher being 24 g per hectare and year. The data on atmospheric deposition was gathered between 2005 and 2015 at 255 different sites in Germany.

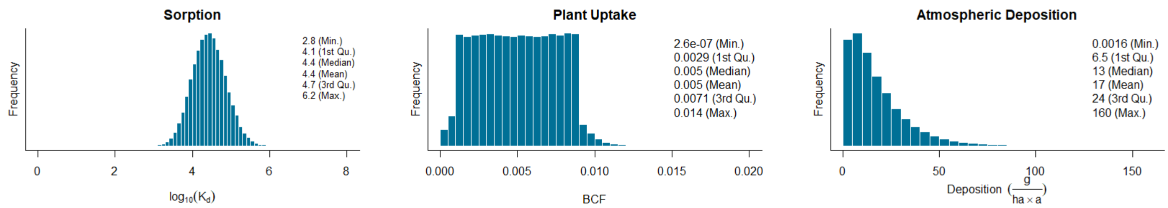

Figure 90: Distribution of sorption coefficient, bioconcentration factor and atmospheric deposition used to predict the environmental lead concentration.

Zinc

The European Chemical Agency has derived PNEC for zinc from sensitivity distributions of 14.4 µg/L and 83.1 mg/kg for freshwater and soil ecosystems, respectively (ECHA, 2022h).

The sorption of zinc is described by Sauvé et al. (2000) as a logarithmic correlation between the dissolved concentration, the pH value, the organic matter content and the total zinc concentration in soil. Since the NEXTGEN model needs the organic carbon content as input parameter, organic matter must be divided by 1.72 (IHCP, 2003b).

Equation 18 $\log_{10} c_{diss} = -0.55\,pH + 0.94 \log_{10} c_t - 0.34\,\log_{10} f_{oc} + 3.68 - \log_{10} 1.72$

f_{oc}: Organic carbon content in %
c_{diss}: Cadmium concentration in porewater in mg/L
c_t: Cadmium content in soil in mg/kg

As for most metals of this study, zinc plant uptake was estimated by data from Kühnen and Goldbach (2004). A linear regression between the logarithmic zinc concentration in soil and the logarithmic BCF could be derived by the measured data. The adjusted R^2 of the regression is 0.69, and is therefore lower as for nickel. However, the range of soils zinc content in this study was from 19.1 to 77.3 mg/kg which covers most of typical zinc contents

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in soil. Remaining uncertainties are taken account for by the standard errors of the coefficients.

Equation 19 $$\log_{10} BCF = -0.749 \ \log_{10} c_t + 0.985$$

BCF: Bioconcentration factor from soil to plant of Nickel
c_t: Nickel concentration in soil in mg/kg

Since zinc is a micro nutrient, plants are dependent on sufficient zinc uptake. Thus, in soils with low zinc content the BCF can easily exceed a value of 1.

Figure 91 shows the distribution of the log K_d, BCF and the atmospheric deposition used for exposure modelling. For the K_d regression soil properties were as described in the chapter about environmental data, while for the plant uptake the zinc content in soil is the only input variable. The zinc content was set to the PNEC for soil ecosystems, so the distribution shows the uncertainty coming from the standard errors of the regression coefficients. Similar to the BCF of copper, zinc BCFs are quite high ranging from 0.17 to 0.72 within inner 50% quantile. Data on atmospheric deposition was gathered between 2000 and 2015 at 183 different sites in Germany, including urban and rural areas. There is a zinc deposition of more than 50 g per hectare and year for 95 % of all cases. In average 170 g deposit on one hectare per year.

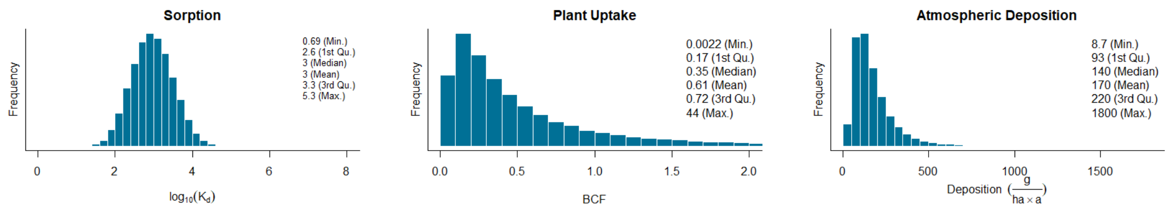

Figure 91: Distribution of sorption coefficient, bioconcentration factor and atmospheric deposition used to predict the environmental zinc concentration.

Benzo(a)pyrene

Amaringo et al. (2022) found that marine organisms are most sensitive towards Benzo(a)pyrene. The PNEC calculated by Amaringo et al. (2022) based on a sensitive species distribution is 0.029 µg/L which is in accordance with the European average EQS for surface waters other than inland surface waters of 0.027 µg/L (Directive: 2008/105/EC). The smaller value was used as PNEC as conservative assumption for groundwater feeding surface waters. For the assessment of the soil ecosystem a European risk assessment report on coal tar pitches derived a PNEC of 0.053 mg/kg, using an assessment factor of 10 (IHCP, 2008).

The sorption of Benzo(a)pyrene was investigated by Tebaay et al. (1993) in cambisols and luvisols. They found log - K_{oc} values between 5.3 and 6.28 while Mackay (1992) reported a value of 5.65. Based on partitioning coefficient between octanol and water a log K_{oc} could also be calculated according to Equation 20 (IHCP, 2003b).

Equation 20 $$\log_{10} K_{OC} = 0.81 \ \log_{10} K_{OW} + 0.1$$

K_{OC}: Partitioning coefficient between organic carbon and water in L/kg
K_{OW}: Partitioning coefficient between octanol and water in L/L

For a log - K_{OW} of 6.13 (Physprop database) the corresponding log - K_{oc} is 5.06. Depending on the sorption of Benzo(a)pyrene, very different biological half-lives can appear in soil. Wild et

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al. (1993) found half-lives from 120 to 270 days which is in the same range as Olesczcuk (2003) described for contaminated polish soils. In field experiments of sewage sludge amanded agricultural soils Wild et al. (1991) found, however, half-lifes up to almost 3000 days. Sushkova et al. (2018) found half-lifes in between 1.4 and 5.4 years, depending on the amount of contamination. The BCF was determined in a German study of Benzo(a)pyrene uptake in wheat grain, ranging from 2E-05 to 1E-04 (Delschen et al., 1996). Compared to other parts of the plant, PAHs are less concentrated in grains. However, Sushkova et al. (2018) also identified a rather high accumulation potential for Benzo(a)pyrene in barley. In spiked field trials they found accumulation factors up to 0.025. All three substance characteristics K_{OC}, Half-life and BCF were described with extended logarithmic uniform distributions for the exposure assessment, using ranges from 5 to 6.5, from 120 to 3000 and from 2E-05 to 0.025, respectively.

Figure 92 shows the distributions for sorption, plant uptake, atmospheric deposition, biological degradation and volatilization that were assumed for benzo(a)pyrene. For obtaining the log K_d value, the organic carbon content as described in the chapter about the environmental data was used. 50% of all K_d values are within the logarithmic range from 3.6 to 4.4. 95% of all BCF are below 0.02, while the median in remarkably lower, indicating a low plant uptake. The deposition data comes from 29 sites in the centre of Germany (Maneke-Fiegenbaum and Berger, 2019). While the majority of the distribution for biological half-life is below 1000 days, extreme values above 10 000 days are also part of the exposure assessment, considering worst-case circumstances for biodegradation. The volatilization rate is based on an experimental Henry constant of 0.0463 (Pa m³)/mol (Hulscher et al., 1992) at 25°C. However, the soil temperature is assumed to be only 10 °C resulting in a decreased Henry constant of only 0.022 (Pa m³)/mol.

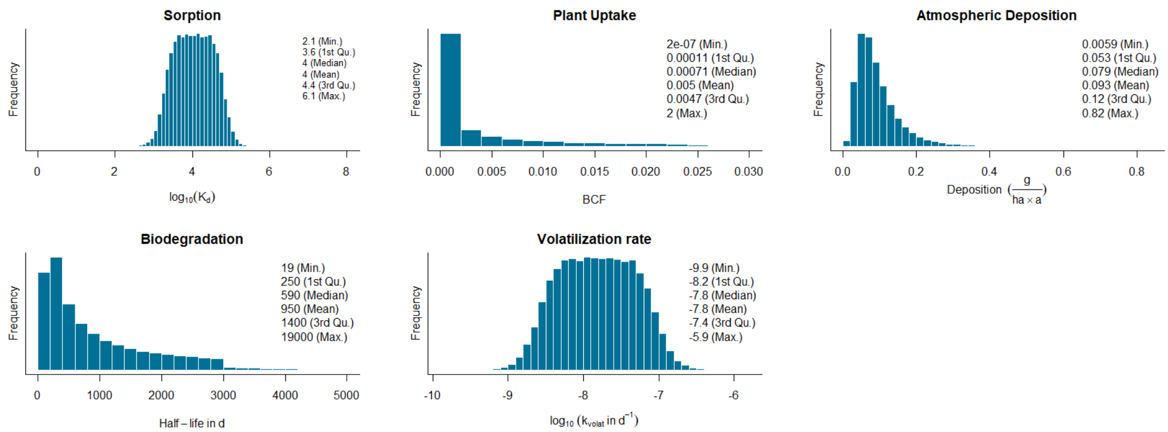

Figure 92: Distributions of sorption coefficient, bioconcentration factor, atmospheric deposition, biodegradation and volatilization rate used to predict the environmental benzo(a)pyrene concentration.

PCDD/F + dl-PCB

Since dioxins, furanes and dioxin-like PCB are part of a very heterogeneous group of chemicals it is complicated to find general substance characteristics. For the toxicity of the group, each substance is assigned a toxicity equivalency factor (TEQ) proposed by the World Health Organization (WHO). This factor is used to get a toxicity equivalent substance concentration. Finally, the weighted concentrations of all substances are summed up to obtain one WHO-TEQ concentration. In 2015, a risk assessment was conducted within the EU funded P-Rex Project and published in a Deliverable report (Kraus and Seis, 2015). The

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calculated PNECs for topsoil and leachate water being 20 ng WHO-TEQ/kg and 54 ng WHO-TEQ /L, respectively, are used in the NEXTGEN risk assessment.

The distribution of sorption coefficients is based on a German study about the exposition of PCDD and PCB (including dl-PCB) (Hennecke et al., 2011). They found log-10 organic carbon to water partition coefficients (K_{OC}) for PCDD/F between 5.58 and 9.04. The large group of dl-PCB have a comparable octanol to water partitioning as PCDD/F and thus similiar K_{OC} values were assumed. For the derivation of sorption coefficients in Figure 93 the organic carbon content as described in the chapter "Environmnetal Data" was used for.

The study of Hennecke et al. (2011) was also used to derive a distribution of Henry coefficients, ranging between 2.57 and 3.29 Pa*m³/mol. The high sorption indicates that soil acts as a sink for dioxins and dioxin-like PCB and hence the soil ecosystem is especially exposed. For the concentration the pathway air to plant is more important than soil to plant (Meneses et al., 2002); (Hennecke et al., 2011). While Harrad and Smith (1997) used root uptake factors below 0.01 for all PCDD/Fs for estimating foodstuff concentrations, Akkan et al. (2004) found factors up to 0.2 when including dl-PCB. For the NEXTGEN risk assessment 0.0001 and 0.2 were used as minimum and maximum of an extended logarithmic uniform distribution. The half-life of the chlorinated compounds lies between 6 months and tens of years according to Rychen et al. (2008). Besides soil properties, the ratio of chlorination is the main factor influencing the half-life. Thus, a very broad and logarithmic scaled extended uniform distribution between 180 and 30 000 days was assumed. The upper limit is a suggestion by the technical guidance Document on risk assessment for inherently biodegradable substances (IHCP, 2003a).

The median of the initially assumed atmospheric deposition is 32 ng per hectare and year and originates from a sample program in western Germany between 2004 and 2016 (LANUV, 2017). The maximum of this distribution was below 1 µg per hectare and year. However, Dufour et al. (2021) found median atmospheric deposition levels of about 23 µg per hectare and year in the vicinity (< 1000 m) of shredding facilities. To include potential highly contaminated sites the standard deviation of the predefined logarithmic normal distribution was increased. The final distribution is shown in Figure 93. While the median value did not change, the maximum atmospheric deposition of the updated distribution increased to 13 µg per hectare and year.

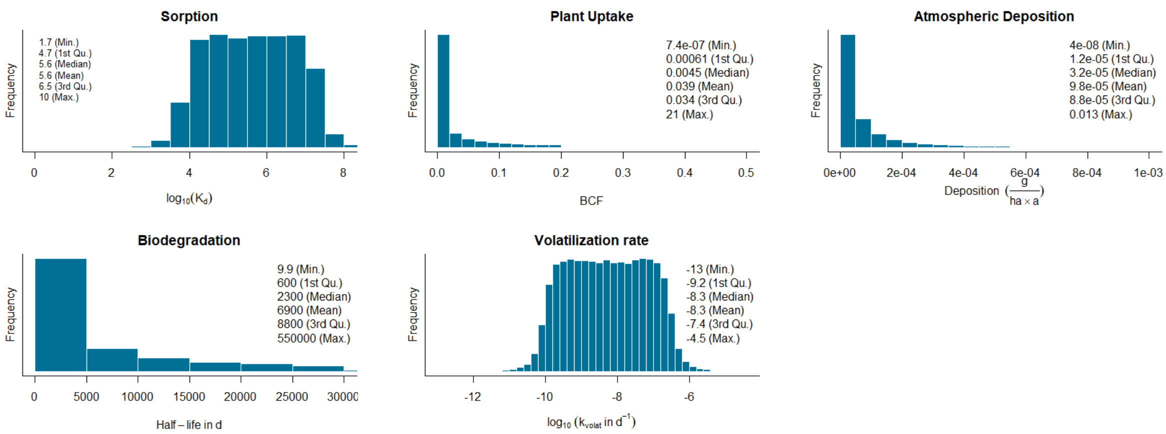

Figure 93: Distributions of sorption coefficient, bioconcentration factor, atmospheric deposition, biodegradation and volatilization rate used to predict the environmental PCDD/Fs + dl-PCBs concentration.

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PFOS and PFOA

The PFAS substance group is very heterogenous and consists of several thousands of substances. They have in common a very high resistance and, thus, are also called "everlasting chemicals".

PFOS and PFOA are chosen for the risk assessment since they are the most studied PFAS. However, even for PFOS and PFOA the environmental behaviour in soil is only at the beginning of understanding with highly contaminated sites described best. Thus, some estimated substance properties have a large range between minimum and maximum and an extended log uniform distribution was chosen to describe them. In order to account for potential different behaviour at highly contaminated sites compared to sites with lowers PFAS content, minimum and maximum values found in literature were shifted one log unit lower and higher, respectively. This was done for the biological half-life and the bioconcentration factor.

Hubert (2021) found a log-K_d dependency on the grain size fraction for PFOS, ranging from 0.2 for a sandy fraction up to 1.2 for a silty fraction. The sorption to organic fibre was significantly higher and increased even more if the fibre contained air. Besides the sorption to organic matter he suspected the air-water interphase to have a major impact. The log-K_d value for air containing organic fibres was higher than 3. This corresponds well with a literature review by Zareitalabad et al.(2013) who found an average log K_{OC} value of 3 with a standard deviation of 0.7. Furthermore, they described an average log K_{OC} value of PFOA which is slightly lower, beeing 2.8 with a standard deviation of 0.9. Higgins and Luthy (2006) also described organic carbon to be the most important impact on PFOS sorption. Thus, K_{OC} values were used to describe the sorption of both PFAS in the soil matrix to include the variability due to organic carbon content in the risk assessment.

The TGD suggests a biological half-life of 3 000 days and 30 000 days for inherently biodegradable substances with K_d values exceeding 2 and 3, respectively. Since PFAS are described to be practically everlasting 3 000 days was used as the minimum of an extended uniform distribution truncated at 0 for both, PFOS and PFOA. The maximum was set one log unit higher to 300 000 days (more than 800 years). It was decided not to use a logarithmic distribution since very long half-lives > 30 000 days are more likely, which can be expressed better by a regular uniform distribution.

The Henry constants were taken from the CompTox Chemicals Dashboard from the EPA. For both PFOA and PFOS there were no experimental data available. The predicted mean values beeing 1.82E-06 Pa*m/mol and 1.95E-05 Pa*m/mol for PFOS and PFOA, respectively, were used as center value between minimum and maximum, each in 1 magnitude distance. An extended logarithmic uniform distribution was thus built between 1.82E-07 Pa*m/mol 1.82E-05 Pa*m/mol for PFOS and between 1.95E-06 Pa*m/mol and 1.95E-04 Pa*m/mol for PFOA.

Stahl et al. (2009) studied the plant uptake of PFOS and PFOA by wheat, potato, corn and oat plants. For the pot trials, they used spiked soil with PFAS concentration ranging from 0.25 mg/kg to 50 mg/kg. Only those results obtained by pot trials with PFAS soil concentrations up to 1 mg/kg were used for the derivation of BCF. The highest BCF were found for straw of wheat beeing 0.27 and 3.2 for PFOA and PFOS, respecitvely. The lowest concentration in plants were below the limit of detection. Using the limit of detection (1 µg/kg DM) this reveals a BCF of 0.001 for a soil concentration of 1 mg/kg. Based on these

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findings an extended logarithmic uniform distribution was derived with a minimum value of 0.0001 and maximum values of 2.7 and 32, for PFOA and PFOS, respectively.

The worldwide variation of PFOA wet deposition was estimated by Thackray et al., (2020), and compared to observed deposition data. They found that especially for long chain PFAS like PFOA the distance to the source has a major impact on the yearly deposition. The estimated PFOA deposition varies between 20 and 2000 ng per square meter and year. In a study close to Hamburg, Germany, Dreyer et al. (2010) predicted a yearly PFOA deposition rate of 1000 ng/m² based on 20 precipitation samples. Lindim et al. (2016) gathered atmospheric deposition data for PFOA and PFOS to compare the atmospheric deposition to European seas to emissions from via rivers from catchments. For PFOA the assumed yearly atmospheric deposition was around 2900 ng/m² while it was only 750 ng/m² for PFOS. To include all PFOA deposition rates, an extended logarithmic uniform distribution between 20 and 3000 ng/(m²a) was used. Since PFOS deposition is lower, the minimum and maximum values for PFOS were obtained by multiplying the PFOA limits by 750 / 2900. This leads to a range between 5 and 775 ng/(m²a).

The extremely low degradability of PFOS and PFOA causes a high risk of accumulation in ecological compartments and along the food chain. The Heads of EPAs Australia and New Zealand (HEPA) developed a "PFAS National Environmental Management Plan" in 2020 (HEPA, 2020). This plan contains amongst others guideline values of PFOS and PFOA for soil and freshwater ecosystems. Especially PFOS tends to accumulate in tissues, therefore, the strict guideline value of 0.01 mg/kg soil is due to indirect exposure (secondary consumers). It is relevant under the assumption of large-scale fertilization. For PFOA direct exposure is more important leading to a significantly higher guideline value of 10 mg/kg soil. For the $PNEC_{groundwater}$, the HEPA guideline values for freshwater were used at which 99% of the species are protected. Those are 0.23 ng/L and 0.19 µg/L for PFOS and PFOA, respectively (HEPA, 2020). The value for PFOS is below the annual average Environmental Quality Standard (EQS) of the European EQS Direcative 2013/39/EU and was chosen for conservative reasons. In Germany a value of 0.1 µg/L as insignificant threshold for PFOA in groundwater (BMUV, 2022). This value is, however, based on human toxicological data. Therefore, the ecologically derived HEPA value was used.

Figure 94 shows the final distributions of several PFOS and PFOA characteristics relevant for the exposure model in soil. For PFOA the range of sorption coefficients is a little larger, the plant uptake the atmospheric deposition and the volatilization rate are higher.

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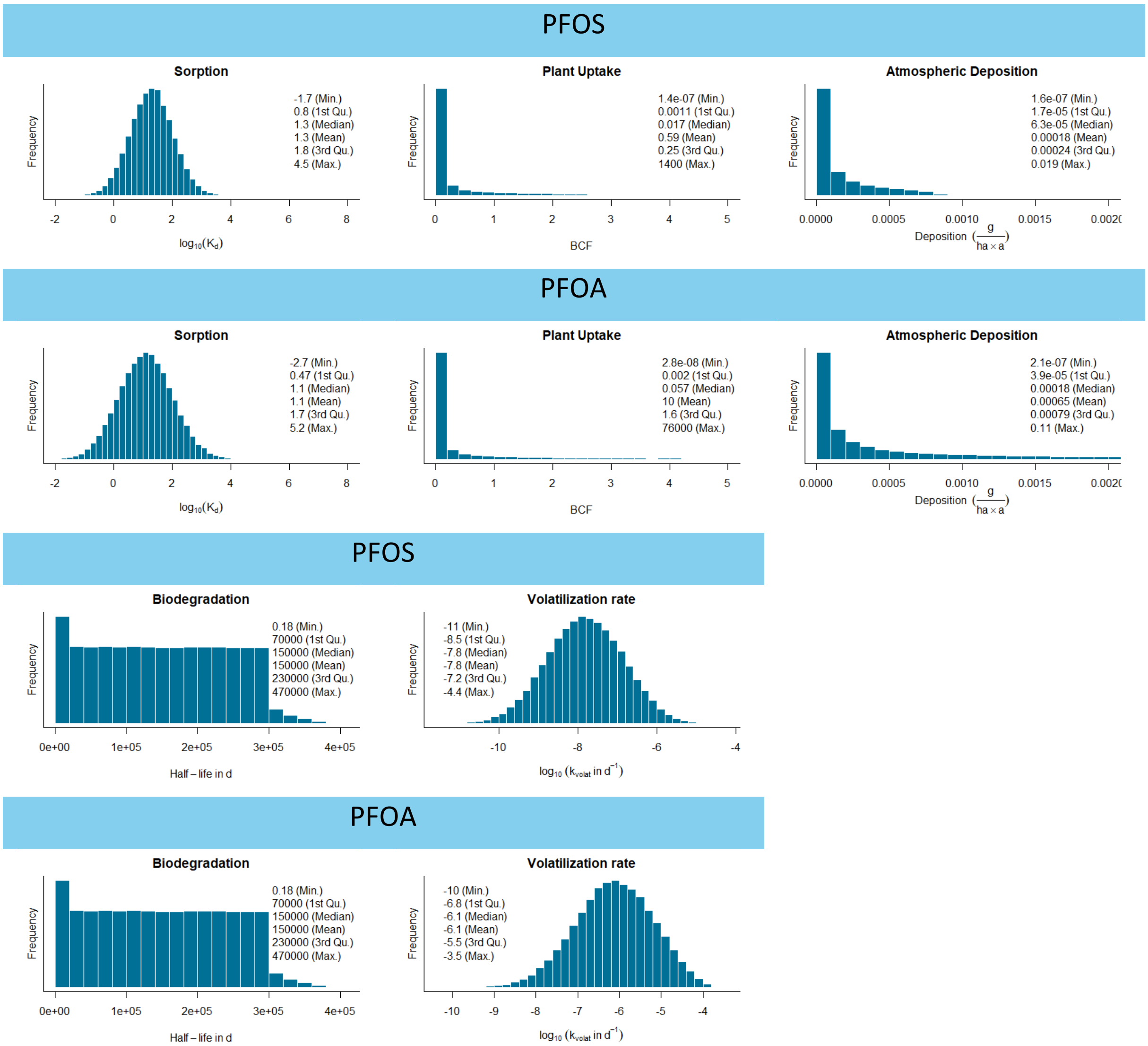

Figure 94: Distributions of sorption coefficient, bioconcentration factor, atmospheric deposition, biodegredation and volatilization rate used to predict the environmental PFOS and PFOA concentrations.

Fertilizer Data (recovered nutrient products)

Both, nitrogen and phosphorous fertilizers are produced within the NEXTGEN project. Besides information about the pollutant content in fertilizer, the yearly fertilizer amount applied is crucial for the assessment. For P-fertilizer this was defined to range from 30 to 60 kg P_2O_5/ha, while for N-fertilizers the yearly application was assumed to be between 100 and 200 kg N/ha. The amount of fertilization depends on the type of crops and environmental conditions. It is therefore understood to be spatially variable and is treated as such in the exposure model. Instead of using a probability distribution for the pollutant content in the fertilizer the mean value was used. This was done for two reasons. First, outliers will even out over a long period of time, and secondly, fertilizers are stored in large batches and mixed before further processing or application.

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However, depending on the number of measurements, the estimation of the mean pollutant concentration can be very uncertain. To account for this, the risk assessment was conducted with 3 different scenarios per pollutant:

1. "Most likely"-Scenario: The actual mean value of all analysed fertilizer samples
2. "10% Probability"-Scenario: The 90^{th} quantile of a normal distribution described by mean value of all measurements and the standard error of the mean.
3. "1% Probability"-Scenario: The 99^{th} quantile of a normal distribution described by mean value of all measurements and the standard error of the mean.

The scenarios are illustrated by an example of three measurements: 2.8, 2.9 and 3.3 mg/kg. The mean value of the measurements is 3 mg/kg. This is most likely the average concentration of to which the environment is exposed. However, the true average concentration could be higher, and the 3 measurements were not sufficient to detect this. Therefore, a standard error of the mean, defined as the standard deviation divided by the square root of the number of measurements, is calculated. In the above case, the standard error is 0.15 mg/kg. The 90^{th} quantile of a normal distribution with mean and standard error is 3.19 mg/kg. Similarly, the 99^{th} quantile is calculated. The concentrations of the scenarios are 1) most likely 3 mg/kg, 2) 10% probability 3.19 mg/kg and 3) 1% probability 3.35 mg/kg.

Braunschweig – Struvite and Ammonia Sulfate Solution

At the wastewater treatment plant of Braunschweig two fertilizers are produced from the centrate of the sewage sludge dewatering (see LCA chapter). Struvite is precipitated by addition of $MgCl_2$ and serves as a phosphorus fertilizer. The remaining process water is stripped to obtain ammonia sulphate solution (ASS) for nitrogen fertilization. The average P_2O_5 content of the struvite is 262 g/kg, leading to a calculated yearly fertilizer application of 115 to 230 kg struvite per ha. The nitrogen concentration in ASS is 104 g/L or 84 g/kg, using a density of 1.25 kg/L. Therefore, 1190 to 2380 kg ASS (1.5 to 3 m³) can be applied per year and ha.

The heavy metal content was analysed in 4 and 9 samples (only 4 and 6 for mercury) in struvite and ASS, respectively. Mean values and standard error were used to define the three scenarios "Most likely", "10% Probability" and "1% Probability" (Table 50). A concentration below the limit of quantification (LOQ) was halved. If all measurements were below the LOQ, the standard error was set to 50% of half of the LOQ.

For the organic pollutants only one sample was available in struvite. It was decided to use 50% of the measured values as standard error to define the scenarios. For PFOS and PFOA only the "Most-likely" scenario was simulated.

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Table 50: Pollutant content in struvite and ASS for 3 scenarios: most likely (mean value), 10% probability (90th quantile) and 1% probability (99th quantile).

	Struvite			ASS		
Pollutant (in mg/kg DM)	Most likely	10% probability	1% probability	Most likely	10% probability	1% probability
Arsenic	0.5*	0.66	0.79	0.032*	0.039	0.044
Cadmium	0.05*	0.066	0.079	0.0047	0.0055	0.0062
Chromium (4)	3.1	3.4	3.7	0.043	0.044	0.045
Copper	1.4	1.5	1.6	3.1	4.1	5
Lead	0.25*	0.33	0.4	0.2	0.28	0.34
Mercury	0.1*	0.13	0.16	0.0018	0.002	0.0021
Nickel	0.59	0.63	0.67	0.046	0.052	0.057
Zinc	3.1	4	4.7	2.5	3.1	3.6
Benzo(a)pyrene	0.025*	0.041	0.054	-	-	-
PCDD/F + dl-PCB	2.4E-06	3.9E-06	5.2E-06	-	-	-
PFOS	0.005*					
PFOA	0.005*					

* All values below LOQ

Athens – Compost

In Athens raw sewage is exploited by a sewer mining unit to collect a carbon and nutrient-rich compost. After digestion in an anaerobic MBR the sludge is mixed with pruning waste and composted. The final product is used for horticultural purposes in a nearby tree nursery. Thus, the applied amount differs from agricultural fertilization and is limited by the fertilizer production. A production of 150 kg per week is targeted. If the entire fertilizer is applied at the tree nursery which is about 1 ha of size, this will result in a yearly fertilizer supply of 7 800 kg/ha. However, currently the production capacity is about 100 kg compost per week. In the future, some of the compost may be further distributed to urban parks. For the risk assessment an application range between 50 and 150 kg/week and ha (2600 and 7800 kg/year) was assumed. The range is used as minimum and maximum value for a uniform distribution.

The heavy metal concentrations given in Table 51 originate from only one sample of the final compost. It cannot be concluded that this is the actual mean value. To include this high uncertainty, a standard deviation of 50% of the mean was assumed for definition of the additional scenarios.

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Table 51: Pollutant content in compost for 3 scenarios: most likely (mean value), 10% probability (90th quantile) and 1% probability (99th quantile)

Pollutant (in mg/kg DM)	Most likely	10% probability	1% probability
Cadmium	2.6	4.3	5.6
Chromium	12	20	26
Copper	27	44	58
Lead	22	36	48
Mercury	0.2	0.33	0.43
Nickel	8.6	14	19
Zinc	108	180	230

Spernal - Hydroxyapatite

In Spernal hydroxyapatite is produced as P-Fertilizer from the effluent of an anaerobic microbial batch reactor. As process steps ion exchange, filtration and precipitation are involved, leading to a very clean product.

The process was not fully operating at the time the report was written, that is why data from previous projects were used for the pollutant content. All substances were measured below limit of detection. For the “Most likely” scenario the LOQs were halved. The use of data from previous studies increases, however, the uncertainty. This was considered by defining a standard error that equals the LOQ. The P_2O_5 content is targeted to be 35%, which would result in a yearly fertilizer application of 85 to 170 kg/ha.

Table 52: Pollutant content in hydroxyapatite for 3 scenarios: most likely (mean value), 10% probability (90th quantile) and 1% probability (99th quantile)

Pollutant (in mg/kg DM)	Most likely	10% probability	1% probability
Arsenic	0.002	0.0071	0.011
Cadmium	0.00012	0.00085	0.0014
Chromium	0.004	0.029	0.045
Copper	0.00018	0.0013	0.002
Lead	0.0012	0.0085	0.014
Mercury	0.02	0.14	0.23
Nickel	0.00006	0.00043	0.00068
Zinc	0.00036	0.0026	0.0041
Benzo(a)pyrene	0.0002	0.0014	0.0023

Dewatered Sewage Sludge

In order to compare the results with known secondary fertilizers, the application of dewatered sewage sludge was additionally simulated. The dewatered sewage sludge is described in a German study about the environmental impact of primary and secondary P-

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fertilizers. The sludge composition is based on 150 and 197 samples for heavy metals (except for mercury: 7) and organic pollutants (benzo(a)pyrene and PCDD/F + dl-PCB), respectively. The average phosphorus content was 8.14%, which results in a yearly fertilizer application of 368 to 737 kg/ha.

Table 53: Pollutant content in sewage sludge for 3 scenarios: most likely (mean value), 10% probability (90th quantile) and 1% probability (99th quantile)

Pollutant (in mg/kg DM)	Most likely	10% probability	1% probability
Arsenic	7.2	8.1	8.8
Cadmium	0.94	1	1.1
Chromium	85	92	98
Copper	380	400	410
Lead	53	56	58
Mercury	0.86	1.2	1.4
Nickel	29	30	32
Zinc	1100	1100	1200
Benzo(a)pyrene	0.18	0.21	0.22
PCDD/F + dl-PCB	1.9E-05	2.2E-05	2.3E-05

Results

The results of the risk assessment are shown and discussed separately for ecosystems, soil and groundwater. Compost from Athens was assessed only in regard to soil, as its localized application in an urban area is not expected to have a major impact on groundwater. In this chapter results, interpreted by the risk matrix are shown (Figure 81), more detailed tables are shown in the supplementary information.

For the interpretation of results, it must be taken into account, that the simulation was running over 100 years and started with a contaminated soil. An unacceptable risk after such a long period of time, with such conservative initial conditions, usually does not mean the sudden occurrence of a severe situation. Rather, an unacceptable risk is intended to draw the attention to the corresponding substance. Therefore, a spearman correlation to every model input variable is performed for each pollutant in a fertilizer leading to an unacceptable risk. In this way, actual local conditions can be matched with risk-promoting circumstances. Furthermore, if an unacceptable risk is identified environmental monitoring can be considered to exclude significant increasing pollutant concentration in soil.

The conclusions drawn and measures taken are part of a subsequent risk management process. The results presented here can serve as a basis for this.

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Risk assessment for the soil ecosystem

For struvite, ASS and hydroxyapatite no critical risk was found. Except for mercury all increases of the RQ caused by fertilization were either below 0.01, or below 0.1 in combination with a maximum total RQ below 2.

Table 54: Risk assessment for the soil ecosystem (blue: negligible risk, green: acceptable risk, orange: risk of increasing concern, red: unacceptable risk; Scenario 1: most likely, Scenario 2: 10% probability, Scenario 3: 1% probability)

Pollutant	Sewage sludge			Struvite (Braunschweig)			ASS (Braunschweig)			Compost (Athens)			Hydroxy-apatite (Spernal)		
Scenario	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3
Arsenic															
Cadmium															
Chromium															
Copper															
Lead															
Mercury															
Nickel															
Zinc															
Benzo(a)pyrene															
PCDD/F + dl-PCB															

For mercury, a concerning situation was identified for long-term fertilization with sewage sludge. Although the mercury concentration is low in sewage sludge it leads to significant increase of the PEC after 100 years. This is caused by the very low PNEC of mercury in soil, which has been significantly lowered recently to account for a possible transformation into more toxic organometallic forms (ECHA, 2022f). Despite this low PNEC, which is assigned a high assessment factor of 50, the application of NEXTGEN fertilizers Struvite, ASS and Hydroxyapatite does not lead to any increase in risk of concern. In the compost from Athens, however, a negative impact after long-term application cannot be excluded in general. The average increase of RQ caused by fertilization is 1.3 and RQ_{max} is 3.7. It was therefore checked, which input variables are most relevant for the exposure assessment. The fertilizer application is most strongly correlated to the amount of increase followed by atmospheric deposition, while the water balance seems to play a minor role for the mercury content in soil.

Table 55: Correlation (spearman) between mercury in soil after compost application and model input variables

Variable	Correlation	Sign
Fertilizer application	0.82	+
Atmospheric deposition	0.42	+
Sorption coefficient	0.18	+
Rain	0.03	-

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It was not possible to find surrounding conditions under which the risk posed by mercury is negligible. This is partly caused by the lack of relation between soil properties and substance behaviour. However, if the yearly fertilizer application was below 4000 kg/ha, the mean RQ increase caused by fertilization would most likely be below 1 (Figure 95). This corresponds to a maximum weekly fertilization of about 75 kg/ha. Nevertheless, it is recommended to either try to reduce the mercury content of the fertilizer, to apply less fertilizer or monitor the soil of the tree nursery on a regular basis. These recommendations are based on the highly uncertain toxic effect of mercury in soil and can be adapted, if new toxicological studies are available.

In addition, the cadmium input leads to a concerning situation for the 1% probability scenario of compost fertilization. Since only one compost sample was available, a large probability distribution was assumed to account for a high uncertainty of the cadmium content. That causes a cadmium content more that is more than twice as high as in the "Most-likely" scenario. Further measurements can help to obtain certainty about the concentration range of cadmium in the compost and reduce the risk.

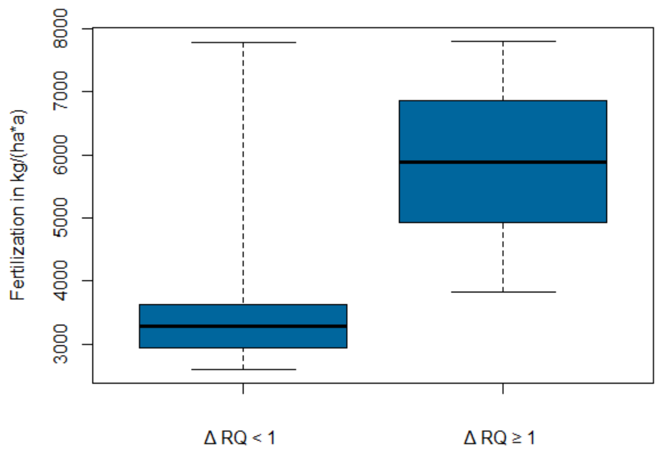

Figure 95: Impact of the fertilizer (mean increase of RQ caused by fertilization) depending on the yearly fertilizer application

Risk assessment for the groundwater ecosystem

The risk assessment of sewage sludge shows how sensitive this approach is. Even though all pollutants are within the allowed range according to the German Fertilizer Ordnincane a long-term fertilization might lead to a relevant increase of risk in the groundwater ecosystem under specific circumstances. This is not the case for the NEXTGEN fertilizers. For all fertilizers and pollutants ΔRQ is below 0.1 and RQ_{max} is below 2. The only exception is an "acceptable risk" for ASS application. In this scenario ΔRQ is only 0.025 and RQ_{max} is 3.9. Despite this result, the cause of risk posed by zinc was checked in detail, since zinc is also micro nutrient. The comparison between soil and groundwater risk assessments suggests that increased risk to groundwater can be easily missed from a soil ecology perspective.

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Table 56: Risk assessment for the groundwater ecosystem (blue: negligible risk, green: acceptable risk, orange: risk of increasing concern, red: unacceptable risk; Scenario 1: most likely, Scenario 2: 10% probability, Scenario 3: 1% probability)

Pollutant	Sewage sludge (Braunschweig)			Struvite (Braunschweig)			ASS (Braunschweig)			Hydroxy-apatite (Spernal)		
Scenario	1	2	3	1	2	3	1	2	3	1	2	3
Arsenic												
Cadmium												
Chromium												
Copper												
Lead												
Mercury												
Nickel												
Zinc												
Benzo(a)pyrene												
PCDD/F + dl-PCB												

The sorption coefficient was most important for the PEC after 100 years in soil. It is described as a function of pH, the organic carbon content and the zinc content in soil, wherein the pH is the most affecting variable. A clear relation could be found between the RQ_{max} and the pH value in soil. Figure 96 shows the RQ_{max} if the pH was equal or higher than the defined value in the x-axis. In case of zinc input via ASS, a minimum ph of 6.34 would lead to a RQ_{max} of 2 and thus to a classification as negligible risk.

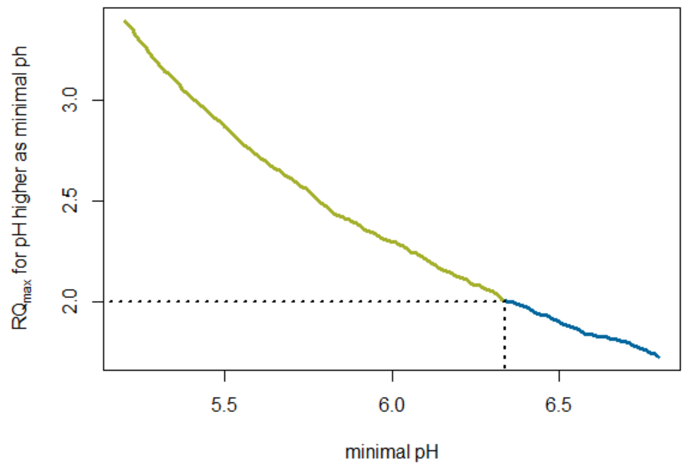

Figure 96: RQ_{max} dependency on pH value

Risk assessment for PFAS in struvite

The objective of the PFAS risk assessment is to understand to what extent even low concentrations in fertilizer can lead to an increased environmental risk. The result can be considered independently of the struvite produced in Braunschweig. PFAS concentrations in struvite were below the limit of detection. Half of the limit was used for modelling the exposure of soil and groundwater ecosystems. For PFOA this results in a negligible risk

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caused by fertilization. This is not the case for PFOS considering the groundwater ecosystem. The mean RQ increase caused by fertilization is 1.74 even though input via fertilization is very low. This is due to the ratio of pollutant input to PNEC. It is estimated that both pollutants are equally concentrated in struvite (5 µg/kg) while the PNECs differ by several orders of magnitude between 0.19 µg/L for PFOA and 0.23 ng/L for PFOS. From this ratio the amount of fertilizer can be calculated that contaminates one litre of clean water. Up to 38 g of struvite would not result in a PFOA concentration that exceeds the PNEC for freshwater. For PFOS, the tolerable amount of struvite drops to 0.046 g per litre of. This difference is responsible for the deviating course of the risk quotients between PFOA and PFOS if fertilizer is applied (Figure 97). While for both PFAS, atmospheric deposition alone does not pose a high risk to soil or groundwater, the addition of fertilizer has a deviating impact. For PFOS, the RQ increases significantly, whereas the increase for PFOA is negligible and cannot be recognized in the graph. To reduce the risk for groundwater posed by PFOS from fertilizers either more toxicological data need to be collected to derive a less conservative PNEC or the detection limit needs to be lowered to better characterize the contaminant input to the ecosystem. In addition, a high number of samples may reinforce the assumption that the concentration is well below the detection limit. This could allow a lower value to be used for the risk assessment.

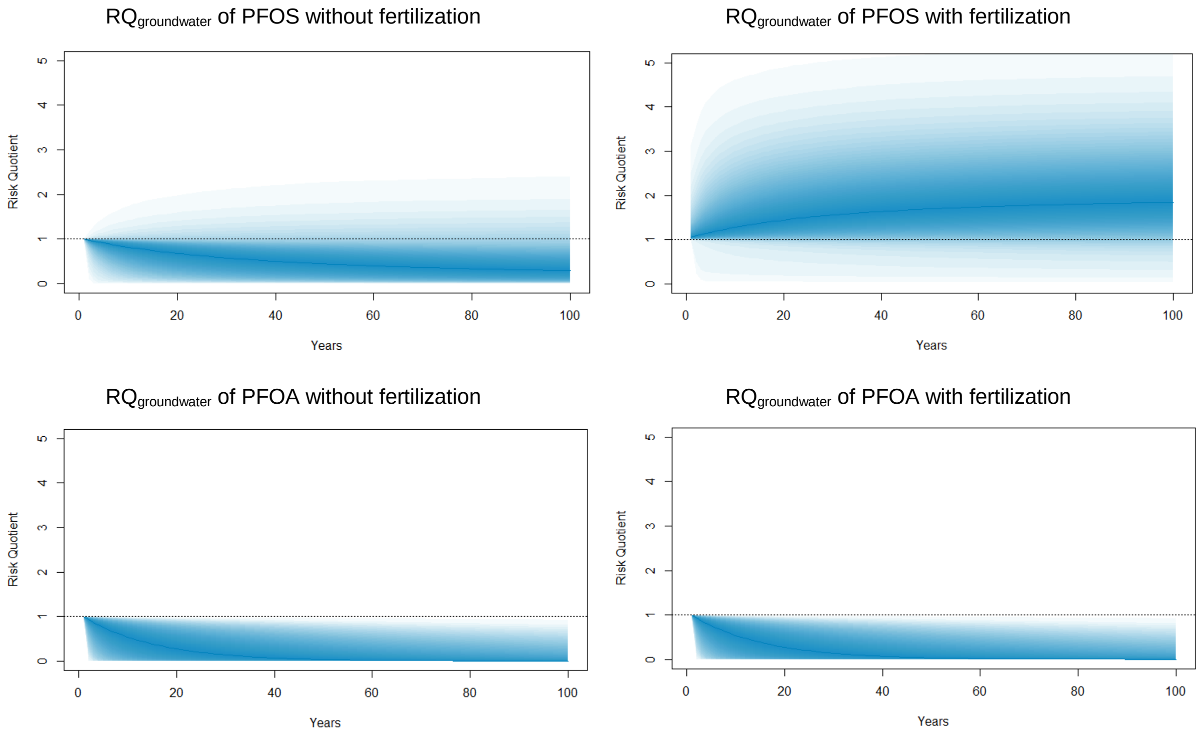

Figure 97: Course of $RQ_{groundwater}$ for PFOS and PFOA with and without fertilization

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Conclusions

In this study, the risk to soil and groundwater ecosystems due to long-term application of secondary fertilizer (struvite, ASS, hydroxyapatite, compost from sewer mining) was assessed. Hazards included were heavy metals (As, Cd, Cr, Co, Hg, Ni, Pb, Zn), PAH (Benzo(a)pyrene), dioxins (PCDD/F + dl-PCB) and PFAS (PFOS, PFOA).

The probabilistic approach of the exposure model allowed to consider spatial variability of the environment and uncertainty of substance properties. The defined initial concentration, which is equivalent to the PNEC, enables a normed procedure for risk interpretation. The risk was defined by i) the increase in risk due to fertilization to account for the fertilizer impact and ii) the highest 5% of all risk quotients to include possible severe situations based on the input assumptions. Both indicators were combined in a risk matrix to identify a high risk either due to a high input of pollutants to the environment or due to a lack of knowledge of the input data. The approach identifies critical situations and allows a more detailed examination to characterize the sources of risk

For ASS, struvite and hydroxyapatite, the results of risk assessment were as follows:

- No unacceptable or critical risk could be identified for the considered substances except for PFOS.
- In the model, a PFOS content of below the limit of detection (50% LOD) already leads to an unacceptable risk for the groundwater compartment. Therefore, a potential risk posed by PFOS cannot be fully excluded with the currently available analytical detection limit and also the current knowledge about its toxicity and environmental behavior.

For compost from sewer mining

- No high risk could be identified for the here considered substances except for mercury.
- It is recommended to reduce the mercury input as long as the on-mercury toxicity to soil ecosystems is uncertain.

Water ecosystems a more sensitive to zinc as soil ecosystems. To prevent leaching of zinc, the input to the soil should comply with the soil pH.

The risk assessment results are only a basis for futher considerations. Conclusions drawn and measures taken are part of a subsequent risk management process.

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Annex

LCA input data

Table 57: LCA datasets for background processes for all case studies (Ecoinvent, 2021)

Process	Dataset in ecoinvent v3.8	Remark
Case study: Altenrhein		
Electricity	market for electricity, medium voltage [CH]	
Electricity from PV	electricity production, photovoltaic, 570kWp open ground installation, multi-Si [DE]	PV modules at WWTP Altenrhein
Polymer	market for acrylonitrile [GLO]	0.75 kg acrylonitrile per kg polymer (active matter)
$FeSO_4$	market for iron sulfate [RER]	
Oxygen (liquid)	market for oxygen, liquid [RER]	For ozonation
GAC production and regeneration	KWB dataset	(DWA, 2016b)
Transport truck	transport, freight, lorry 16-32 metric ton, EURO5 [RER]	For transport of chemicals and materials
Co-incineration of dried sludge	electricity production, hard coal [IT]	Recalculated via LHV of hard coal (27 MJ/kg) and sludge (8 MJ/kg)
NaOH	market for sodium hydroxide, without water, in 50% solution state [GLO]	For stripping
H2SO4	market for sulfuric acid [RER]	For stripping
Citric acid	citric acid production [RER]	For stripping
KOH	potassium hydroxide production [RER]	For Pyrophos
$NaHCO_3$	market for sodium bicarbonate [GLO]	For Pyrophos
Activated carbon	activated carbon production, granular from hard coal [RER]	For Pyrophos
NH_4OH	market for ammonia, anhydrous, liquid [RER]	For Pyrophos
Natural gas	heat production, natural gas, at boiler atmospheric non-modulating <100kW [RoW]	For Pyrophos
District heating	market for heat, district or industrial, natural gas [Europe without Switzerland]	Credits for heat surplus
Mineral N fertilizer	nutrient supply from ammonium sulfate [RER]	Credits for ammonium sulfate from stripping
Mineral P fertilizer	market for inorganic phosphorus fertiliser, as P2O5 [CH]	

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Mineral K fertilizer	market for inorganic potassium fertiliser, as K2O [CH]	
Hard coal	market for hard coal briquettes [RoW]	Raw material for conventional GAC
Emission data for GAC production/regeneration	heat production, at hard coal industrial furnace 1-10MW [RoW]	Emission data for hard coal combustion
Steam	market for steam, in chemical industry [RoW]	Steam for GAC production
Electricity	market group for electricity, high voltage [CN]	For GAC production in Asia
Ship transport	market for transport, freight, sea, container ship [GLO]	For GAC transport
Natural gas	heat production, natural gas, at industrial furnace low-NOx >100kW [Europe without Switzerland]	For GAC regeneration
Case study: Braunschweig	Ecoinvent v3.6	
Electricity	market for electricity, medium voltage [DE]	Mix for Germany
Polyacrylamide	market for polyacrylamide [GLO]	
$FeCl_3$	market for iron(III) chloride, without water, in 14% iron solution state [GLO]	
$MgCl_2$	Residue from KCl production requires drying: market group for heat, district or industrial, natural gas [RER]	
NaOH	market for sodium hydroxide, without water, in 50% solution state [GLO]	
H_2SO_4	market for sulfuric acid [RER]	
Natural gas	market for natural gas, high pressure [DE]	
P Fertiliser	diammonium phosphate production [RER]	Allocation on P
N Fertiliser	diammonium phosphate production [RER]	Allocation on N as Ammonium
Case study: Tossa de Mar	Ecoinvent v3.6	
Electricity	market for electricity, medium voltage [ES]	Mix for Spain
polyacrylamide	market for polyacrylamide [GLO]	
Citric acid	market for citric acid [GLO]	As proxy for antiscalant
HCl	market for hydrochloric acid, without water, in 30% solution state [RER]	
$AlCl_3$	market for polyaluminium chloride [GLO]	
$NaHSO_3$	market for sodium hydrogen sulfite [GLO]	
NaOCl	market for sodium hypochlorite, without water, in 15% solution state [RER]	

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NH_4Cl	ammonium chloride production [GLO]	
NaOH	market for sodium hydroxide, without water, in 50% solution state [GLO]	
H_2SO_4	market for sulfuric acid [RER]	
H_2O_2 (50 %)	market for hydrogen peroxide, without water, in 50% solution state [RER]	
Tossa Wells	market for electricity, medium voltage [ES]; market for sodium hypochlorite, without water, in 15% solution state [RER]	Based on estimations (Kraus et al., 2016)
Tossa Lloret DWTP	market for electricity, medium voltage [ES]; market for chlorine, gaseous [RER]	Calculated based on (Serra, 2021)
Case study: LaTrappe		
Electricity	market for electricity, medium voltage [NL]	
Polymer	market for polyacrylamide [GLO]	For sludge dewatering and DAF
FeCl3	market for iron (III) chloride, without water, in 40% solution state [GLO]	For DAF
FeCl2	market for iron(II) chloride [GLO]	For sulphide binding in EGSB
NaOH	market for sodium hydroxide, without water, in 50% solution state [GLO]	For pH control and membrane
H2SO4	market for sulfuric acid [RER]	For pH control
Urea	market for urea [RER]	For nutrient dosing
Citric acid	market for citric acid [GLO]	For membrane cleaning
NaOCl	market for sodium hypochlorite, without water, in 15% solution state [RER]	For membrane cleaning
Concrete	market for concrete block [DE]	For infrastructure
Reinforcing steel	market for reinforcing steel [GLO]	For infrastructure
Stainless steel	market for steel, chromium steel 18/8 [GLO]	For infrastructure
Iron	market for cast iron [GLO]	For infrastructure
HDPE	market for polyethylene, high density, granulate, recycled [Europe without Switzerland]	For infrastructure
PP	market for polypropylene, granulate [GLO]	For infrastructure
PVC	market for polyvinylidenchloride, granulate [RER]	For infrastructure
GRP	market for glass fibre reinforced plastic, polyester resin, hand lay-up [GLO]	For infrastructure
Glass	market for flat glass, uncoated [RER]	For infrastructure
Sand-lime bricks	market for sand-lime brick [GLO]	For infrastructure

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Transport truck	transport, freight, lorry 16-32 metric ton, EURO5 [RER]	For transport of chemicals and materials
Mineral N fertilizer	market for inorganic nitrogen fertiliser, as N [NL]	For sludge credits
Mineral P fertilizer	market for inorganic phosphorus fertiliser, as P2O5 [NL]	For nutrient dosing and sludge credits
Heat	heat production, natural gas, at industrial furnace >100kW [Europe without Switzerland]	For credits from biogas recovered with EGSB
Process water	tap water production, underground water without treatment [Europe without Switzerland]	For credits from water reuse in scenario MNR+NF
Case study: Spernal		
Electricity	market for electricity, medium voltage [GB]	For all operational electricity demand and credits from biogas
Polymer	market for acrylonitrile [GLO]	746 g acrylonitrile + water = 1kg of polymer active substance
Iron sulphate	iron sulphate production [RER]	Precipitation agent
Sulfuric acid	market for sulfuric acid [GLO]	Acid to produce ammonium sulphate
Potassium chloride	market for potassium chloride, as K2O [GLO]	For regeneration solution for N-IEX
Sodium chloride	market for sodium chloride, brine solution [GLO]	For regeneration solution for N-IEX
Sodium hydroxide	market for sodium hydroxide, without water, in 50% solution state [GLO]	For regeneration solution for P-IEX
Hydrated lime	market for lime, hydrated, lose weight [RoW]	For precipitating CaP
Cationic resin	market for cationic resin [GLO]	Resin of N-IEX
Anionic resin	market for anionic resin [GLO]	Resin of P-IEX
Disposal of anionic resin	market for spent anionic exchange resin from potable water production [GLO]	Disposal of spent resin
Disposal of cationic resin	market for spent cationic exchange resin from potable water production [GLO]	Disposal of spent resin
Ammonia solution (100% N)	diammonium phosphate, as N, at regional storehouse [RER]	Credit for recovered ammonium
Calcium phosphate	market for phosphate fertiliser, as P2O5 [GLO]	Credit for recovered CaP
Truck transport	transport, freight, lorry 16-32 metric ton, EURO5 [RER]	Sludge transports
Nitrogen	diammonium phosphate, as N, at regional storehouse [RER]	Fertiliser credit for N in sludge/wastewater in agriculture

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Phosphate	market for phosphate fertiliser, as P2O5 [GLO]	Fertiliser credit for P in sludge/wastewater in agriculture
Concrete	market for concrete [RoW]	Infrastructure material for IEX foundation
Stainless steel	steel production, electric, chromium steel 18/8 [RoW]	Infrastructure material for IEX
Reinforced steel	reinforcing steel production [RoW]	Infrastructure material for IEX
PE	polyethylene production, low density, granulate [RER]	Infrastructure material for IEX
Case study: Athens		
Electricity	market for electricity, medium voltage [GR]	
Polymer	market for polyacrylamide [GLO]	For sludge dewatering in WWTP
Transport truck	transport, freight, lorry 16-32 metric ton, EURO5 [RER]	For transport of chemicals and materials
Co-incineration of dried sludge	electricity production, hard coal [IT]	Recalculated via LHV of hard coal (27 MJ/kg) and sludge (13 MJ/kg)
Disposal of pruning waste	treatment of waste wood, untreated, sanitary landfill [RoW]	
Citric acid	citric acid production [RER]	For membrane cleaning
NaOCl	market for sodium hypochlorite, without water, in 15% solution state [RER]	For membrane cleaning
Concrete	market for concrete, for de-icing salt contact [CH]	For infrastructure of NEXTGEN scenario
Reinforcing steel	reinforcing steel production [RoW]	For infrastructure of NEXTGEN scenario
HDPE	polyethylene production, low density, granulate [RER]	For infrastructure of NEXTGEN scenario
Mineral N fertilizer	market for inorganic nitrogen fertiliser, as N [GR]	Credited in NEXTGEN scenario
Mineral P fertilizer	market for inorganic phosphorus fertiliser, as P2O5 [GR]	Credited in NEXTGEN scenario
Peat as fertilizer	market for peat [RoW]	Credited in NEXTGEN scenario
Heat credits	market for heat, district or industrial, natural gas [Europe without Switzerland]	Credited in NEXTGEN scenario for excess heat from heat pump

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Table 58: Normalisation factors for all impact categories

Impact category	Unit	Annual impact per person equivalent	Source
Cumulative energy demand, fossil & nuclear	MJ/(pe a)	122’950	(Eurostat, 2016)
Global warming potential 100a	kg CO_2-Eq/(pe a)	11’215	(ReCiPe, 2015)
Terrestrial acidification potential	kg SO_2-Eq/(pe a)	34,4	
Freshwater eutrophication potential	kg P-Eq/(pe a)	0,415	
Marine eutrophication potential	kg N-Eq/(pe a)	10,12	
Human toxicity potential	kg 1,4-DCB-Eq/(pe a)	595	

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Chemical risk assessment: exposure model input

Table S 1: Environmental properties used for the risk assessment. For the definition of Value 1, Value 2, Shift, Distribution and Variable type see method chapter in QCRA.

Variable	Description	unit	Value 1	Value 2	Shift	Distribution	Variable Type
k_aslAir	Partial mass transfair to air	m/d	120				Single Value
k_aslSoilAir	Partial mass transfair to soilair	m/d	0.48				Single Value
k_aslSoilWater	Partial mass transfair to soilwater	m/d	4.80E-05				Single Value
R	Gas constant	$(kg*m^2)/(s^2mol*K)$	8.3144				Single Value
f_air	Fraction air in soil	-	0.2				Single Value
f_water	Fraction water in soil	-	0.2				Single Value
f_solid	Fraction solids in soil	-	0.6				Single Value
f_oc	Fraction organic carbon in solids	-	-3.933	0.407		Lognormal	Spatial
rho_solid	Solid density	kg/m^3	2500				Single Value
rho_soil	Soil bulk density	kg/m^3	1700				Single Value
d	Depth	m	0.2				Single Value
pH	pH-value	-	5	7		Extended Uniform	Spatial
f_inf	Infiltraion rate	-	0.25				Single Value
temp	Annual mean temperature	k	283.2				Single Value
rain *	Mean daily rain	m/d	1.80835	2025.54	0.00124	Gamma	Spatial
t_g	Plant growing period	d	180				Single Value
Y **	Yield	kg/m^2	0.6	0.15		Normal	Spatial

* Uniform distribution without shift between 0.0011 and 0.00274 m/d for case study Athens

** Set to 0 for case study Athens

Table S 2: Arsenic specifications used for exposure modelling. For the definition of Value 1, Value 2, Shift, Distribution and Variable type see method chapter in QCRA.

Variable	Description	unit	Value 1	Value 2	Shift	Distribution	Variable Type
k_volat	Volatilisation	1/d	3.00E-09	1.40E-06	0	logderived	TRUE
k_leach	Leaching	1/d	NA		0	none	TRUE
k_bio	Bio-degredation	1/d	0.00E+00		0	none	TRUE
k_plant	Plant-accumulation	1/d	NA		0	none	TRUE
k	Decay	1/d	NA		0	none	TRUE
K_H	Henry constant	$Pa*m^3/mol$	0		0	none	TRUE
p	Vapour pressure	Pa	NA		0	none	TRUE
M	Molar weight	g/mol	NA		0	none	TRUE
sol	Solubility	mg/L	NA		0	none	TRUE
DT50	Half-life period	d	NA		0	none	TRUE
K_oc	Organic carbon to water coefficient	L/kg	NA		0	none	TRUE
K_ow	Octanol to water coefficient		NA		0	none	TRUE
K_d	Sorption coefficient	L/kg	7.368514	1.611042	0	lognormal	TRUE
const_K_d	Logarithmic constant (Kd)	-	NA	NA	0	none	TRUE

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beta_c	Concentration coefficient (Kd)	-	NA	NA		none	TRUE
beta_pH	pH – coefficient (Kd)	-	NA	NA	0	none	TRUE
beta_oc	Organic carbon coefficient (Kd)	-	NA	NA	0	none	TRUE
K_SoilWater	Soil to water coefficient	m³/m³	NA		0	none	TRUE
K_AirWater	Air to water	m³/m³	NA		0	none	TRUE
BCF	Bio concentration factor	-	0.0036	0.023	0	tderived	TRUE
const_BCF	Logarithmic constant (BCF)	-	NA	NA			TRUE
gamma_c	Concentration coefficient (BCF)	-	NA	NA			TRUE
gamma_pH	pH – coefficient (BCF)	-	NA	NA			TRUE
gamma_oc	Organic carbon coefficient (BCF)	-	NA	NA			TRUE
c_i *	Initial concentration	mg/kg	2.9		0	none	TRUE
D_air_tot	Areal-Deposiiton	mg/(m³d)	NA		0	none	TRUE
D_air	Mass-based deposition	mg/(kg*d)	-13.63747	0.5382929	0	lognormal	TRUE
PNEC_human	Predicted no effect concentration for human uptake = TDI	[µg/d]	21		0	none	TRUE
PNEC_soil	Predicted no effect concentration for soil organisms	[mg/kg DM soil]	2.9		0	none	TRUE
PNEC_water	Predicted no effect concentration for groundwater	[µg/L]	5.6		0	none	TRUE

* Initial concentration depending on environmental compartment. Defined as the corresponding PNEC concentration.

Table S 3: Arsenic specifications used for exposure modelling. For the definition of Value 1, Value 2, Shift, Distribution and Variable type see method chapter in QCRA.

Variable	Description	unit	Value 1	Value 2	Shift	Distribution	Variable Type
k_volat	Volatilisation	1/d	3.00E-09	1.40E-06		Extended logarithmic uniform	Spatial
k_bio	Bio-degredation	1/d	0				Single Value
K_d	Sorption coefficient	L/kg	7.368514	1.611042		Lognormal	Spatial
BCF	Bio concentration factor	-	0.0036	0.023		Extended truncated uniform	Spatial
c_i*	Initial concentration	mg/kg	PNEC				Single Value
D_air	Mass-based deposition	mg/(kg*d)	-13.63747	0.5382929		Lognormal	Spatial
PNEC_soil	Predicted no effect concentration for soil organisms	[mg/kg DM soil]	2.9				Single Value
PNEC_water	Predicted no effect concentration for groundwater	[µg/L]	5.6				Single Value

* Initial concentration depending on environmental compartment. Defined as the corresponding PNEC concentration.

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Table S 4: Cadmium specifications used for exposure modelling. For the definition of Value 1, Value 2, Shift, Distribution and Variable type see method chapter in QCRA.

Variable	Description	unit	Value 1	Value 2	Shift	Distribution	Variable Type
k_volat	Volatilisation	1/d	0				Single Value
k_bio	Bio-degredation	1/d	0				Single Value
K_H	Henry constant	Pa*m³/mol	0				Single Value
const_K_d	Logarithmic constant (Kd)	-	3.184	0.11		Normal	Spatial
beta_c	Concentration coefficient (Kd)	-	1.08	0.02		Normal	Spatial
beta_pH	pH – coefficient (Kd)	-	-0.47	0.02		Normal	Spatial
beta_oc	Organic carbon coefficient (Kd)	-	-0.81	0.05		Normal	Spatial
const_BCF	Logarithmic constant (BCF)	-	0.114				Single Value
gamma_c	Concentration coefficient (BCF)	-	0.76				Single Value
gamma_pH	pH – coefficient (BCF)	-	-0.15				Single Value
gamma_oc	Organic carbon coefficient (BCF)	-	-0.39				Single Value
c_i*	Initial concentration	mg/kg	PNEC				Single Value
D_air	Mass-based deposition	mg/(kg*d)	-14.429	0.7948452		Lognormal	Spatial
PNEC_soil	Predicted no effect concentration for soil organisms	[mg/kg DM soil]	0.9				Single Value
PNEC_water	Predicted no effect concentration for groundwater	[µg/L]	0.19				Single Value

* Initial concentration depending on environmental compartment. Defined as the corresponding PNEC concentration.

Table S 5: Chromium specifications used for exposure modelling. For the definition of Value 1, Value 2, Shift, Distribution and Variable type see method chapter in QCRA.

Variable	Description	unit	Value 1	Value 2	Shift	Distribution	Variable Type
k_volat	Volatilisation	1/d	0				Single Value
k_bio	Bio-degredation	1/d	0				Single Value
K_H	Henry constant	Pa*m³/mol	0				Single Value
const_K_d	Logarithmic constant (Kd)	-	2.64	0.792		Normal	Spatial
beta_c	Concentration coefficient (Kd)	-	0				Single Value
beta_pH	pH – coefficient (Kd)	-	0.21	0.063		Normal	Spatial
beta_oc	Organic carbon coefficient (Kd)	-	0				Single Value
BCF	Bio concentration factor	-	0.001	0.015		Uniform	Single Value
c_i*	Initial concentration	mg/kg	PNEC				Single Value
D_air	Mass-based deposition	mg/(kg*d)	2.56E-06	1.76E-06		Truncated normal	Single Value
PNEC_soil	Predicted no effect concentration for soil organisms	[mg/kg DM soil]	21.1				Single Value
PNEC_water	Predicted no effect concentration for groundwater	[µg/L]	6.5				Single Value

* Initial concentration depending on environmental compartment. Defined as the corresponding PNEC concentration.

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Table S 6: Copper specifications used for exposure modelling. For the definition of Value 1, Value 2, Shift, Distribution and Variable type see method chapter in QCRA.

Variable	Description	unit	Value 1	Value 2	Shift	Distribution	Variable Type
k_volat	Volatilisation	1/d	0.00E+00				Single Value
k_bio	Bio-degredation	1/d	0.00E+00				Single Value
K_H	Henry constant	Pa*m³/mol	0				Single Value
const_K_d	Logarithmic constant (Kd)	-	1.13	0.14		normal	Spatial
beta_c	Concentration coefficient (Kd)	-	0.93	0.05		normal	Spatial
beta_pH	pH – coefficient (Kd)	-	-0.21	0.02		normal	Spatial
beta_oc	Organic carbon coefficient (Kd)	-	-0.21	0.02		normal	Spatial
BCF	Bio concentration factor	-	0.05	0.6		Extended truncated Uniform	Spatial
c_i*	Initial concentration	mg/kg	PNEC				Single Value
D_air	Mass-based deposition	mg/(kg*d)	-1.09E+01	8.47E-01		lognormal	Spatial
PNEC_soil	Predicted no effect concentration for soil organisms	[mg/kg DM soil]	65				Single Value
PNEC_water	Predicted no effect concentration for groundwater	[µg/L]	7.8				Single Value

* Initial concentration depending on environmental compartment. Defined as the corresponding PNEC concentration.

Table S 7: Lead specifications used for exposure modelling. For the definition of Value 1, Value 2, Shift, Distribution and Variable type see method chapter in QCRA.

Variable	Description	unit	Value 1	Value 2	Shift	Distribution	Variable Type
k_volat	Volatilisation	1/d	0				Single Value
k_bio	Bio-degredation	1/d	0				Single Value
K_H	Henry constant	Pa*m³/mol	0				Single Value
const_K_d	Logarithmic constant (Kd)	-	1.19	0.22		Normal	Spatial
beta_c	Concentration coefficient (Kd)	-	0.44	0.07		Normal	Spatial
beta_pH	pH – coefficient (Kd)	-	0.37	0.04		Normal	Spatial
beta_oc	Organic carbon coefficient (Kd)	-	0				Single Value
BCF	Bio concentration factor	-	0.001	0.009		Extended truncated Uniform	Spatial
c_i*	Initial concentration	mg/kg	PNEC				Single Value
D_air	Mass-based deposition	mg/(kg*d)	1.34E+00	9.66E+04		Gamma	Spatial
PNEC_soil	Predicted no effect concentration for soil organisms	[mg/kg DM soil]	212				Single Value
PNEC_water	Predicted no effect concentration for groundwater	[µg/L]	2.4				Single Value

* Initial concentration depending on environmental compartment. Defined as the corresponding PNEC concentration.

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Table S 8: Mercury specifications used for exposure modelling. For the definition of Value 1, Value 2, Shift, Distribution and Variable type see method chapter in QCRA.

Variable	Description	unit	Value 1	Value 2	Shift	Distribution	Variable Type
k_volat	Volatilisation	1/d	1.93E-06	3.85E-07		Normal	Spatial
k_bio	Bio-degredation	1/d	0				Single Value
p	Vapour pressure	Pa	0.0703	0.0007		Normal	Temporal
M	Molar weight	g/mol	200.592				Single Value
sol	Solubility	mg/L	0.037				Single Value
K_d	Sorption coefficient	L/kg	8.289351	1.61181		Lognormal	Spatial
BCF	Bio concentration factor	-	0.008	0.064		Extended truncated Uniform	Spatial
c_i	Initial concentration	mg/kg	PNEC				Single Value
D_air	Mass-based deposition	mg/(kg*d)	-15.97992	0.9295441		Lognormal	Spatial
PNEC_soil	Predicted no effect concentration for soil organisms	[mg/kg DM soil]	0.022				Single Value
PNEC_water	Predicted no effect concentration for groundwater	[µg/L]	0.057				Single Value

* Initial concentration depending on environmental compartment. Defined as the corresponding PNEC concentration.

Table S 9: Nickel specifications used for exposure modelling. For the definition of Value 1, Value 2, Shift, Distribution and Variable type see method chapter in QCRA.

Variable	Description	unit	Value 1	Value 2	Shift	Distribution	Variable Type
k_volat	Volatilisation	1/d	0				Single Value
k_bio	Bio-degredation	1/d	0				Single Value
K_H	Henry constant	Pa*m³/mol	0				Single Value
const_K_d	Logarithmic constant (Kd)	-	-4.396	0.6		normal	Spatial
beta_c	Concentration coefficient (Kd)	-	0			normal	Spatial
beta_pH	pH – coefficient (Kd)	-	1.02	0.09		normal	Spatial
beta_oc	Organic carbon coefficient (Kd)	-	0.8	0.2		normal	Spatial
const_BCF	Logarithmic constant (BCF)	-	-0.575	0.16		normal	Spatial
gamma_c	Concentration coefficient (BCF)	-	-1.095	0.19		normal	Spatial
gamma_pH	pH – coefficient (BCF)	-	0				Single Value
gamma_oc	Organic carbon coefficient (BCF)	-	0				Single Value
c_i*	Initial concentration	mg/kg	PNEC				Single Value
D_air	Mass-based deposition	mg/(kg*d)	-1.21E+01	7.14E-01		lognormal	Spatial
PNEC_soil	Predicted no effect concentration for soil organisms	[mg/kg DM soil]	29.9				Single Value
PNEC_water	Predicted no effect concentration for groundwater	[µg/L]	7.1				Single Value

* Initial concentration depending on environmental compartment. Defined as the corresponding PNEC concentration.

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Table S 10: Zinc specifications used for exposure modelling. For the definition of Value 1, Value 2, Shift, Distribution and Variable type see method chapter in QCRA.

Variable	Description	unit	Value 1	Value 2	Shift	Distribution	Variable Type
k_volat	Volatilisation	1/d	0				Single Value
k_bio	Bio-degredation	1/d	0				Single Value
K_H	Henry constant	Pa*m³/mol	0				Single Value
const_K_d	Logarithmic constant (Kd)	-	3.44	0.31		Normal	Spatial
beta_c	Concentration coefficient (Kd)	-	0.94	0.08		Normal	Spatial
beta_pH	pH – coefficient (Kd)	-	-0.55	0.04		Normal	Spatial
beta_oc	Organic carbon coefficient (Kd)	-	-0.34	0.12		Normal	Spatial
const_BCF	Logarithmic constant (BCF)	-	0.985	0.284		Normal	Spatial
gamma_c	Concentration coefficient (BCF)	-	-0.749	0.185		Normal	Spatial
gamma_pH	pH – coefficient (BCF)	-	0				Single Value
gamma_oc	Organic carbon coefficient (BCF)	-	0				Single Value
c_i*	Initial concentration	mg/kg	PNEC				Single Value
D_air	Mass-based deposition	mg/(kg*d)	-9.07E+00	6.28E-01		Lognormal	Spatial
PNEC_soil	Predicted no effect concentration for soil organisms	[mg/kg DM soil]	83.1				Single Value
PNEC_water	Predicted no effect concentration for groundwater	[µg/L]	14.4				Single Value

* Initial concentration depending on environmental compartment. Defined as the corresponding PNEC concentration.

Table S 11: Benzo(a)pyrene specifications used for exposure modelling. For the definition of Value 1, Value 2, Shift, Distribution and Variable type see method chapter in QCRA.

Variable	Description	unit	Value 1	Value 2	Shift	Distribution	Variable Type
K_H	Henry constant	Pa*m³/mol	0.022				Single Value
p	Vapour pressure	Pa	5.60E-04				Single Value
M	Molar weight	g/mol	252				Single Value
sol	Solubility	mg/L	0.00162				Single Value
DT50	Half-life period	d	120	3000		Extended logarithmic uniform	Spatial
K_oc	Organic carbon to water coefficient	L/kg	1.00E+05	3.16E+06		Extended logarithmic uniform	Spatial
BCF	Bio concentration factor	-	0.00002	0.025		Extended logarithmic uniform	Spatial
c_i *	Initial concentration	mg/kg	PNEC				Single Value
D_air	Mass-based deposition	mg/(kg*d)	-1.66E+01	5.84E-01		Lognormal	Spatial
PNEC_soil	Predicted no effect concentration for soil organisms	[mg/kg DM soil]	0.053				Single Value
PNEC_water	Predicted no effect concentration for groundwater	[µg/L]	0.027				Single Value

* Initial concentration depending on environmental compartment. Defined as the corresponding PNEC concentration.

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Table S 12: PCDD/F + dl-PCB specifications used for exposure modelling. For the definition of Value 1, Value 2, Shift, Distribution and Variable type see method chapter in QCRA.

Variable	Description	unit	Value 1	Value 2	Shift	Distribution	Variable Type
K_H	Henry constant	Pa*m³/mol	2.57	3.29		Extended uniform	Spatial
DT50	Half-life period	d	180	30000		Extended logarithmic uniform	Spatial
K_oc	Organic carbon to water coefficient	L/kg	3.80E+05	1 10E+09		Extended logarithmic uniform	Spatial
BCF	Bio concentration factor	-	0.0001	0.2		Extended logarithmic uniform	Spatial
c_i *	Initial concentration	mg/kg	2.00E-05				Single Value
D_air	Mass-based deposition	mg/(kg*d)	-2.44E+01	1.50E+00		Lognormal	Spatial
PNEC_soil	Predicted no effect concentration for soil organisms	[mg/kg DM soil]	2.00E-05				Single Value
PNEC_water	Predicted no effect concentration for groundwater	[µg/L]	3.25E-06				Single Value

* Initial concentration depending on environmental compartment. Defined as the corresponding PNEC concentration.

Table S 13: PFOA specifications used for exposure modelling. For the definition of Value 1, Value 2, Shift, Distribution and Variable type see method chapter in QCRA.

Variable	Description	unit	Value 1	Value 2	Shift	Distribution	Variable Type
K_H	Henry constant	Pa*m³/mol	1.95E-06	1.95E-04		Extended logarithmic uniform	Spatial
DT50	Half-life period	d	300	300000		Extended truncated uniform	Spatial
K_oc	Organic carbon to water coefficient	L/kg	6.447	2.072		Lognormal	Spatial
BCF	Bio concentration factor	-	0.0001	32		Extended logarithmic uniform	Spatial
c_i *	Initial concentration	mg/kg	PNEC				Single Value
D_air_tot	Areal-Deposiiton	mg/(m²d)	2.74E-09	8.22E-07		Extended logarithmic uniform	Spatial
PNEC_soil	Predicted no effect concentration for soil organisms	[mg/kg DM soil]	10				Single Value
PNEC_water	Predicted no effect concentration for groundwater	[µg/L]	0.19				Single Value

* Initial concentration depending on environmental compartment. Defined as the corresponding PNEC concentration.

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Table S 14: PFOS specifications used for exposure modelling. For the definition of Value 1, Value 2, Shift, Distribution and Variable type see method chapter in QCRA.

Variable	Description	unit	Value 1	Value 2	Shift	Distribution	Variable Type
K_H	Henry constant	Pa*m³/mol	1.82E-07	1.82E-05		Extended logarithmic uniform	Spatial
DT50	Half-life period	d	300	300000		Extended truncated uniform	Spatial
K_oc	Organic carbon to water coefficient	L/kg	6.908	1.612		Lognormal	Spatial
BCF	Bio concentration factor	-	0.0001	2.7		Extended logarithmic uniform	Spatial
c_i *	Initial concentration	mg/kg	PNEC				Single Value
D_air_tot	Areal-Deposiiton	mg/(m²d)	1.37E-09	2.12E-07		Extended logarithmic uniform	Spatial
PNEC_soil	Predicted no effect concentration for soil organisms	[mg/kg DM soil]	0.01				Single Value
PNEC_water	Predicted no effect concentration for groundwater	[µg/L]	2.30E-04				Single Value

* Initial concentration depending on environmental compartment. Defined as the corresponding PNEC concentration.

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Chemical risk assessment results

Sewage Sludge as a reference

Table S 15: Aggregated results of environmental risk assessment regarding the soil ecosystem for long-term sewage sludge application (ΔRQ: Average increase of risk quotients caused by fertilization, RQ_{max}: Upper 5% of all RQ, RC: Risk class according to risk matrix (chapter "Risk characterisation"): 1: negligible, 2: acceptable, 3: increasing concern, 4: unacceptable)

	Most likely			10% Probability			1% Probability		
	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC
Arsenic	0.04	1.1	1	0.045	1.1	1	0.049	1.1	1
Cadmium	0.017	1.1	1	0.018	1.1	1	0.019	1.1	1
Chromium	0.065	1.1	1	0.07	1.1	1	0.075	1.1	1
Copper	0.092	1.1	1	0.097	1.1	1	0.099	1.1	1
Lead	0.004	1	1	0.004	1	1	0.004	1	1
Mercury	0.599	2.8	3	0.835	3	3	0.974	3.2	3
Nickel	0.016	1	1	0.016	1	1	0.017	1	1
Zinc	0.207	1.3	2	0.207	1.3	2	0.226	1.3	2
Benzo(a)pyrene	-	<0.1	1	-	<0.1	1	-	0	1
PCDD/F + dl-PCB	0.01	0.7	1	0.011	0.7	1	0.012	0.7	1

Table S 16: Aggregated results of environmental risk assessment regarding the water ecosystem for long-term sewage sludge application application (ΔRQ: Average increase of risk quotients caused by fertilization, RQ_{max}: Upper 5% of all RQ, RC: Risk class according to risk matrix (chapter "Risk characterisation"): 1: negligible, 2: acceptable, 3: increasing concern, 4: unacceptable)

	Most likely			10% Probability			1% Probability		
	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC
Arsenic	0.075	1	1	0.089	1	1	0.101	1	1
Cadmium	0.168	2.2	3	0.177	2.3	3	0.192	2.3	3
Chromium	0.176	2.3	3	0.189	2.5	3	0.2	2.6	3
Copper	0.493	2.5	3	0.518	2.6	3	0.531	2.6	3
Lead	0.04	4.1	2	0.042	4.1	2	0.044	4.1	2
Mercury	0.36	3	3	0.45	3.6	3	0.501	4	3
Nickel	0.718	3.3	3	0.741	3.4	3	0.786	3.5	3
Zinc	2.129	13.2	4	2.13	13.2	4	2.316	14.2	4
Benzo(a)pyrene	-	<0.1	1		<0.1	1	-	< 0.1	1
PCDD/F + dl-PCB	0.043	0.6	1	0.049	0.6	1	0.051	0.6	1

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Struvite from Braunschweig

Table S 17: Aggregated results of environmental risk assessment regarding the soil ecosystem for long-term struvite application (ΔRQ: Average increase of risk quotients caused by fertilization, RQ_{max}: Upper 5% of all RQ, RC: Risk class according to risk matrix (chapter "Risk characterisation"): 1: negligible, 2: acceptable, 3: increasing concern, 4: unacceptable)

	Most likely			10% Probability			1% Probability		
	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC
Arsenic	0.001	1	1	0.001	1	1	0.001	1	1
Cadmium	<0.001	1	1	<0.001	1	1	<0.001	1	1
Chromium	0.001	1	1	0.001	1	1	0.001	1	1
Copper	<0.001	1	1	<0.001	1	1	<0.001	1	1
Lead	<0.001	1	1	<0.001	1	1	<0.001	1	1
Mercury	0.022	2.2	2	0.029	2.2	2	0.035	2.2	2
Nickel	<0.001	1	1	<0.001	1	1	<0.001	1	1
Zinc	<0.001	1	1	<0.001	1.1	1	<0.001	1.1	1
Benzo(a)pyrene	-	<0.1	1	-	<0.1	1	-	<0.1	1
PCDD/F + dl-PCB	<0.001	0.7	1	0.001	0.7	1	0.001	0.7	1

Table S 18: Aggregated results of environmental risk assessment regarding the water ecosystem for long-term struvite application (ΔRQ: Average increase of risk quotients caused by fertilization, RQ_{max}: Upper 5% of all RQ, RC: Risk class according to risk matrix (chapter "Risk characterisation"): 1: negligible, 2: acceptable, 3: increasing concern, 4: unacceptable)

	Most likely			10% Probability			1% Probability		
	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC
Arsenic	0.001	1	1	0.001	1	1	0.001	1	1
Cadmium	0.003	2	1	0.004	2	1	0.005	2	1
Chromium	0.006	1	1	0.007	1	1	0.007	1	1
Copper	0.001	1.4	1	0.001	1.4	1	0.001	1.4	1
Lead	<0.001	3.9	1	<0.001	3.9	1	<0.001	3.9	1
Mercury	0.021	1.7	1	0.028	1.7	1	0.035	1.7	1
Nickel	0.005	1.9	1	0.005	1.9	1	0.005	1.9	1
Zinc	0.002	3.9	1	0.003	3.9	1	0.003	3.9	1
Benzo(a)pyrene		<0.1	1		<0.1	1	-	<0.1	1
PCDD/F + dl-PCB	0.002	0.6	1	0.003	0.6	1	0.003	0.6	1

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Ammonium Sulfate Solution from Braunschweig

Table S 19: Aggregated results of environmental risk assessment regarding the soil ecosystem for long-term ASL application (ΔRQ: Average increase of risk quotients caused by fertilization, RQ_{max}: Upper 5% of all RQ, RC: Risk class according to risk matrix (chapter "Risk characterisation"): 1: negligible, 2: acceptable, 3: increasing concern, 4: unacceptable)

	Most likely			10% Probability			1% Probability		
	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC
Arsenic	0.001	1	1	0.001	1	1	0.001	1	1
Cadmium	<0.001	1	1	<0.001	1	1	<0.001	1	1
Chromium	<0.001	1	1	<0.001	1	1	<0.001	1	1
Copper	0.002	1	1	0.003	1	1	0.004	1	1
Lead	<0.001	1	1	<0.001	1	1	<0.001	1	1
Mercury	0.004	2.2	1	0.005	2.2	1	0.005	2.2	1
Nickel	<0.001	1	1	<0.001	1	1	<0.001	1	1
Zinc	0.002	1.1	1	0.002	1.1	1	0.002	1.1	1

Table S 20: Aggregated results of environmental risk assessment regarding the water ecosystem for long-term ASL application (ΔRQ: Average increase of risk quotients caused by fertilization, RQ_{max}: Upper 5% of all RQ, RC: Risk class according to risk matrix (chapter "Risk characterisation"): 1: negligible, 2: acceptable, 3: increasing concern, 4: unacceptable)

	Most likely			10% Probability			1% Probability		
	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC
Arsenic	0.001	1	1	0.001	1	1	0.001	1	1
Cadmium	0.003	2	1	0.003	2	1	0.004	2	1
Chromium	0.001	1	1	0.001	1	1	0.001	1	1
Copper	0.013	1.5	1	0.018	1.5	1	0.022	1.5	1
Lead	<0.001	3.9	1	0.001	3.9	1	0.001	3.9	1
Mercury	0.004	1.6	1	0.004	1.6	1	0.005	1.6	1
Nickel	0.004	1.9	1	0.004	1.9	1	0.005	1.9	1
Zinc	0.018	3.9	2	0.022	3.9	2	0.026	3.9	2

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Compost from Athens

Table S 21: Aggregated results of environmental risk assessment regarding the soil ecosystem for long-term compost application (ΔRQ: Average increase of risk quotients caused by fertilization, RQ_{max}: Upper 5% of all RQ, RC: Risk class according to risk matrix (chapter "Risk characterisation"): 1: negligible, 2: acceptable, 3: increasing concern, 4: unacceptable)

	Most likely			10% Probability			1% Probability		
	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC
Cadmium	0.419	1.6	2	0.685	2	2	0.890	2.3	3
Chromium	0.087	1.1	1	0.145	1.2	2	0.188	1.3	2
Copper	0.069	1.1	1	0.107	1.1	2	0.137	1.2	2
Lead	0.016	1	1	0.026	1	1	0.035	1.1	1
Mercury	1.31	3.7	4	2.159	4.8	4	2.812	5.7	4
Nickel	0.046	1.1	1	0.073	1.1	1	0.073	1.1	1
Zinc	0.198	1.3	2	0.323	1.5	2	0.409	1.6	2

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Hydroxyapatite from Spernal

Table S 22: Aggregated results of environmental risk assessment regarding the soil ecosystem for long-term hydroxyapatite application (ΔRQ: Average increase of risk quotients caused by fertilization, RQ_{max}: Upper 5% of all RQ, RC: Risk class according to risk matrix (chapter "Risk characterisation"): 1: negligible, 2: acceptable, 3: increasing concern, 4: unacceptable)

	Most likely			10% Probability			1% Probability		
	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC
Arsenic	<0.001	1	1	<0.001	1	1	<0.001	1	1
Cadmium	<0.001	1	1	<0.001	1	1	<0.001	1	1
Chromium	<0.001	1	1	<0.001	1	1	<0.001	1	1
Copper	<0.001	1	1	<0.001	1	1	<0.001	1	1
Lead	<0.001	1	1	<0.001	1	1	<0.001	1	1
Mercury	0.003	2.2	1	0.02	2.2	2	0.037	2.2	2
Nickel	<0.001	1	1	<0.001	1	1	<0.001	1	1
Zinc	<0.001	1.1	1	<0.001	1.1	1	<0.001	1.1	1
Benzo(a)pyrene	-	<0.1	1	-	<0.1	1	-	<0.1	1

Table S 23: Aggregated results of environmental risk assessment regarding the water ecosystem for long-term hydroxy apatite application (ΔRQ: Average increase of risk quotients caused by fertilization, RQ_{max}: Upper 5% of all RQ, RC: Risk class according to risk matrix (chapter "Risk characterisation"): 1: negligible, 2: acceptable, 3: increasing concern, 4: unacceptable)

	Most likely			10% Probability			1% Probability		
	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC	ΔRQ	RQ_{max}	RC
Arsenic	<0.001	1	1	<0.001	1	1	<0.001	1	1
Cadmium	<0.001	1.9	1	<0.001	1.9	1	<0.001	1.9	1
Chromium	<0.001	1	1	<0.001	1	1	<0.001	1	1
Copper	<0.001	1.4	1	<0.001	1.4	1	<0.001	1.4	1
Lead	<0.001	3.9	1	<0.001	3.9	1	<0.001	3.9	1
Mercury	0.003	1.6	1	0.02	1.7	1	0.037	1.7	1
Nickel	<0.001	1.8	1	<0.001	1.8	1	<0.001	1.8	1
Zinc	<0.001	3.8	1	<0.001	3.8	1	<0.001	3.8	1
Benzo(a)pyrene	-	<0.1	1	-	<0.1	1	-	<0.1	1

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