Supplementary Material

Resource flow characterisation and sustainable value creation analysis for the holistic circularity assessment of wastewater systems

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1. Nitrogen

Table S1 summarises the values extracted from a Food and Agriculture Organization database [1] for nitrogen applied to cropland in EU-27 countries in the year 2020, used to calculate the percentages of N_2 emissions that are circular or neutral.

Table S1. Nitrogen applied to cropland in EU-27 countries in 2020.

Total to crops				**Circularity**
14,241,375.64		tons		Neutral/Circular
Fractions of fertilisers		**Mass**		
Synthetic Fertilisers	69%	8,796,622.49	tons	Neutral
Manure applied to Soils	31%	3,979,757.14	tons	Circular
Total fractions		**Mass**		
Synthetic Fertilisers	62%	8,796,622.49	tons	Neutral
Manure Applied to Soils	28%	3,979,757.14	tons	Circular
Atmospheric Deposition	7%	1,031,166.88	tons	Neutral
Biological Fixation	3%	433,829.13	tons	Circular

2. Conventional Process Model

In this section, the data provided was used to create the mass balance model enabling MFA of the conventional 10,000 PE WWTP process. The wastewater influent loadings were taken from literature and are provide in Table S2 [2].

Table S2. Influent loading reported for the WWTP.

Parameter	**Value**	**Unit**
COD	640	g/m^3
BOD	340	g/m^3
TN	80	g/m^3
NH_3	63	g/m^3
NO_3	0.99	g/m^3
TP	12	g/m^3
TSS	320	g/m^3

Quantities of solids removed during pretreatment stages were calculated using parameters in Table S3 taken from literature, and mass balancing across process units was used to calculate resultant effluent quality [3].

Table S3. Pretreatment process solids removal parameters.

Screening – 6 mm bar screen					
Removal	90	L/1000 m^3	Moisture	75 %	
Density	750	kg/ m^3	Volatiles	75 %	
Grit					
Removal	0.01	m^3/1000 m^3	Moisture	40 %	
Bulk Density	1,660	kg/ m^3	Volatiles	28.5 %	

Extended aeration is an activated sludge process, with kinetic parameters used to calculate removal efficiencies and biomass production shown in Table S4 [3]. Only nitrification occurs and there is no enhanced chemical or biological phosphorus removal, meaning soluble nutrient concentrations in the effluent are high, however, chemical oxygen demand (COD) limits are met before discharge.

Table S4. Kinetic parameters for extended aeration.

Extended Aeration					
bCOD:BOD	1.6		b_h	0.12	gVSS/gVSS d
TSS:VSS	0.85		b_{aob}	0.135	g/g d
VSS: BOD	0.85		Y_n	0.15	gVSS/gNOX
Y_h	0.45	gVSS/gCOD	f_d	0.15	

Sludge is thickened, stabilised with liming, then dewatered and the parameters used are shown in Table S5 [3,4].

Table S5. Parameters required for liming sludge treatment calculations.

Sludge Treatment					
Thickened WAS	3.7 %	DS	Dewatered Cake	22 %	DS
Thickener Efficiency	98 %		Dewatering Efficiency	98 %	
Polyelectrolyte Requirement	22	kg/t	Polyelectrolyte Requirement	7.3	kg/t
Liming Carbon Loss	15%	As CO_2 emissions	Sludge Lime Dose	300	kgCa(OH)$_2$/tDS
Liming Nitrogen Loss	2.8%	As NH_3 emissions			

Lastly, the energy requirement for the process was calculated using values taken from literature, based on kWh/m^3 for a range of wastewater treatment plant sizes [5].

3. Circular Intervention Model

In this section, the data provided was used to update the conventional process mass balance model enabling MFA of the circular intervention technology. Table S6 provides the parameters for the updated pretreatment process that includes FOG removal [3,6,7].

Table S6. FOG removal pretreatment operation parameters.

FOG Removal					
Concentration	57	mg/L	Removal	50%	
DS	45 %				

The effluent quality of the primary settler was taken from literature [2] and used to calculate the removal efficiencies of wastewater components shown in Table S7.

Table 7. Removal efficiencies of primary settler.

Component	Primary Clarifier Removal Efficiency
Suspended Solids (SS)	63 %
Biological Oxygen Demand (BOD)	18 %
COD	20 %
Nitrogen	11 %
Phosphorus	25 %

The PBR operation was modelled using parameters reported by project partners, which are summarised in Table S8.

Table S8. PBR and clarifier operation parameters.

Soluble COD removal	80 %		Nitrogen removal	40 %	
COD removal	80 %		Phosphorus removal	70 %	
BOD removal	90 %		TSS removal	80 %	
Biomass Yield	0.21	gVSS/gCOD	Recycle Ratio	0.1	
Settler Efficiency	97 %		Sludge DS	0.40 %	

For sludge treatment, thickeners were assumed to operate as reported for the conventional process. A stoichiometric method was used to complete the mass balance for the AD and biogas production calculations [8]. A heat balance was completed across the digester, showing the heat requirements could be covered by biogas combustion in a boiler (with the excess sent to a generator for electricity production). The digestate is then dewatered before being sold for land application. The parameters required for these calculations are provided in Table S9 [3].

Table S9. Sludge treatment and energy balance parameters.

AD Kinetic Parameters					
f_{s0}	0.11		b	0.05	d^{-1}
f_d	0.8		SRT	20	D
Heat Balance					
Generator Efficiency	30 %	Electricity	Methane Energy Density	38.8	MJ/m^3
Boiler Efficiency	86 %	Heat			
Heat Transfer Coefficients of Digester [3]					
Wall	1	$W/ m^2 C$	Roof	4.5	$W/ m^2 C$
Floor	1.25	$W/ m^2 C$	Air Temperature	15.2	℃
Inlet Temperature	15	℃	Digester Temperature	37	℃
Dewatering					
Cake	22 %	Dry solids	Polyelectrolyte Dose	0.05	L/m^3
Efficiency	98 %				

The thermal hydrolysis is assumed to perform as reported [9]. Lastly, the energy balance was completed using the values reported for conventional equipment [5], whilst energy consumption by the PBR at this scale was provided by project partners.

4. Resource Flow Characterisation of the Conventional Process

Here the resource flow characterisation tables used for conventional WWTP indicator calculation are presented in Tables S10-S13.

Table S10. Water resource flow characterisation for conventional process.

Influent			
Stream	**Fraction**	**Status**	
WWTP inlet	80 %	Circular	
Losses (Consumption - WWT Inlet)	20 %	Linear	
Outlets			
Stream	**Water Fraction of the Stream**	**Destination**	**Status**
Screenings	75 %	Landfill	Linear
Grit	40 %	Landfill	Linear
Effluent	>99.9 %	Restoration (groundwater, lake, river)	Circular
Biosolids	78 %	Land application	Linear *assumed it does not reduce the raw water abstraction

Table S11. Phosphorus resource flow characterisation for conventional process.

Influent			
Stream	**Fraction**	**Status**	
Urine	30 %	Circular	
Faeces	10 %		
Food scraps	1 %	Linear	
Food additives	29 %		
Auto dishwashing	9 %		
Laundry Detergents	14 %		
Tap water dosing	6 %		
Personal Care product	1 %		
Outlets			
Stream	**P fraction**	**Destination**	**Status**
Effluent	4.98 mg/L	Fresh water body	Linear
Biosolids	2.96 %DS	Land application	Circular

Table S12. Nitrogen resource flow characterisation for conventional process.

Influent			
Stream	**Fraction**	**Status**	
Urine	80 %	Circular	
Faeces	14 %		
Greywater (kitchen/laundry/bathroom)	6 %	Linear	
Outlets			
Stream	**N fraction**	**Destination**	**Status**
Effluent	67.31 mg/L	Fresh water body	Linear
Biosolids	5 %DS	Land application	Circular
Emissions	NH_3	Atmosphere	Linear
	N_2O	Atmosphere	Linear

Table S13. Carbon resource flow characterisation for conventional process.

Influent			
Stream	**Fraction**	**Status**	
Fossil	5.5 %	Linear	
Biogenic	94.5 %	Circular	
Outlets			
Stream	**OC fraction**	**Destination**	**Status**
Screenings	41.3 % TS	Landfill	Linear
Effluent	3.87 mg/L	Fresh water body	Linear (biogenic)
	5 % of total fossil OC		Linear (fossil)
Biosolids	20 %	Land application	Circular (biogenic)
	56.76 % of total fossil OC		Linear (fossil)
Gas Emissions	>99% CO_2	Atmosphere	Circular (Biogenic)
	30.5 % of total fossil OC	Atmosphere	Linear (Fossil)
	CH_4 (0.0075 $kgCH_4/kgCOD$)	Atmosphere	Linear
Liming Emissions	CO_2	Atmosphere	Circular (biogenic)
	7.74 % of total fossil OC	Atmosphere	Linear fossil

5. Resource Flow Characterisation of the Circular Intervention Process

Here the resource flow characterisation tables used for the WWTP with circular interventions indicator calculations are presented in Tables S14-S17.

Table S14. Water resource flow characterisation for the circular intervention process.

Influent			
Stream	**Fraction**	**Status**	
WWTP inlet	80 %	Circular	
Losses (Consumption - WWT Inlet)	20 %	Linear	
Outlets			
Stream	**Water Fraction of the stream**	**Destination**	**Status**
Screenings	75 %	Landfill	Linear
FOG	55 %	Landfill	Linear
Grit	40 %	Landfill	Linear
Effluent	>99.9 %	Restoration (groundwater, lake, river)	Circular
Biosolids	78 %	Land application	Linear *assumed it does not reduce the raw water abstraction

Table S15. Phosphorus resource flow characterisation for the circular intervention process.

Influent			
Stream	**Fraction**	**Status**	
Urine	30 %	Circular	
Faeces	10 %		
Food scraps	1 %	Linear	
Food additives	29 %		
Auto dishwashing	9 %		
Laundry Detergents	14 %		
Tap water dosing	6 %		
Personal Care product	1 %		
Outlets			
Stream	**P fraction**	**Destination**	**Status**
Effluent	2.49 mg/L	Fresh water body	Linear
Biosolids	5 %DS	Land application	Circular

Table S16. Nitrogen resource flow characterisation for the circular intervention process.

Influent			
Stream	**Fraction**	**Status**	
Urine	80 %	Circular	
Faeces	14 %		
Greywater (kitchen/ laundry bathroom)	6 %	Linear	
Outlets			
Stream	**N fraction**	**Destination**	**Status**
Effluent	40.9 mg/L	Fresh Water	Linear
Biosolids	22 %DS	Land application	Circular

Table S17. Carbon resource flow characterisation for the circular intervention process.

Influent			
Stream	**Fraction**	**Status**	
Fossil	5.5 %	Linear	
Biogenic	94.5 %	Circular	
Outlets			
Stream	**C fraction**	**Destination**	**Status**
FOG	77 % TS	Landfill	Linear
Screenings	41.3 % TS	Landfill	Linear
Effluent	19.6 mg/L	Fresh water body	Linear (biogenic)
	7.1 % of total fossil OC		Linear (fossil)
Biosolids	43 %	Land application	Circular (biogenic)
	81.7 % of total fossil OC		Linear (fossil)
Biogas	45 wt% C	Used Biogas	Circular (biogenic)
	11.1 % of total fossil OC	Used Biogas	Linear (Fossil)
	1.4 % of biogas	Biogas fugitive	Linear

6. Sustainability Analysis Calculation Methodology

6.1. Carbon Footprint

Scope 1 emissions consider direct emissions from the system including, gases produced during wastewater treatment, transportation, and sludge treatment (fugitive emissions). These emission factors were taken from the IPCC report and ecoinvent 3 database, with transport factors taken from literature [10]. Scope 2 emissions are those indirectly produced by the production of energy and parameters are summarised in Table S18.

Table S18. Parameters required to calculate scope 1 and 2 emissions from processes.

Global Warming Potential					
Methane	25	$kgCO_2$ eq/$kgCH_4$	N_2O	298	$kgCO_2$ eq/kgN_2O
Transportation					
Grit	0.195	kgkm/m^3	Chemicals	0.755	kgkm/m^3
Grease	0.009405	kgkm/m^3	Sludge	156.515	kgkm/m^3
Emission factors					
N_2O Direct Emissions (conventional process)	0.016	kgN_2O/kgN	Transport	0.168	$kgCO_2$/tkm
CH_4 Direct Emissions (conventional process)	0.0075	$kgCH_4$/kg/COD	Fugitive AD Emissions	1.40%	
Scope 2					
Grid Electricity	0.403	$kgCO_2$/kWh			

Scope 3 emissions are indirect emissions resulting from effluent discharge, sludge application to land and chemical consumption. Emission factors were taken from IPCC documentation for effluent and sludge application, whilst chemical emission factors were taken from the ecoinvent 3 database, and are summarised in Table S19.

Table S19. Parameters required to calculate scope 3 emissions from processes.

N_2O Effluent	0.005	kgN_2O/kgN	CH_4 Effluent	0.028	$kgCH_4$/kgCOD
Limed sludge to land	20	$kgCH_4$/tDS	Polyelectrolyte	2.83	$kgCO_2$/kg
AD sludge to land	5	$kgCH_4$/tDS	Lime	0.95	$kgCO_2$eq/kg
Sludge to land	0.01	kgN/kgN			

Additionally, the offsets from application of biofertiliser and biosolids were calculated by mitigating the production and application of industrial fertilisers. The information was collected from the ecoinvent 3 database and literature [11], and is summarised in Table S20.

Table S20. Parameters required to calculate carbon offsets from biosolids application to land.

Ammonium Nitrate (as nitrogen)	7.97	$kgCO_2$ eq/kg	Phosphate Fertiliser P_2O_5 (as phosphorous)	1.84	$kgCO_2$ eq/kg
Replacement ratio	0.5		Replacement Ratio	0.7	

6.2. Economic Value Added

The value added method of Medina-Mijango et al. [12] was followed and is calculated using Equation S1:

$$VC = (WWT_V \times GF) - (CAPEX + OPEX + ST) + In \quad \text{(S1)}$$

Where, WWT_V is the volume of wastewater treated (m^3), GF are the gate fees of the WWTP (€/m^3), ST are state taxes for landfill and discharge (€), and In is income from sales of products (€). For economic calculations, it was assumed that both the conventional and biorefinery facilitates were constructed in Spain in the year 2021. The CAPEX for the construction of a conventional wastewater treatment plant of this size and type was calculated using a method provided by the OCED [13]. The expenditure in EUR/PE for a Mechanical-Biological-Nitrification process between 2,000-10,000 PE is given by Equation S2:

$$CAPEX = \frac{10}{7.44}^{-0.2612\log(PE)+4.26} \tag{S2}$$

Equation S2 provides the CAPEX for the year 1990, therefore, Construction Cost Indices (CCI) were used to scale the results accordingly [14]. The construction costs for the biorefinery facility were provided by the project consortium partners, based on scale up of the demonstration site CAPEX (load 3,000 m^3/d). Amortisation was calculated using Equation S3:

$$Investment_{EUR/Year} = CAPEX \times \frac{r(1+r)}{(1+r)^n - 1}^{n} \tag{S3}$$

Where r is the discount rate (4 %) and n is the time horizon (15 years as recommended by project engineers). OPEX, revenue, and tax data for conventional and biorefinery plants were provided by wastewater operators for plants of this size: reported for conventional plant of this size and estimated from demonstration photobioreactor system scale up. Economic data used for the value added calculations is summarised in Table S21.

Table 21. Parameters required for value added calculations.

Parameter	Unit	Conventional Plant	Biorefinery
CAPEX	€	Estimated	3,200,000
OPEX	€/m^3	0.4	0.135
Landfill Cost	€/t	42	
Discharge Cost	€/m^3	0.01751	
Gate Fee	€/m^3	0.8	
Fertiliser Sale	€/t	N/A	150

6.3. Social Assessment

Parameters required for the calculation of social indicators are presented in Tables S22 and S23.

Table S22. Material and electricity inflows of urban WWTP systems.

Consumables	Unit	Conventional Plant	Novel Plant
Lime	kg/m^3 wastewater	0.0701	0
Polyelectrolyte	kg/m^3 wastewater	0.00693	0.00253
Electricity	kWh/m^3 wastewater	0.382	0.331

Table S23. Environmental releases of urban WWTP systems to soil, water and air.

Substance	Unit	Conventional Plant	Novel Plant
Emissions to Soil			
Phosphorus	kg/m^3 wastewater	0.00677	0.00782
Emissions to Water			
COD	kg/m^3 wastewater	0.0192	0.0774
Nitrogen	kg/m^3 wastewater	0.0633	0.0386
Phosphorus	kg/m^3 wastewater	0.00468	0.00236
Nitrate (includes fertiliser application to soil)	kg/m^3 wastewater	0.0149	0.0439
Emissions to Air			
N_2O	kg/m^3 wastewater	0.00268	0.000633
CO_2 (Fossil)	kg/m^3 wastewater	0.00974	0.00491
CH_4	kg/m^3 wastewater	0.00991	0.00349

7. Sustainability Analysis Results

Carbon Footprint

Results of carbon footprint analysis are summarised in Figure 7A of the manuscript. Scope 1 (direct) emissions have the greatest reduction between systems, as even though fugitive emissions from sludge treatment are approximately 10 times greater for the PBR system, direct emissions from wastewater treatment can be assumed negligible. Therefore, Scope 1 emissions are only 6 % of the conventional system. Scope 2 (electricity consumption) emissions decreased by more than 10 % due to the reduction in demand of grid electricity. Scope 3 (indirect) emissions account for indirect process emissions and the PBR system achieves a reduction of a third, attributed to higher removal of nitrogen from the wastewater effluent and decreased emissions generation from digested biosolids when applied to land compared with limed sludge. Lastly, carbon offsets were measured by calculating emissions avoided by the process. Offsets of the PBR process are four times greater than for the conventional treatment process, as the higher nutrient content of PPB biosolids means it is able to substitute a greater amount of industrial NP fertiliser applied to land than conventional biosolids.

To summarise, the PBR process is much more efficient in terms of emissions release to air. Total emissions for the PBR system are almost a third of the emissions from conventional treatment.

Additionally, whenever this is adjusted to incorporate offsets from application of biosolids to land this drops even further to approximately a quarter.

LCA

Results from LCA comparing each impact category for the conventional and PBR WWTPs are presented in Figure 7B of the manuscript. PBR operation performs better in six out of the seven impact categories investigated, ranging from 15 % to 41 % reduction. Eutrophication sees the largest decrease of 41 %, attributed to the reduction of NP emissions in wastewater effluents. Ozone depletion, photochemical oxidation and acidification decrease by 34 %, 20 % and 15 % respectively which occurs due to the reduction of emissions to air during wastewater and sludge treatment. Lastly, abiotic depletion of elements and fossil fuels decrease by 20 % and 19 % respectively, which is correlated with reductions in chemical and energy consumption from the grid for the PBR system. Lastly, water consumption undergoes a small increase of 0.4 %, however a change of this size is considered negligible.

Combining this analysis with the carbon footprint results it can be concluded that the operation of the Deep Purple PBR system improves the environmental performance of wastewater treatment at this scale.

Economic Value Added

In the manuscript Figure 7C provides the economic value added results, showing the change in revenue and costs between PBR and conventional processes. The same volume of wastewater is treated by both systems, therefore, the gate fees are constant meaning the increase in revenue for the PBR system is a result of biofertiliser sales, adding approximately 0.1 M€/y. There is a reduction in OPEX due to the lower energy demand associated with the mitigation of aeration during biological treatment and energy recovery from biogas, as well as the removal of lime requirements for sludge treatment. The economic value generated by the PBR system is the increase in revenue added to the reduction in CAPEX and OPEX, which is almost M€ 0.5 per year for water the utility. This shows that the PBR technology system for the treatment of wastewater is a more economically sustainable process compared with the conventional prolonged aeration system at this scale.

Social Impacts

In the manuscript Figure 7D provides impact results for human health, ecosystems, and resources indicators. The PBR system results in a reduction to all impact indicators compared to the conventional system, with the largest reduction being to the human health indicator which decreases DALY by 58 %. This trend occurs due to similar reasons explained for the favourable LCA and carbon footprint results. Smaller grid energy and material consumption, coupled with the mitigation of significant proportions of direct and indirect emissions results in the reduction of endpoint impacts.

Employment was also used to quantify the social impacts of the system. Based on the employment data for local wastewater workers, it is estimated that 3 employees would be required to operate a WWTP of this size. Project partners responsible for plant operation estimate that over the course of the project employment growth of 1-5 people is expected. Therefore, for projects that implement PBR technologies, employment is expected to rise by an average of 100 % over a time frame of approximately 5 years.

Lastly, contribution to the local economy of the WWTP was calculated by dividing the economic value added of the systems by the expected GDP of the local area (Soria). PBR system increased this to 0.0018%, compared with 0.00014% for the conventional system. Therefore, these 5 indicators confirm that the PBR system results in greater social value.

8. References

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