Life cycle assessment of wastewater reclamation in a petroleum refinery in Turkey

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1. Wastewater reuse quality criteria

Table 1. Quality requirements for wastewater reuse by Tüpraş.

Parameter	Unit	Firefight reuse	Cooling reuse	Boiler reuse
pH	-	7.5-8.5	7.5-8.5	7-9
Total suspended solids (TSS)	mg/L	10		
Oil and grease	mg/L	3	0.5	0.2
Conductivity	µs/cm	1,500	200-250	1
Chloride	mg/L	300	50	
Total organic carbon (TOC)	mg/L	15	4	
Ca hardness	mg $CaCO_3$/L		80	
Mg hardness	mg $CaCO_3$/L		20	
Total alkalinity	mg $CaCO_3$/L		80	
Total hardness	mg $CaCO_3$/L			0
m-Alkalinity	mg $CaCO_3$/L		80	
Silica	mg/L		5	0.02
Fe	mg/L		0.3	0.02
Al	mg/L		0.1	0.02
Sodium	mg/L		10	0.01
Copper	mg/L			0.003
Total dissolved solids	mg/L			0.5

2. Speciation of hydrocarbons in oil and grease

The parameter 'oil and grease' essentially refers to a mixture of petroleum hydrocarbons. In order to be able to capture the environmental effects of these substances in the impact assessment, it is necessary in the life cycle inventory to disaggregate this parameter into a set of individual pollutants.

The speciation of oil and grease in the inventory has been carried out based on a detailed analysis of petroleum hydrocarbons in the treated effluent of the Tüpraş refinery at Izmit. A summary of this characterization is shown in the table below, displaying the percentage in mass that each fraction represents. For each of these groups, the flow considered in the inventory analysis is shown. The choice of flow is of importance, since it determines the contribution of these pollutants in different impact categories, such as eco-toxicity or human toxicity.

Table 2. Characterization of petroleum hydrocarbons in the refinery effluent.

Compounds	% in mass	Compound used in the inventory
Aliphatic		
C5-C6	0.0%	
C6-C8	0.0%	
C8-C10	0.0%	
C10-C12	0.0%	
C12-C16	3.9%	Hydrocarbons, aliphatic, alkanes, cyclic
C16-C35	40.7%	Hydrocarbons, aliphatic, alkanes, cyclic
C35-C40	4.2%	Hydrocarbons, aliphatic, alkanes, cyclic
Aromatic		
C5-C7	0.0%	
C7-C8	0.0%	
C8-C10	0.7%	Xylene
C10-C12	0.0%	
C12-C16	0.0%	
C16-C21	6.6%	Fluorene
C21-C35	33.6%	Anthracene
C35-C40	10.3%	Anthracene
TOTAL	100.0%	

3. Electricity production inventories

3.1. Turkey

Production of electricity in Turkey is modelled according to consequential LCI principles, whereby we only include in the production mix those technologies expected to contribute to new capacity in the coming years. Table 3 shows the electricity generation in Turkey in 2014 and the predicted generation in 2030, both obtained from the National Official Plan as reported in WWF (2014). The specific contributions of biomass, geothermal, and oil are not specified in the original source. The contribution from solar energy in 2014 is not specified either. The contribution from oil has been neglected, and this is justified by the fact that its low contribution to the overall mix remains unchanged over time in the period 2014-2030, therefore it does not constitute a long-term marginal supplier. As for geothermal, biomass, and solar (in 2014) it has been assumed that each of these generation technologies contribute with 1% to the total production in 2014 and in 2030. The general calculation procedure of the consequential electricity mix is documented in Muñoz (2019).

Table 3. Power generation in Turkey, 2012 and 2030 and calculation of the future marginal mix of power generation.

Electricity source	TWh 2014[a]	TWh 2030[a]	Annual growth 2014-2030	Plant lifetime (years)[b]	Capital replacement rate (%)[c]	Net annual growth 2014-2030 (%) [d]	Net annual growth 2014-2030 (TWh/yr)[e]	Marginal mix[f]
Coal	72.9	167.4	8%	60	-1.7%	9.8%	7.12	25%
Oil	0.0	0.0	0%	60	-1.7%	1.7%	0	0%
Gas	110.7	111.6	0.1%	30	-3.3%	3.4%	3.74	13%
Biomass	2.7	6.2	8%	45	-2.2%	10.3%	0.27	1%
Nuclear	0.0	93.0	Infinite[g]	60	-1.7%	Infinite[g]	5.81[g]	20%
Hydro	70.2	105.4	3%	60	-1.7%	4.8%	3.37	12%
Wind	8.1	105.4	75%	20	-5.0%	80.1%	6.49	23%
Geothermal	2.7	6.2	8%	20	-5.0%	13.1%	0.35	1%
Solar	2.7	24.8	51%	30	-3.3%	54.5%	1.47	5%
Marine	0.0	0.0	0	20	-5.0%	0	0	0%
Total	**270.0**	**620.0**	**n.a.**	**n.a.**	**n.a.**	**n.a.**	**28.64**	**100%**

[a] WWF (2014). [b] NREL (2010). [c] Calculated as the inverse of the plant lifetime, with a minus sign. [d] Calculated as the annual growth 2014-2030 minus the capital replacement rate. [e] Calculated as the generation in 2014 times the net annual growth. [f] Calculated as the technology's net annual growth divided by the total (TWh/yr). [g] When a technology departs from zero production the annual growth rate becomes infinite. In this case the net annual growth (TWh/yr) is simply calculated as the absolute increase in production divided by the number of years.

This electricity mix has been modelled with ecoinvent by adapting the existing data set for production of electricity in Turkey at high voltage, whereas the original data sets for transforming from high to medium voltage have been kept unchanged. Besides changing the original contribution of the individual technologies to the electricity mix, below we report other adaptations required to implement this marginal mix in ecoinvent:

- In ecoinvent, production of electricity at high voltage in Turkey does not contain production from photovoltaics. Photovoltaics have been added by means of two Rest-of-the-World (RoW) data sets for production in multi-Si and single-Si panels. We assumed a share of 50% each.
- In addition to the above, photovoltaics are assumed to supply the grid at high voltage rather than at low voltage. This was done to simplify the implementation of the marginal electricity mix in ecoinvent. Although this might deviate from reality, we expect this deviation to have a negligible impact in the results.

- In ecoinvent, production of electricity at high voltage in Turkey does not contain production from nuclear sources. Nuclear has been added by means of two RoW data sets for production in boiling water reactors and pressure water reactors. We assumed a share of 50% each.
- The ecoinvent database does not contain data sets for production of electricity from biomass. This was solved by adapting a RoW data set for heat production from biomass (heat production from hardwodd chips at forest, at furnace 1000 kW), assuming the calorific value of the biomass can be transformed to electricity with 30% efficiency (see inventory for this activity in this Section 6).
- The original electricity mix for Turkey in ecoinvent goes beyond our generation technology classification in the sense that, for example, what in Table 3 is classified as coal, in the ecoinvent data set corresponds to the sum of hard coal and lignite, where hard coal contributes to 74% of the coal-based production and lignite contributes to the remaining 26%. In our adaptation we have kept these relative contributions from hard coal and lignite constant. The same applies to wind power and hydropower, which also consist of the sum of different technology options, such as onshore and offshore for wind power and run-of-river and dams in hydropower.

Table 4. LCI for production of electricity in Turkey, high voltage.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Electricity, TR, high voltage	kWh	1	
Inputs of products and services:			
Transmission network	km	3.17E-10	Transmission network, long-distance {GLO}| market for | Conseq
Transmission network	km	6.58E-09	Transmission network, electricity, high voltage {GLO}| market for | Conseq
Losses	kWh	0.05655	Electricity, TR, high voltage (this data set)
Electricity production, geothermal	kWh	0.0124	Electricity, high voltage {TR}| electricity production, deep geothermal | Conseq
Electricity production, hard coal	kWh	0.0641	Electricity, high voltage {TR}| electricity production, hard coal | Conseq
Electricity production, lignite	kWh	0.184	Electricity, high voltage {TR}| electricity production, lignite | Conseq
Electricity production, hydropower	kWh	0.0588	Electricity, high voltage {TR}| electricity production, hydro, reservoir, non-alpine region | Conseq
Electricity production, hydropower	kWh	0.0588	Electricity, high voltage {TR}| electricity production, hydro, run-of-river | Conseq
Electricity production, natural gas	kWh	0.131	Electricity, high voltage {TR}| electricity production, natural gas, combined cycle power plant | Conseq
Electricity production, wind	kWh	0.0442	Electricity, high voltage {TR}| electricity production, wind, <1MW turbine, onshore | Conseq
Electricity production, wind	kWh	0.00929	Electricity, high voltage {TR}| electricity production, wind, >3MW turbine, onshore | Conseq
Electricity production, wind	kWh	0.173	Electricity, high voltage {TR}| electricity production, wind, 1-3MW turbine, onshore | Conseq
Electricity production, biomass	kWh	0.0097	Electricity from biomass {RoW} (LCI data in Section 6)
Electricity production, nuclear	kWh	0.102	Electricity, high voltage {WECC, US only}| electricity production, nuclear, boiling water reactor | Conseq
Electricity production, nuclear	kWh	0.102	Electricity, high voltage {RoW}| electricity production, nuclear, pressure water reactor | Conseq
Electricity production, photovoltaic	kWh	0.0257	Electricity, low voltage {RoW}| electricity production, photovoltaic, 3kWp slanted-roof installation, multi-Si, panel, mounted | Conseq
Electricity production, photovoltaic	kWh	0.0257	Electricity, low voltage {RoW}| electricity production, photovoltaic, 3kWp slanted-roof installation, single-Si, panel, mounted | Conseq
Emissions to air:			
Dinitrogen monoxide	kg	0.000005	As in original ecoivnent data set Electricity, high voltage {TR}| market for | Conseq
Ozone	kg	4.16-06	As in original ecoivnent data set Electricity, high voltage {TR}| market for | Conseq

3.2. Europe

Table 5 shows the electricity generation in Europe in 2008 and the predicted generation in 2020. Generation in 2008 was obtained from IEA (2010a, p IV.59) and for 2020 from IEA (2010b, p 636-8). These data cover European countries being part of OECD, namely Austria, Belgium, the Czech Republic, Denmark, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Luxembourg, the Netherlands, Norway, Poland, Portugal, the Slovak Republic, Spain, Sweden, Switzerland, Turkey, and the United Kingdom. The electricity mixes for these countries are assumed to be representative for a European electricity mix.

Table 5. Power generation in Europe, 2008 and 2020 and calculation of the future marginal mix of power generation.

Electricity source	TWh 2008[a]	TWh 2020[b]	Annual growth 2008-2020	Plant lifetime (years)[c]	Capital replacement rate (%)[d]	Net annual growth 2008-2020 (%)[e]	Net annual growth 2008-2020 (TWh/yr)[f]	Marginal mix[g]
Coal	934	710	-1.5%	60	-1.7%	0.2%	1.56	1.6%
Oil	104	44	-4%	60	-1.7%	-1.9%	0.00	0.0%
Gas	869	942	0.5%	30	-3.3%	3.9%	33.54	33.7%
Biomass	113	183	4%	45	-2.2%	6.1%	6.88	6.9%
Nuclear	922	909	0%	60	-1.7%	1.6%	14.56	14.6%
Hydro	554	593	0%	60	-1.7%	2.1%	11.66	11.7%
Wind	120	455	17%	20	-5.0%	22.4%	26.94	27.0%
Geothermal	10	16	4%	20	-5.0%	8.9%	0.88	0.9%
Solar	8	61	45%	30	-3.3%	47.9%	3.59	3.6%
Marine	1	2	19%	20	-5.0%	23.8%	0.12	0.1%
Total	**3,634**	**3,915**	**n.a.**	**n.a.**	**n.a.**	**n.a.**	**99.61**	**100.0%**

[a] IEA (2010a, p IV.59). [b] IEA (2010b, p 636-8). [c] NREL (2010. [d] Calculated as the inverse of the plant lifetime, with a minus sign. [e] Calculated as the annual growth 2014-2030 minus the capital replacement rate. [f] Calculated as the generation in 2008 times the net annual growth. [g] Calculated as the technology's net annual growth divided by the total (TWh/yr).

In ecoinvent there are no data sets for production of electricity at high voltage in Europe, but only for individual countries. In order to produce an operational data set, and given that this data set is only meant to be used in a sensitivity analysis, we used the Turkish data set in Table 4 as a template, in which we only modified the composition of the mix according to Europe as shown in Table 5. In those cases where the data set contained more than one option for a given generation technology, for example lignite and hard coal for 'Coal', we assumed an equal share for the different options, i.e. a 50/50 split in the case of hard coal and lignite.

Table 6. LCI for production of electricity in Europe, high voltage.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Electricity, Europe, high voltage	kWh	1	
Inputs of products and services:			
Transmission network	km	3.17E-10	Transmission network, long-distance {GLO}| market for | Conseq
Transmission network	km	6.58E-09	Transmission network, electricity, high voltage {GLO}| market for | Conseq
Losses	kWh	0.05655	Electricity, TR, high voltage (this data set)
Electricity production, geothermal	kWh	0.00785	Electricity, high voltage {TR}| electricity production, deep geothermal | Conseq
Electricity production, hard coal	kWh	0.0042	Electricity, high voltage {TR}| electricity production, hard coal | Conseq
Electricity production, lignite	kWh	0.00785	Electricity, high voltage {TR}| electricity production, lignite | Conseq
Electricity production, hydropower	kWh	0.0585	Electricity, high voltage {TR}| electricity production, hydro, reservoir, non-alpine region | Conseq
Electricity production, hydropower	kWh	0.0585	Electricity, high voltage {TR}| electricity production, hydro, run-of-river | Conseq
Electricity production, natural gas	kWh	0.337	Electricity, high voltage {TR}| electricity production, natural gas, combined cycle power plant | Conseq
Electricity production, wind	kWh	0.0901	Electricity, high voltage {TR}| electricity production, wind, <1MW turbine, onshore | Conseq
Electricity production, wind	kWh	0.0901	Electricity, high voltage {TR}| electricity production, wind, >3MW turbine, onshore | Conseq
Electricity production, wind	kWh	0.0901	Electricity, high voltage {TR}| electricity production, wind, 1-3MW turbine, onshore | Conseq
Electricity production, biomass	kWh	0.0691	Electricity from biomass {RoW} (LCI data in Section 6)
Electricity production, nuclear	kWh	0.0731	Electricity, high voltage {WECC, US only}| electricity production, nuclear, boiling water reactor | Conseq
Electricity production, nuclear	kWh	0.0731	Electricity, high voltage {RoW}| electricity production, nuclear, pressure water reactor | Conseq
Electricity production, photovoltaic	kWh	0.0181	Electricity, low voltage {RoW}| electricity production, photovoltaic, 3kWp slanted-roof installation, multi-Si, panel, mounted | Conseq
Electricity production, photovoltaic	kWh	0.0181	Electricity, low voltage {RoW}| electricity production, photovoltaic, 3kWp slanted-roof installation, single-Si, panel, mounted | Conseq
Emissions to air:			
Dinitrogen monoxide	kg	0.000005	As in original ecoinvent data set Electricity, high voltage {TR}| market for | Conseq
Ozone	kg	4.16-06	As in original ecoinvent data set Electricity, high voltage {TR}| market for | Conseq

4. Reference scenario inventory

4.1. Wastewater treatment equipment

We have not been able to find specific inventory data for infrastructure of industrial WWTPs. The ecoinvent database contains data sets for construction of urban wastewater treatment plants in Switzerland, for five different sizes, which we use as an approximation. We calculated an inventory for the Tüpraş WWTP by interpolating the figures from the two closest capacities (5E+09 L/year and 1E+09 L/year). The only specific information regarding the Tüpraş facility is land occupation, which we estimate as 9,470 m^2, based on the satellite image in Google Maps.

Figure 1. Satellite image of the Tüpraş WWTP in the Izmit refinery, obtained from Google Maps. The estimated total area is 9,470 m^2.

The dismantling of the WWTP and disposal of the embedded materials and equipment has been determined based on the amounts quantified for its construction and existing or adapted ecoinvent data sets for waste disposal. Concrete and excavated soil are quantified in kg in the waste disposal data sets, while they are quantified as m^3 in the construction data set. Mass was calculated for these materials with the following densities: 2,200 kg/m^3 for concrete, 1,000 kg/m^3 for soil.

The overall LCIs for construction and dismantling (end of life) of the refinery WWTP are displayed in Table 7 and Table 8. These correspond to the total amount of materials, etc., for the plant as a whole. In order to attribute these activities to the wastewater being treated, it is necessary to define a life span for the plant, which we set at 30 years, the same value considered for urban WWTPs in the ecoinvent database.

Table 7. LCI for construction of the refinery WWTP, reference scenario.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Refinery WWTP construction	unit	1	Reference flow is 1 WWTP
Inputs of resources:			
Transformation, from unknown previous use	m^2	9,470	
Transformation, to industrial area, built up	m^2	9,470	
Occupation, industrial area, built up	m^2yr	284,100	9,470 m^2 during 30 years
Inputs of products and services:			
Aluminium	kg	28,952	Aluminium, cast alloy {GLO}| market for | Conseq, U
Unspecified inorganic chemicals	kg	16,556	Chemical, inorganic {GLO}| market for chemicals, inorganic | Conseq
Unspecified organic chemicals	kg	135,890	Chemical, organic {GLO}| market for | Conseq, U
Concrete	m^3	33,299	Concrete, high exacting requirements {CH}| market for | Conseq
Copper	kg	30,737	Copper {GLO}| market for | Conseq
Electricity, TR	kWh	1,264	LCI data in Table 3
Excavation	m^3	116,180	Excavation, hydraulic digger {GLO}| market for | Conseq
Processing of plastics	kg	82,125	Extrusion, plastic film {GLO}| market for | Conseq
Glass fibre	kg	65,372	Glass fibre {GLO}| market for | Conseq
Limestone	kg	715,035	Limestone, crushed, washed {GLO}| market for | Conseq
Pitch	kg	16,743	Pitch {GLO}| market for | Conseq
Polyethylene components, high density	kg	81,578	Polyethylene, high density, granulate {GLO}| market for | Conseq
Polyethylene components, low density	kg	537	Polyethylene, low density, granulate {GLO}| market for | Conseq
Reinforcing steel	kg	2,586,390	Reinforcing steel {GLO}| market for | Conseq
Rock wool	kg	29,116	Rock wool, packed {GLO}| market for | Conseq
Stainless steel	kg	207,503	Steel, chromium steel 18/8, hot rolled {GLO}| market for | Conseq
Rubber	kg	29,456	Synthetic rubber {GLO}| market for | Conseq
Tap water	kg	4,062,450	Tap water {RoW}| market for | Conseq

Table 8. LCI for dismantling the refinery WWTP, reference scenario.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Refinery WWTP dismantling	unit	1	Reference flow is 1 WWTP
Waste treatment:			
Aluminium waste	kg	28,952	Waste aluminium {GLO}| market for | Conseq
Inert waste	kg	117,112,352	Accounts for inorganic chemicals, organic chemicals, excavated material, glass fibre and limestone. Ecoinvent data set: Inert waste {GLO}| market for | Conseq
Concrete waste	kg	73,257,690	Waste concrete, not reinforced {GLO}| market for | Conseq
Copper waste	kg	30,737	Copper scrap, sorted, pressed {GLO}| market for | Conseq
Pitch waste	kg	16,743	Waste bitumen {GLO}| market for | Conseq
Polyethylene waste	kg	82,114	Waste polyethylene {GLO}| market for | Conseq
Reinforcing steel waste	kg	2,586,390	Waste reinforcement steel {GLO}| market for | Conseq
Rock wool waste	kg	29,116	Waste mineral wool {GLO}| market for | Conseq
Steel waste	kg	207,503	Steel scrap recovery (LCI data in Section 6)
Rubber waste	kg	29,456	Waste rubber, unspecified {GLO}| market for | Conseq

4.2. Use of energy and chemicals

Electricity consumption for the refinery WWTP (DAF unit, biological treatment, sludge dewatering) was provided by Tüpraş as confidential information and for this reason is not disclosed here. Concerning chemical reagents, the following doses are considered, based either on literature or data provided by Tüpraş:

- Iron chloride as coagulant to enhance flotation: 200 ppm (Hernando 2011). It must be highlighted that the choice of product and dose is not necessarily reflecting the actual operation at Tüpraş.
- Polyelectrolyte as flocculant to enhance flotation: 2 ppm according to Tüpraş.
- Phosphoric acid as nutrient for biological treatment: this has been estimated, based on a COD:P ratio of 250. With a COD of 370 mg/L and a phosphate-P concentration of 1.3 mg/L, the additional P requirement is 0.2 mg P/L. Phosphorus is assumed to be added in a 54% solution of phosphoric acid, thus leading to a dose of 0.001 kg solution per m^3 wastewater.

4.3. Effluent composition

Table 9 presents the effluent composition considered for the reference WWTP. It must be highlighted that while some parameters correspond to actual measurements at the Izmit refinery, while for others the legal discharge limit is used instead.

Table 9. Emissions in the effluent of the WWTP currently in operation at the Tüpraş refinery.

Parameters	Unit	Effluent	Source and comments
Oil and grease, to sea	mg/L	10	Legal discharge limit in Turkey
Total organic carbon (TOC), to sea	mg/L	15	Provided by Tüpraş
Suspended solids, to sea	mg/L	60	Legal discharge limit in Turkey
Chemical oxygen demand (COD), to sea	mg/L	200	Legal discharge limit in Turkey
Biological oxygen demand (BOD), to sea	mg/L	33	Provided by Tüpraş
Ammonium, to sea	mg/L	20	Legal discharge limit in Turkey
Nitrate, to sea	mg/L	1.6	Provided by Tüpraş
Phosphate, to sea	mg/L	<0.1	Provided by Tüpraş. Considered as zero in the LCI

4.4. VOC emissions

According to Barthe et al. (2015), WWTPs in refineries are a source of volatile organic carbon (VOC) emissions. The main sources are the oil separation unit, the flotation unit and the biological reactor. They provide emission factors for each of these treatment units as a function of their area. In the study we have made an estimate of the magnitude of these emissions at the Tüpraş WWTP using these emission factors, but excluding emissions from the API oil separation unit, as it is excluded from our study. Table 10 shows that we estimate an emission of 22 kg VOC/day, or 1.83 mg VOC/L.

Table 10. Estimate of VOC emissions in the Tüpraş WWTP.

Parameter	Flotation unit	Biological unit	Total
Emission factor ($kg/m^2/h$)[a]	0.002	0.0002	n.a.
Area (m^2)[b]	126	3,312	3,438
Emission (kg/day)	6	16	22
Emission (mg/L)[c]	0.50	1.32	1.83

[a] Barthe et al. (2015, p. 219)

[b] Provided by Tüpraş.

[c] The daily wastewater flow is 12,000 m^3.

4.5. Dissolved air flotation

The contribution of this process to consumption of energy, chemicals and emissions of VOC has already been described. In this section we only describe the calculation of the amount of sludge produced. Sludge production is calculated based on a mass balance considering the amount of oil removed and the contribution of the coagulant and flocculant.

The initial oil and grease concentration at the inlet of the flotation unit is 20 mg/L and this is estimated to be 11.3 mg/L at the outlet. The final effluent value after biological treatment is 10 mg/L (Table 9). The additional 1.3 mg/L are taken into account as VOC emissions in the biological treatment unit as calculated in Table 10. Also, in the flotation tank 0.50 mg/L VOC are emitted (Table 10).

The amount of sludge produced by the coagulant is calculated considering that the addition of iron chloride results in the formation of iron hydroxide (Equation 1), which is removed with the sludge. The chloride anion remains dissolved in water and is not considered in the calculation of sludge production.

$$FeCl_3 + 3\ H_2O \rightarrow Fe(OH)_3 + 3\ HCl$$

Equation 1

Based on stoichiometry, 200 mg/L iron chloride result in 162 mg/L iron hydroxide. Finally, the flocculant dose, of 2 mg/L, is also considered entirely as partitioned to sludge. The total amount of sludge (in dry mass) created per L wastewater in the flotation unit is thus calculated as:

20 mg oil - 0.5 mg VOC - 11.3 mg oil + 131 mg $Fe(OH)_3$ + 2 mg pol. = 139.2 mg sludge dry mass

4.6. Biological treatment

The biological treatment considered consists of an activated sludge basin followed by secondary settling. The contribution of this process to consumption of energy and emissions of VOCs has been described in the previous sections, as well as the composition of the treated effluent. In this section we focus on the following aspects:

- Production of excess sludge.
- Emissions to air of CO_2 and N_2O from the aeration basin.

Production of excess sludge is estimated based on the concept of observed yield, shown in Equation 2:

$$Y_{obs} = Y / (1 + k_d \cdot \theta_c)$$

Equation 2

Where:

- Y_{obs} is the observed yield (g VSS/g COD removed) or net amount of biomass produced per unit of mass substrate removed.
- Y is the yield (g VSS/g COD removed) or amount of biomass produced per unit of mass substrate removed. This parameter ranges from 0.3 to 0.7 (von Sperling 2007, p. 94). A value of 0.5 is chosen for the calculations.

- k_d is the endogenous respiration coefficient or bacterial decay coefficient (day^{-1}), ranging from 0.05 to 0.12 (von Sperling 2007, p. 92. A value of 0.085 is chosen for the calculations.
- θ_c is the sludge residence time in the system (days). The specific value for the Tüpraş WWTP is 30 days.

The Y_{obs} value calculated with Equation 2 is 0.14 g VSS/g COD removed. The amount of COD removed is 278 g/m^3, therefore 39 g excess VSS are produced per m^3 wastewater.

Emissions of CO_2, in kg /m^3, produced by respiration of microorganisms in the biological reactor are calculated with Equation 3:

$$CO_2 = COD_{rem} \cdot [1 - (Y_{obs} \cdot 1.42)] \cdot C_{COD} \cdot 44/12$$

Equation 3

Where:

- COD_{rem} is the amount of COD removed, namely 0.278 kg/m^3 as stated above.
- 1.42 is the COD content of sludge biomass (kg COD/kg VSS)
- C_{COD} is the carbon content of COD in the wastewater (kg organic carbon/kg COD). The average value for Tüpraş is 0.23.
- 44/12 are stoichiometric factors to convert organic carbon into carbon dioxide.

The resulting emission is 0.187 kg CO_2/m^3 wastewater.

N_2O emissions are estimated based on an emission factor of 0.005 kg N_2O-N/kg N input to the biological reactor (Muñoz et al. 2016). Counting the input of ammonia and nitrate in the influent the total-N input is 0.017 kg N/m^3, resulting in an emission of 1.3E-04 kg N_2O/m^3.

4.7. Degradation in the environment

Besides the emissions quantified so far, eventually all substances containing organic carbon, which are released to the sea or to the atmosphere are expected to degrade in the environment. In the ocean mainly through the action of microorganisms as well as abiotic processes such as photolysis. If some substance volatilizes it is also expected to be degraded in the atmosphere through reaction with hydroxyl radicals.

The total organic carbon in the effluent is 15 mg/L (Table 9), while the organic carbon content in the VOC emissions (Table 10) is estimated as 1.5 mg/L. Assuming all carbon is converted to CO_2, this results in 0.06 kg CO_2/m^3.

Besides carbon, the WWTP releases nitrogen in the form of ammonium and nitrate, which is expected to lead to some N_2O emissions in the environment. Based on Table 9, the total-N in the effluent is 13 mg/L. Considering the same emission factor as in the biological treatment, of 0.005 kg N_2O-N/kg N input, this results in an emission of 1.0E-04 kg N_2O/m^3.

4.8. Sludge disposal

Sludge produced during flotation and biological treatment adds up to 180 g dry mass/m^3. This material is dewatered with the aid of a polyelectrolyte, added at a rate of 0.005 kg/kg dry mass, according to Tüpraş. Thus, the overall sludge production attributable to the WWTP is 181 g dry mass/m^3. After dewatering, a dry mass content of 37% is achieved according to Tüpraş. Therefore, the sludge production in wet mass is 490 g/m^3.

Dewatered sludge is sent by Tüpraş to a cement factory, where it is used as fuel. The transport distance is 215 km. This transport step is modelled with average road transport data from ecoinvent, assuming an empty return trip by the truck.

In the cement factory, the sludge is dried to improve its fuel value. It is assumed that it is dried from 37% dry mass to 90% dry mass, reducing the wet weight from 0.49 kg/m^3 to 0.20 kg/m^3. This operation is highly energy-intense, however it is assumed that the source of this energy is hot waste gases from the cement kiln (Global cement 2013). The energy used to process the sludge is estimated as 0.1 kWh electricity and 3.6 MJ heat per kg water evaporated (Doblado 2004). Based on the target of 90% dry mass to be achieved, the net energy used is 0.029 kWh electricity and 1.04 MJ in hot gas per m^3 wastewater. The use of hot gases from the cement kiln is not attributed any environmental impact.

The use of sludge as fuel substitutes conventional fuels used at the cement factory on an energy-content basis. For this reason, it is necessary to define the net calorific value of the sludge. Also, in order to quantify the CO_2 emissions released by combustion of sludge it is necessary to quantify the organic carbon content in the sludge. Finally, the ash contained in the sludge is incorporated in the clinker. Since the ash content of sludge is higher than that of conventional fuels, its use leads to a decrease in the input of raw meal (limestone, clay, etc.) for clinker production. It is therefore necessary to quantify the ash content of the sludge.

The low heating value (LHV) of sludge, in MJ/kg, is calculated with Equation 4 and Equation 5:

$$LHV = HHV - 2.447 \cdot (W + 9H)$$

Equation 4

$$HHV = 34.016 \cdot C - 9.8324 \cdot O + 124.265 \cdot H + 6.276 \cdot N + 19.079 \cdot S$$

Equation 5

Where:

- *HHV* is the high heating value (HHV), in MJ/kg,
- *W* is the moisture content in sludge, in kg water/kg,
- *H* is the hydrogen content in sludge, excluding that from moisture, in kg H/kg,
- *C* is the carbon content in sludge, in kg C/kg,
- *O* is the oxygen content in sludge, excluding that from moisture, in kg O/kg,
- *N* is the nitrogen content in sludge, in kg N/kg,
- *S* is the sulfur content in sludge, in kg S/kg.

Equation 5 calculates the total heating value of the fuel, whereas Equation 4 adjusts this value by subtracting the latent heat of evaporation for water (44.03 kJ/mol) initially present in the fuel or formed during combustion. Equation 4 is obtained from Muñoz et al. (2007).

In Table 11 we summarize the data used to calculate the low calorific value of sludge with 90% dry mass, as combusted in the cement kiln. The resulting fuel value of the sludge is 1.27 MJ/m^3 wastewater originating this sludge.

Table 11. Calculation of low calorific value of sludge in the reference scenario, when dried to 90% dry mass.

Component	Low calorific value (MJ/kg component)[a]	Content in sludge (kg/m^3 wastewater)	Low calorific value (MJ/m^3 wastewater)[a]	Comments
Oil and grease	41.0	0.082	0.33	Composition of crude oil from ChemEngineering (2017): 83% C, 12% H, 1% N, 1% O, 3% S
$Fe(OH)_3$	0	0.131	0	Does not have fuel value
Biomass	22.4	0.039	0.88	Empirical formula of biomass volatile solids from Muñoz et al. (2016) is $C_5H_7O_2N$
Polyelectrolyte	37.9	0.003	0.11	We assume polyelectrolyte used is polyacrylamide, with the empirical formula $(C_3H_5NO)_n$
Water	-2.45	0.020	-0.05	Based on Equation 4
Total	6.3	0.201	1.27	The value of 6.3 is calculated as the ratio 1.27/0.201

[a] Calculated as the product of the values in the two previous columns, except the total, which is calculated as the sum of the contributions from all components.

The carbon content in sludge is calculated with a similar procedure as in the table above, that is, defining the carbon content of the individual components, considering the compositions used in the previous table (column Comments). The resulting carbon content on a per m^3 wastewater basis is 0.029 kg C, which stoichiometrically implies an emission of 0.107 kg CO_2/m^3 associated to combustion of the sludge.

In terms of emissions in the cement kiln, it is not straightforward to determine whether combustion of sludge leads to different levels in the emission of air pollutants compared to the operation of a cement kiln not using sludge. In the inventory we consider that levels of pollutants such as particles, SO_2, NOx, heavy metals, etc., remain unaltered on a per MJ fuel basis, regardless of the fuel used. The only exception to this is CO_2 emissions, where the difference between using sludge and conventional fuels can be taken into account, given that the carbon content of sludge and of the replaced fossil fuels is well known.

As for the ash content, based on Table 11, the main contribution to ash is expected to be the iron hydroxides, which are present in a concentration of 0.65 kg/kg dry mass. The combustion of sludge in the cement kiln is expected to lead to the oxidation of these iron hydroxides, as follows:

$$2\ Fe(OH)_3 \rightarrow Fe_2O_3 + 3\ H_2O$$

Equation 6

According to stoichiometry, and neglecting the contribution from other sludge components, the amount of ash produced is 0.098 kg/m^3 wastewater.

Both the replacement of conventional fuels and of raw meal by the use of sludge as fuel have been modelled taking into account the inputs to the cement industry in Europe according to the ecoinvent database, in particular with the data set for clinker production in Europe without Switzerland. Detailed LCI tables for these processes (fuels for clinker production, raw meal for clinker production) are available in Section 6. The overall inventory for sludge disposal is shown in Table 12.

Table 12. LCI for disposal of sludge in the cement factory.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Refinery sludge disposal, reference situation	kg	0.49	Dewatered sludge containing 37% dry mass
Inputs of products and services:			
Transport, road	kgkm	211	Transport to cement factory. Ecoinvent data set *Transport, freight, lorry, unspecified {GLO}| market for | Conseq*
Waste heat	MJ	1.04	Excess heat from cement kiln, no burdens associated
Electricity, TR	kWh	0.029	Table 3
Fuels for clinker production	MJ	-1.27	LCI data available in Section 6
Raw meal for clinker production	kg	-0.098	LCI data available in Section 6
Emissions to air [a]:			
CO_2, fossil	kg	0.107	Calculated based on data from Table 11

[a] Emissions to air other than CO_2 are neglected, since we assume they remain constant in the cement kiln regardless of the use of sludge as fuel.

4.9. Overall LCI for the reference scenario

In Table 13 we summarize the overall LCI for refinery wastewater treatment in the reference situation, based on the inventory data presented in the previous sections.

Table 13. LCI for refinery wastewater treatment, reference situation.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Refinery wastewater treatment, reference	m^3	1	
Inputs of products and services:			
Polyelectrolyte	kg	0.003	Ecoinvent data set Chemical, organic {GLO}| market for | Conseq
Iron chloride, pure	kg	0.2	Ecoinvent data set Iron (III) chloride, without water, in 40% solution state {GLO}| market for | Conseq
Phosphoric acid, 54%	kg	0.001	Phosphoric acid, 54% (LCI data in Section 6)
Electricity, TR	kWh	1.5	Table 3
Refinery WWTP construction	unit	7.61E-09	Table 7
Emissions to air:			
CO_2, fossil	kg	0.187	Emission from biological treatment
CO_2, fossil	kg	0.06	Emission from degradation in the environment of treated effluent
N_2O	kg	1.3E-04	Emission from biological treatment
N_2O	kg	1.0E-04	Emission from degradation in the environment of treated effluent and VOC emissions
VOC	kg	0.0018	Emission from flotation plus biological treatment
Emissions to sea water:			
Water	kg	999.7	Treated effluent. Equals input water minus water in dewatered sludge
Nitrate	kg	0.0016	Treated effluent, Table 9
Ammonium	kg	0.0166	Treated effluent, Table 9
Chemical oxygen demand (COD)	kg	0.092	Treated effluent, Table 9
Oil and grease	kg	0.01	Treated effluent, Table 9. Speciation of oil and grease according to Table 2
Waste to treatment:			
Sludge disposal	kg	0.49	Table 12
Refinery WWTP dismantling	unit	7.61E-09	Table 8

5. INTEGROIL scenarios inventory

5.1. INTEGROIL plant equipment

Table 14 shows the LCI data for construction of the INTEGROIL plant, including the five treatment modules (DAF, MBR, CWAO, AOP, RO), expressed per year of plant use. The table also includes the inventory for a common electrical installation. These data originate from the design by each technology developer, as a scale-up from the demonstration plant to the assessed scale (500 m^3/h). Table 15 in turn shows the LCI data for plant dismantling, also expressed on the basis of one year of use.

Table 14. LCI for construction of the up-scaled INTEGROIL plant (500 m^3/h), 1 year of use.

Exchanges	Unit	DAF	MBR	CWAO	AOP	RO	Electrical installation	Ecoinvent data sets/comments
Reference flow:								
INTEGROIL plant construction	Year	1	1	1	1	1	1	Reference flow is 1 year of INTEGROIL plant use
Inputs of resources:								
Transformation, from unknown previous use	m^2	2.8E-05	1.9E-04	1.8E-05	8.7E-05	1,724		Assuming the useful life is 30 years.
Transformation, to industrial area, built up	m^2	8.3E-05	1.9E-04	1.8E-05	8.7E-05	3.9E-04		Assuming the useful life is 30 years.
Occupation, industrial area, built up	m^2yr	365	829	80	380	3.9E-04		
Inputs of products and services:								
Automated valves	kg	9	226			33		Actuator valve (LCI data in Section 6)
Compressors	kg	150	735					Air compressor, screw-type compressor, 300kW (LCI data in Section 6)
Compressors	kg				67			Air compressor, screw-type compressor, 4kW (LCI data in Section 6)
Particle filter	kg				25			Air filter (LCI data in Section 6)
Aluminium parts	kg		101					Aluminium product (LCI data in Section 6)
Concrete			46,080					Concrete (LCI data in Section 6)
IBC container	kg					3.8		IBC (LCI data in Section 6)
Reinforcing steel			569					Reinforcing steel {GLO}| market for | Conseq
Polyethylene parts	kg		9.9					Polyethylene product (LCI data in Section 6)
Polypropylene parts	kg	1,310	9			668		Polypropylene product (LCI data in Section 6)
Pumps	kg	177	4,902		60	829		Pump (LCI data in Section 6)
Polyvinylchloride parts and valves	kg	43	185		444	51		PVC product (LCI data in Section 6)
Air drier	kg				437			Refrigeration machine, R134a as refrigerant (LCI data in Section 6)
Steel parts	kg	15	4,102	2,170		1,660	966	Steel product (LCI data in Section 6)
Stainless steel parts	kg	199	3,014	2,878	29	62		Steel product, chromium steel (LCI data in Section 6)

Exchanges	Unit	DAF	MBR	CWAO	AOP	RO	Electrical installation	Ecoinvent data sets/comments
Variable speed drive	kg		27					Electric motor, electric passenger car {GLO}| electric motor production, vehicle (electric powertrain) | Conseq
Electric and electronic equipment	kg	14	97			61	48	Electronics, for control units {GLO}| market for | Conseq
Glass fibre reinforced plastic parts	kg	740	3		853	2,950		Glass fibre reinforced plastic, polyester resin, hand lay-up {GLO}| market for | Conseq
Glass rotameter	kg			0.18				Glass tube, borosilicate {GLO}| market for | Conseq
Klingersil	kg			2	1.4			Klingersil (LCI data in Section 6)
Ozonator	kg				667			Metal working machine, unspecified {GLO}| market for | Conseq
Polymethylmethacrylate probe	kg				0.12			Polymethyl methacrylate, sheet {GLO}| market for | Conseq
Polyvinylidene fluoride parts	kg	7.6				3.7		Polyvinylfluoride, film {GLO}| market for | Conseq
Ceramic membranes	kg		1,807					Refractory, high aluminium oxide, packed {GLO}| market for | Conseq
RO membranes	m^2					845		Seawater reverse osmosis module {GLO}| market for | Conseq
Silicone parts	kg				0.066			Silicone product {GLO}| market for | Conseq
Rubber parts	kg		9					Synthetic rubber {GLO}| market for | Conseq
IT screens	kg						32	Display, liquid crystal, 17 inches (LCI data in Section 6)
Electronic components	kg						2.7	Printed wiring board, surface mounted, unspecified, Pb free {GLO}| market for | Conseq
Router	kg						1.3	Router (LCI data in Section 6)

Table 15. LCI for dismantling of the up-scaled INTEGROIL plant (500 m³/h), 1 year of use.

Exchanges	Unit	DAF	MBR	CWAO	AOP	RO	Electrical installation	Ecoinvent data sets/comments
Reference flow:								
INTEGROIL plant dismantling	year	1	1	1	1	1	1	Reference flow is dismantling of materials for 1 year of INTEGROIL plant use
Waste to treatment:								
IBC	kg					3.8		Waste IBC (LCI data in Section 6)
Machinery	kg	327	5,664		1,231	829		Machinery disposal (LCI data in Section 6)
Steel parts	kg	214	7,685	5,048	29	1,722	966	Steel scrap recovery (LCI data in Section 6)
Air filters	kg				25			Waste air filter (LCI data in Section 6)
Automated valves	kg	9.2	226			33		Waste actuator valve (LCI data in Section 6)
Glass fibre reinforced plastic	kg	740	3.48		853	2,950		Waste glass fibre reinforced plastic (LCI data in Section 6)
Aluminium parts	kg		101					Aluminium scrap, post-consumer {GLO}| market for | Conseq
Electronic components	kg	14	97			63	49	Electronics scrap {GLO}| market for | Conseq
Membranes, klingersil, silicone	kg		1,807	2	1.5			Inert waste {GLO}| market for | Conseq
Concrete			46,080					
Glass rotameter	kg			0.18				Waste glass {GLO}| market for | Conseq
Plastic parts, unspecified	kg	7.6			0.12	634		Waste plastic, mixture {GLO}| market for | Conseq
Polyethylene parts	kg		9.9					Waste polyethylene {GLO}| market for | Conseq
Polypropylene parts	kg	1,310	9			668		Waste polypropylene {GLO}| market for | Conseq
Polyvinylchloride and polyvinylidene fluoride parts	kg	43	185		444	52		Waste polyvinylchloride {GLO}| market for | Conseq
Rubber parts	kg		9					Waste rubber, unspecified {GLO}| market for | Conseq
IT screens	kg						32	Liquid crystal display {GLO}| market for | Conseq
Electronic components	kg						2.7	Used printed wiring boards {GLO}| market for | Conseq

5.2. DAF operation

The LCI for operation of the DAF module includes the following inputs, expressed as an average per m^3 at the inlet of the INTEGROIL plant:

- Electricity consumption: due to confidentiality reasons this figure cannot be disclosed. However it can be stated that the value is in the same order of magnitude than existing values in literature (Vlasopoulos et al. 2006; Barthe et al. 2015).
- Dose of starch-based coagulant: 62.5 mg/L
- Dose of polyelectrolyte: 0.6 mg/L

- Dose of sodium hydroxide (pure): 0.9 mg/L

The DAF module produces 0.01 m^3 of flotation sludge per m^3 produced water. The dry mass content of this sludge is estimated, based on the oil and grease removal efficiency and that 100% of the coagulant and polyelectrolyte are also partitioned to the sludge phase. Thus, the sludge contains, per m^3 wastewater: 0.02 kg oil and grease, 0.0625 kg coagulant and 0.0006 kg polyelectrolyte.

Electricity consumption was modelled according to data presented in Section 6, while all chemicals were modelled with existing ecoinvent data sets. The starch-based coagulant was approximated with the data set for starch production available in ecoinvent.

Table 16. LCI for operation of the DAF module in the INTEGROIL plant.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
DAF operation	m^3	1	Reference flow is treating 1 m^3 refinery wastewater at the inlet of the INTEGROIL plant
Inputs of products and services:			
Electricity, TR	kWh	Confidential	LCI data in Table 3
Coagulant	kg	0.0625	Maize starch {GLO}| market for | Conseq
Polyelectrolyte	kg	6.0E-04	Polyacrylamide {GLO}| market for | Conseq, U
Sodium hydroxide	kg	9.0E-04	Sodium hydroxide, without water, in 50% solution state {GLO}| market for | Conseq
Waste to treatment:			
Sludge, dry mass	kg	0.0825	See section 5.8

5.3. MBR operation

The LCI for operation of the MBR module includes the following inputs expressed as an average per m^3 at the inlet of the INTEGROIL plant:

- Electricity consumption: 2.09 kWh/m^3
- Dose of sodium hypochlorite solution (161 g Cl/L)): 19.5 mg/L
- Dose of acid cleaner Divos 35 VM30: 4.1 mg/L
- Dose of alkaline cleaner Divos 120CL VM9: 0.7 mg/L
- Dose of phosphoric acid (54%): 1 mg/L

As opposed to the other chemicals, the dose of phosphoric acid is estimated, as reported in section 4.2. All chemicals as well as electricity production were modelled with specific data sets created for this study, which are available in Section 6.

According to simulations conducted based on the ASM2 model adapted to the MBR technology, 1 m^3 refinery wastewater produces 0.024 kg excess sludge, expressed in dry mass, containing 72% volatile solids.

Table 17. LCI for operation of the MBR module in the INTEGROIL plant.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
MBR operation	m^3	1	Reference flow is treating 1 m^3 refinery wastewater at the inlet of the INTEGROIL plant
Inputs of products and services:			
Electricity, TR	kWh	2.09	LCI data in Table 3
Sodium hypochlorite	kg	0.0195	Sodium hypochlorite solution (LCI data in Section 6)
Acid cleaner	kg	0.0041	Acid cleaner (LCI data in Section 6)
Alkaline cleaner	kg	0.0007	Alkaline cleaner (LCI data in Section 6)
Phosphoric acid, 54%	kg	0.001	Phosphoric acid, 54% (LCI data in Section 6)
Waste to treatment:			
Sludge, dry mass	kg	0.024	See section 5.8

5.4. CWAO operation

The LCI for operation of the CWAO module is based on data provided by APLICAT and includes the following items, expressed as an average per m^3 at the inlet of the INTEGROIL plant:

- Electricity consumption: 0.16 kWh/m^3
- Catalyst consumption: 0.043 kg/m^3
- Transport and incineration of the spent catalyst

The catalyst used in the CWAO module is based on granular activated carbon (GAC) and placed in the reactor in a similar fashion as in a conventional GAC filter. It is expected that it has to be changed every two years in order to prevent a loss in performance. A further 5% extension of the life span of the catalyst is assumed thanks to the DSS. The reactor contains 140,000 kg of catalyst, resulting in a consumption of 0.043 kg/m3 at the inlet of the INTEGROIL plant. The production of this material has been modelled with the existing data set for activated carbon in the ecoinvent database.

The spent catalyst is expected to be disposed of by means of incineration. We have included the transport to incineration plant assuming a distance of 100 km with a generic road transport data set in ecoinvent. The incineration process has been specifically created for this study, using the hazardous waste incineration model developed by Doka (2007). Detailed data for the incineration process is available in Section 6.

Table 18. LCI for operation of the CWAO module in the INTEGROIL plant.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
CWAO operation	m^3	1	Reference flow is treating 1 m^3 refinery wastewater at the inlet of the INTEGROIL plant
Inputs of products and services:			
Electricity, TR	kWh	0.16	LCI data in Table 3
CWAO catalyst	kg	0.043	Activated carbon, granular {GLO}| market for activated carbon, granular | Conseq
Waste to treatment:			
CWAO catalyst transport	kgkm	4.3	Transport, freight, lorry, unspecified {GLO}| market for | Conseq
CWAO catalyst incineration	kg	0.043	CWAO catalyst incineration (LCI data in Section 6)

5.5. AOP operation

The LCI for operation of the AOP module includes the following items, expressed as an average per m^3 at the inlet of the INTEGROIL plant:

- Electricity consumption: 3.2 kWh/m^3
- Dose of hydrogen peroxide (30% solution): 90 mg/L

The AOP module does not produce any solid or liquid waste, besides the treated effluent.

Table 19. LCI for operation of the AOP module in the INTEGROIL plant.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
AOP operation	m^3	1	Reference flow is treating 1 m^3 produced water at the inlet of the INTEGROIL plant
Inputs of products and services:			
Electricity, TR	kWh	3.2	LCI data in Table 3
Hydrogen peroxide solution	kg	0.09	Hydrogen peroxide 30% (LCI data in Section 6)

5.6. RO operation

The RO module in the scaled-up plant was designed with the inclusion of a double-pass RO system. Operation with a single pass is used when firefight or cooling water qualities are required, whereas the second pass is strictly reserved for achieving boiler water quality. In terms of LCI, these two operation modes differ mainly in energy consumption, due to the addition of a booster pump, while the consumption of chemicals remains the same in both cases and the permeate recovery is only slightly reduced when the double pass is used, from 75% to 72.83%.

The LCI for operation of the RO module includes the following items, expressed as an average per m^3 at the inlet of the INTEGROIL plant:

- Electricity consumption: 0.42 kWh/m^3 when operating with a single pass, 0.53 kWh/m^3 when operating with a double pass.
- Dose of antiscalant DP5053: 4.2 mg/L
- Dose of biocide Bactirep 2007: 2.5 mg/L
- Dose of sodium bisulfite: 1.3 mg/L
- Dose of citric acid: 1.1 mg/L
- Dose of EDTA: 1.1 mg/L

The RO module produces a concentrate that needs to be disposed of and discharge to the sea is assumed. The LCI data for this aspect is covered in section 5.7.

Table 20. LCI for operation of the RO module in the INTEGROIL plant.

Exchanges	Unit	RO, single pass	RO, double pass	Ecoinvent data sets/comments
Reference flow:				
RO operation	m^3	1	1	Reference flow is treating 1 m^3 produced water at the inlet of the INTEGROIL plant
Inputs of products and services:				
Electricity, TR	kWh	0.42	0.53	LCI data in Table 3
Antiscalant DP5053	kg	0.0042	0.0042	Antiscalant DP5053 (LCI data available in Section 6)
Bactirep 2007	kg	0.0025	0.0025	Bactirep 2007 (LCI data available in Section 6)
Sodium bisulfite	kg	0.0013	0.0013	Sodium sulfite {GLO}| market for | Conseq
Citric acid	kg	0.0011	0.0011	Citric acid {GLO}| market for | Conseq
EDTA	kg	0.0011	0.0011	EDTA, ethylenediaminetetraacetic acid {GLO}| market for | Conseq
Waste to treatment:				
RO brine	m^3	0.247	0.268	See section 5.7

5.7. Direct emissions

Direct emissions from the INTEGROIL plant include the following:

- VOC emissions from the DAF and MBR tanks.
- Emissions in the RO concentrate discharged to the sea.
- CO_2 from degradation of TOC in the wastewater, both during treatment and after discharging the RO concentrate (environmental degradation).
- N_2O from nitrification/denitrification of nitrogen in the wastewater, both during treatment and after discharging the RO concentrate (environmental degradation).

VOC emissions are estimated using the same emission factors used for the reference scenario (Barthe et al. 2015) and the areas of the DAF and MBR tanks according to the scale-up design. Table 21 shows that we estimate an emission of 5.1 kg VOC/day, or 0.43 mg VOC/L.

Table 21. Estimate of VOC emissions in the DAF and MBR tanks in all INTEGROIL scenarios.

Parameter	DAF	MBR	Total
Emission factor ($kg/m^2/h$)[a]	0.002	0.0002	n.a.
Area (m^2)[b]	64	440	504
Emission (kg/day)	3.1	2.1	5.2
Emission (mg/L)[c]	0.26	0.18	0.43

[a] Barthe et al. (2015, p. 219)

[b] Based on scale-up.

[c] The daily wastewater flow is 12,000 m^3.

Direct discharges to seawater occur only through the RO concentrate, since the treated effluent is reused. Direct analytical measurements for this waste flow were not available, and therefore the figures we present in Table 22 constitute a rough estimate. The oil and grease values were obtained from the mass balance, while the other parameters were obtained from analytical results for either the MBR, CWAO and/or AOP modules, and considering the RO achieves a removal of 99.9%.

Table 22. Emissions of pollutants in the RO concentrate, per m³ refinery wastewater.

Parameter	INTEGROIL fire reuse[a]	INTEGROIL cooling reuse[b]	INTEGROIL boiler reuse[c]
Oil and grease	4.5E-06	6.8E-05	9.9E-05
COD	0.003	0.018	0.0005
BOD	0	0	0
Ammonium	0.002	0.0108	0.012
Nitrates	0	0	0

[a] Pollutants contained in 0.040 m^3 concentrate.
[b] Pollutants contained in 0.222 m^3 concentrate.
[c] Pollutants contained in 0.268 m^3 concentrate.

CO_2 emissions have been calculated based on a TOC balance, taking into account the initial TOC in the wastewater (85 mg/L) and the individual TOC removal efficiencies by each module. CO_2 emissions during treatment relate to the TOC that is subject to degradation in the biological treatment (MBR), CWAO and AOP modules, while the remaining modules only remove the TOC without mineralizing it. As in the reference scenario, it is assumed that all TOC emitted in the effluent eventually degrades to CO_2. The balance is summarized in Table 23, where it can be seen that the direct CO_2 emissions are similar in the three scenarios.

Table 23. Carbon balance and calculation of direct CO_2 emissions in the INTEGROIL scenarios.

Exchange	Unit	INTEGROIL fire reuse	INTEGROIL cooling reuse	INTEGROIL boiler reuse
TOC in wastewater (1)	kg/m³	0.085	0.085	0.085
TOC to sludge (DAF+UF) (2)	kg/m³	0.065	0.065	0.065
TOC mineralized (MBR+AOP+CWAO) (3)	kg/m³	0.019	0.018	0.017
TOC to reuse (4)	kg/m³	7.3E-04	4.3E-04	2.3E-06
TOC in RO concentrate (5=1-2-3-4)	kg/m³	0.0001	0.002	0.003
CO_2 from treatment (from 3)[a]	kg/m³	0.071	0.064	0.062
CO_2 from environmental degradation (from 5)[a]	kg/m³	0.001	0.008	0.012
CO_2 total	kg/m³	0.071	0.072	0.074

[a] Calculated as TOC*44/12.

Emissions of N_2O originating in the biological reactor and after release of the RO concentrate to the sea were calculated using the same emission factors as in the reference treatment, namely 0.005 kg N_2O-N/kg N input to the biological reactor and 0.005 kg N_2O-N/kg N input to the environment. Counting the input of ammonia and nitrate in the influent, the total-N input is 0.017 kg N/m^3, resulting in an emission of 1.3E-04 kg N_2O/m^3, that is, the same amount as in the reference treatment. As for emissions taking place in the environment, the total-N in the RO concentrate is shown in Table 22. The resulting emissions for each scenario are the following:

- Fire reuse: 1.2E-05 kg N_2O/m^3 refinery wastewater.
- Cooling reuse: 6.6E-05 kg N_2O/m^3 refinery wastewater.
- Boiler reuse: 7.3E-05 kg N_2O/m^3 refinery wastewater.

5.8. Sludge disposal

Sludge disposal in the INTEGROIL scenarios follows the same principles as in the reference scenario, that is, sludge is dewatered and transported to a cement plant, where it is used as fuel. What changes in the INTEGROIL scenarios is the amount of sludge produced per functional unit and the composition of this sludge, which has implications in terms of transport, combustion emissions and substituted fuels and cement raw meal.

The total amount of sludge produced, in dry mass, in the DAF and MBR modules combined is 0.107 kg/m^3 wastewater. This is dewatered to 37% in dry mass with the aid of polyelectrolyte, at a rate of 0.005 kg/kg dry mass, according to Tüpraş, resulting in a consumption of 5.0E-04 kg polyelectrolyte/m^3 wastewater. The wet weight of dewatered sludge produced is 0.29 kg/m^3/wastewater. The sludge is transported by road to the cement plant, located at 215 km from the refinery. This is modelled with the same ecoinvent data set as in the reference scenario. We also use the same energy consumption factors for processing of sludge at the cement plant, namely 0.1 kWh electricity and 3.6 MJ heat per kg water evaporated to achieve a dryness of 90%, reducing the sludge mass to 0.12 kg/m^3 wastewater.

In Table 24 we summarize the data used to calculate the low calorific value of sludge with 90% dry mass, as combusted in the cement kiln. The resulting fuel value of the sludge is 2.27 MJ/m^3 wastewater originating this sludge.

Table 24. Calculation of low calorific value of sludge in the INTEGROIL scenarios, when dried to 90% dry mass.

Component	Low calorific value (MJ/kg component)[a]	Content in sludge (kg/m^3 wastewater)	Low calorific value (MJ/m^3 wastewater)[a]	Comments
Oil and grease	41.0	0.020	0.81	Composition of crude oil from ChemEngineering (2017): 83% C, 12% H, 1% N, 1% O, 3% S
Starch-based coagulant	17.0	0.063	1.06	Assuming the calorific value of starch, 17.5 MJ/kg (Wikipedia 2019) with an empirical formula $C_6H_{10}O_5$
Biomass	22.4	0.017	0.39	Empirical formula of biomass volatile solids from Muñoz et al. (2016) is $C_5H_7O_2N$
Fixed solids	0	0.007	0	Does not have fuel value
Polyelectrolyte	37.9	0.001	0.04	We assume polyelectrolyte used is polyacrylamide, with the empirical formula $(C_3H_5NO)_n$
Water	-2.45	0.012	-0.029	Based on Equation 4
Total	19.0	0.119	2.27	The value of 19.0 is calculated as the ratio 2.30/0.119

[a] Calculated as the product of the values in the two previous columns, except the total, which is calculated as the sum of the contributions from all components.

The carbon content in sludge is calculated with a similar procedure as in the table above, that is, defining the carbon content of the individual components, considering the compositions used in the table (column Comments). The resulting carbon content on a per m^3 wastewater basis is 0.054 kg C, which stoichiometrically implies an emission of 0.199 kg CO_2/m^3 associated to combustion of the sludge. As in the reference scenario, in the inventory we consider that levels of pollutants such as particles, SO_2, NOx, heavy metals, etc., remain unaltered on a per MJ fuel basis, regardless of the fuel used in the cement plant. The only exception to this is CO_2 emissions, where the difference between using sludge and conventional fuels can be taken into account, given that the carbon content of sludge and of the replaced fossil fuels is well known.

As for the ash content, based on Table 24, the main contribution to ash is expected to be the fixed solids fraction. We assume these solids remain unaltered after combustion, substituting an equal mass of cement raw meal. The final inventory for sludge disposal in the INTEGROIL scenarios is shown in Table 25.

Table 25. LCI for disposal of sludge in the INTEGROIL scenarios.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Refinery sludge disposal, INTEGROIL scenario	kg	0.29	Dewatered sludge containing 37% dry mass
Inputs of products and services:			
Transport, road	kgkm	125	Transport, freight, lorry, unspecified {GLO}| market for | Conseq
Waste heat	MJ	0.61	Excess heat from cement kiln, no burdens associated
Electricity, TR	kWh	0.017	LCI data in Table 3
Fuels for clinker production	MJ	-2.27	LCI data available in Section 6
Raw meal for clinker production	kg	-0.007	LCI data available in Section 6
Emissions to air [a]:			
CO_2, fossil	kg	0.199	Calculated based on data from Table 24

[a] Emissions to air other than CO_2 are neglected, since we assume they remain constant in the cement kiln regardless of the use of sludge as fuel.

5.9. Fire water from freshwater

Wastewater reuse for firefighting purposes substitutes production of firefighting water from freshwater. When freshwater is used, the required treatment is considered to consist of a simple filtration process. We considered the most appropriate data set to represent this activity is ecoinvent's tap water production by direct filtration. This process includes disinfection, which we ignore in this study. Also, we further adapted the original ecoinvent data set by labelling the freshwater input flow as originating in Turkey, and by using the Turkish electricity production mix, as presented in Section 6.

Table 26. LCI data for firefighting water production from freshwater.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow			
Firefighting water, from freshwater	m^3	1	
Inputs of resources:			
Freshwater, TR	m^3	1.013	Abstracted from natural water body
Inputs of products and services:			
Water treatment equipment	unit	1.52E-09	Water works, capacity 1.1E10l/year {Europe without Switzerland}| water works construction, capacity 1.1E10l/year, direct filtration treatment | Conseq
Heat, diesel	MJ	6.64E-03	Diesel, burned in building machine {GLO}| market for | Conseq
Heat, natural gas	MJ	1.16E-03	Heat, district or industrial, natural gas {RER}| market group for | Conseq
Electricity, TR	kWh	0.286	LCI data in Table 3
Waste to treatment:			
wastewater	m^3	0.013	Wastewater, unpolluted {GLO}| market for | Conseq

5.10. Cooling makeup water from freshwater

Wastewater reuse for cooling purposes substitutes production of cooling water from freshwater. In this case we consider a more intense treatment than for firefighting water, in which the feed water quality is assimilated to tap water, and this is in turn subject to a RO process, equivalent to the single-pass RO considered in INTEGROIL. Production of tap-quality water in Turkey has been modelled with the existing ecoinvent data set for production of tap water by conventional treatment, consisting of coagulation, flocculation, settling, filtration and disinfection. We further adapted the original ecoinvent data set by labelling the freshwater input flow as originating in Turkey, and by using the

Turkish electricity production mix, as presented in Section 6. The LCI data for this water production process is shown in Table 27.

Table 27. LCI for tap-quality water production in Turkey.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow			
Tap water, from freshwater	m^3	1	
Inputs of resources			
Freshwater, TR	m^3	1.033	Abstracted from natural water body
Inputs of products and services:			
Water treatment equipment	unit	1.52E-09	Water works, capacity 1.1E10l/year {Europe without Switzerland}| water works construction, capacity 1.1E10l/year, conventional treatment | Conseq
Charcoal	kg	6.61E-04	Charcoal {GLO}| market for | Conseq
Ultraviolet lamp	unit	1.75E-07	Ultraviolet lamp {GLO}| market for | Conseq
Chlorine dioxide	kg	1.11E-04	Chlorine dioxide {GLO}| market for | Conseq
Sodium hydroxide, pure	kg	7.86E-04	Sodium hydroxide, without water, in 50% solution state {GLO}| market for | Conseq
Sodium hypochlorite, pure	kg	4.21E-04	Sodium hypochlorite, without water, in 15% solution state {GLO}| market for | Conseq
Iron sulfate, pure	kg	7.40E-03	Iron(III) sulfate, without water, in 12.5% iron solution state {GLO}| market for | Conseq
Sodium tripolyphosphate	kg	1.11E-04	Sodium tripolyphosphate {GLO}| market for | Conseq
Water for reagent solutions	kg	0.021	Tap water {Europe without Switzerland}| market for | Conseq
Oxygen	kg	0.041	Oxygen, liquid {RER}| market for | Conseq
Aluminium sulfate	kg	0.0402	Aluminium sulfate, powder {GLO}| market for | Conseq
Sand	kg	1.50E-03	Silica sand {GLO}| market for | Conseq
Polyacrylamide	kg	1.58E-04	Polyacrylamide {GLO}| market for | Conseq
Chlorine	kg	2.00E-03	Chlorine, liquid {GLO}| market for | Conseq
Lime	kg	6.20E-03	Lime, hydrated, loose weight {GLO}| market for | Conseq
Sodium silicate	kg	1.44E-03	Sodium silicate, solid {GLO}| market for | Conseq
Heat, diesel	MJ	0.016	Diesel, burned in building machine {GLO}| market for | Conseq
Heat, natural gas	MJ	0.178	Heat, district or industrial, natural gas {Europe without Switzerland}| market for heat, district or industrial, natural gas | Conseq
Electricity, TR	kWh	0.427	LCI data in Table 3
Waste treatment:			
Wastewater	m^3	0.033	Wastewater, unpolluted {GLO}| market for | Conseq
Charcoal waste	kg	6.61E-04	Waste wood, untreated {GLO}| market for | Conseq

Production of cooling water is achieved by subjecting the treated freshwater to RO. This has been approximated by means of the data for the single-pass RO module used in the INTEGROIL plant. In the LCI we include the same water treatment equipment, energy and dosage of chemicals as in Table 20, with the difference that, on the one hand, the RO concentrate in the present case is assumed to be clean water, and on the other hand, the reference flow in the present case is the output of the RO module (0.75 m^3 permeate per m^3 input) rather than the wastewater input. The LCI data for this process is shown in the table below.

Table 28. LCI for cooling water production from freshwater.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow			
Cooling water, from freshwater	m^3	1	
Inputs of products and services:			
Tap water, from freshwater	m^3	1.33	The RO module has a permeate recovery of 75%. LCI data in Table 27
INTEGROIL plant construction, RO module	year	3.0E-07	LCI data in Table 14
Electricity, TR	kWh	0.56	LCI data in Table 3
Antiscalant DP5053	kg	0.0056	Antiscalant DP5053 (LCI data available in Section 6)
Bactirep 2007	kg	0.0033	Bactirep 2007 (LCI data available in Section 6)
Sodium bisulfite	kg	0.0017	Sodium sulfite {GLO}| market for | Conseq
Citric acid	kg	0.0015	Citric acid {GLO}| market for | Conseq
EDTA	kg	0.0015	EDTA, ethylenediaminetetraacetic acid {GLO}| market for | Conseq
Waste treatment:			
Wastewater	m^3	0.033	Wastewater, unpolluted {GLO}| market for | Conseq
INTEGROIL plant dismantling, RO module	year	3.0E-07	LCI data in Table 15

5.11. Boiler feed water from freshwater

Boiler feed water requires the most intensive treatment, in order to obtain deionized water that prevents damage in boilers. The LCI for production of deionized water is based partly on the ecoinvent data set for deionized water and data from Beardsley et al. (1995). Consumption figures for electricity, steam, sulfuric acid, caustic soda and lime were obtained from Beardsley et al. (1995), assuming the feed water has a total dissolved solids (TDS) content of 240 mg/L expressed as $CaCO_3$-equivalents, which is the average scenario in that study. The figures were obtained as the arithmetic average from the cases where TDS equals 160 mg/L and 320 mg/L, respectively. Consumption of cationic and anionic resins per m^3 product water was calculated by extrapolating from the original ecoinvent data set for deionized water, where we estimate the feed water contains 191 mg/L TDS as $CaCO_3$-equivalents (Table 29). Given the slightly higher hardness of our feed water, the resin consumption is adjusted proportionally (Table 30).

Table 29. Calculation of TDS as $CaCO_3$-equivalents in the ecoinvent data set for deionized water production.

Component	Concentration in feed water (mol/m^3)[a]	Molecular weight (g/mol)	$CaCO_3$-eq (g $CaCO_3$-eq/g)[b]	TDS (mg $CaCO_3$-eq/L)
Ca	1.39	40	2.5	139
Mg	0.32	24	4.1	32
Na	0.29	23	2.18	15
K	0.04	39	1.28	2
SiO_2	0.06	60	n.a.	4
Total	2.04	n.a.	n.a.	**191**

[a] Primas (2007, p. 818).
[b] Michaud (2007).

Table 30. Calculation of cationic and anionic resin consumption per m³ deionized water.

Resin type	Consumption in 15 years (kg resin)[a]	Water production in 15 years (m³)[a]	Hardness removed in 15 years (mg $CaCO_3$-eq)[b]	Unitary resin consumption (kg resin/ mg $CaCO_3$-eq)[c]	Unitary resin consumption, TDS = 240 (kg resin/m³ deionized water)
Cationic resin	20,400	1.10E+07	2.10E+12	9.71E-09	**2.33E-03**
Anionic resin	9,240	1.10E+07	2.10E+12	4.40E-09	**1.06E-03**

[a] Taken from ecoinvent data set on ion-exchanger production for water treatment in Switzerland.
[b] Based on 191 mg $CaCO_3$-eq/L (Table 29).
[c] Calculated as first column divided by third column.
[d] Calculated as fourth column*240/1000.

The LCI for deionization is shown in Table 31. As in the original ecoinvent data set, the feed water is assumed to have tap water quality. Feed water is modelled with data in Table 27, and the yield is 0.83 m³ deionized water per m³ feed water (Beardsley et al. 1995). The remaining inputs and outputs have mainly been modelled with existing ecoinvent data sets.

Table 31. LCI for boiler feed water production from freshwater.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow			
Boiler feed water, from freshwater	m³	1	
Inputs of products and services:			
Water treatment equipment	unit	9.0E-08	Ion-exchange plant (LCI data in Section 6)
Tap water, from freshwater	m³	1.2	LCI data in Table 27
Electricity, TR	kWh	0.317	LCI data in Table 3
Steam	MJ	0.685	Heat, district or industrial, natural gas {Europe without Switzerland}| market for heat, district or industrial, natural gas | Conseq
Sulfuric acid, pure	kg	0.631	Sulfuric acid {GLO}| market for | Conseq
Caustic soda, pure	kg	0.244	Sodium hydroxide, without water, in 50% solution state {GLO}| market for | Conseq
Lime	kg	0.21	Lime {GLO}| market for | Conseq
Cationic resin	kg	2.33E-03	Cationic resin {GLO}| market for | Conseq
Anionic resin	kg	1.06E-03	Anionic resin {GLO}| market for | Conseq
Waste treatment:			
Spent cationic resin	kg	2.33E-03	Spent cation exchange resin from potable water production {GLO}| market for | Conseq
Spent anionic resin	kg	1.06E-03	Spent anion exchange resin from potable water production {GLO}| market for | Conseq
Wastewater	m³	0.2	Wastewater, unpolluted {GLO}| market for | Conseq

5.12. Steam substitution

The RO permeate obtained by the INTEGROIL demonstration plant tested in the Tüpraş refinery has a temperature ranging from 18ºC to 42ºC, with an average at 34ºC. When considering reuse of this permeate as boiler feed water this presents an advantage, given that feed water needs to be heated to temperatures of around 80-90ºC. When boiler feed water is obtained from freshwater, the latter is expected to be around 10-15 ºC, thus involving higher heat requirements than if the INTEGROIL RO permeate is used.

In this section we attempt to estimate the energy savings, associated to the warmer temperature of the RO permeate. We take the following assumptions and data:

- The RO permeate has an average temperature of 34ºC.

- Boiler feed water from freshwater is assumed to have a temperature of 15 ºC.
- The heat capacity of water is 4.18 MJ/m^3/ºC

The energy saving from this 19ºC temperature difference is 79.8 MJ/m^3 RO permeate reused as boiler feed water. In the LCI, we consider this heat is provided by cogeneration with natural gas and we model it with an existing ecoinvent data set representing Turkish conditions.

Table 32. LCI for heat savings from reusing RO permeate as boiler feed water in the INTEGROIL boiler reuse scenario.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow			
Boiler feed water, from RO permeate	m^3	1	
Inputs of products and services:			
Heat, natural gas	MJ	-79.8	Heat, district or industrial, natural gas {TR}| heat and power co-generation, natural gas, conventional power plant, 100MW electrical | Conseq

5.13. Overall LCI for the INTEGROIL scenarios

In the table below we summarize the overall LCI for the INTEGROIL scenarios, based on the inventory data presented in the previous sections.

Table 33. LCI for the INTEGROIL scenarios.

Exchanges	Unit	INTEGROIL fire reuse	INTEGROIL cooling reuse	INTEGROIL boiler reuse	Ecoinvent data sets/comments
Reference flow:					
Refinery wastewater treatment	m^3	1	1	1	
Inputs of products and services:					
INTEGROIL plant construction, DAF module	year	2.28E-07	2.28E-07	2.28E-07	LCI data in Table 14
INTEGROIL plant construction, MBR module	year	2.28E-07	2.28E-07	2.28E-07	LCI data in Table 14
INTEGROIL plant construction, CWAO module	year	2.28E-07	2.28E-07	2.28E-07	LCI data in Table 14
INTEGROIL plant construction, AOP module	year	2.28E-07	2.28E-07	2.28E-07	LCI data in Table 14
INTEGROIL plant construction, RO module	year	2.28E-07	2.28E-07	2.28E-07	LCI data in Table 14
INTEGROIL plant construction, electrical installation	year	2.28E-07	2.28E-07	2.28E-07	LCI data in Table 14
INTEGROIL plant dismantling, DAF module	year	2.28E-07	2.28E-07	2.28E-07	LCI data in Table 15
INTEGROIL plant dismantling, MBR module	year	2.28E-07	2.28E-07	2.28E-07	LCI data in Table 15
INTEGROIL plant dismantling, CWAO module	year	2.28E-07	2.28E-07	2.28E-07	LCI data in Table 15
INTEGROIL plant dismantling, AOP module	year	2.28E-07	2.28E-07	2.28E-07	LCI data in Table 15
INTEGROIL plant dismantling, RO module	year	2.28E-07	2.28E-07	2.28E-07	LCI data in Table 15
INTEGROIL plant dismantling, electrical installation	year	2.28E-07	2.28E-07	2.28E-07	LCI data in Table 15
DAF operation	m^3	1	1	1	LCI data in Table 16
MBR operation	m^3	1	1	1	LCI data in Table 17
CWAO operation	m^3	0.85	0.96	1	LCI data in Table 18
AOP operation	m^3	0.44	0.66	1	LCI data in Table 19
RO operation, single pass	m^3	0.16	0.90		LCI data in Table 20
RO operation, double pass	m^3			1	LCI data in Table 20
Firefighting water, from freshwater	m^3	-0.95			LCI data in Table 26
Cooling water, from freshwater	m^3		-0.77		LCI data in Table 28
Boiler feed water, from freshwater	m^3			-0.72	LCI data in Table 31
Heat, natural gas	MJ			-57	From Table 32. Heat, district or industrial, natural gas {TR}| heat and power co-generation, natural gas, conventional power plant, 100MW electrical | Conseq
Emissions to air:					
CO_2, fossil	kg	0.209	0.210	0.212	Calculated in Table 23
VOC	kg	4.3E-04	4.3E-04	4.3E-04	Calculated in Table 21
Emissions to seawater:					
Oil and grease, refinery effluent	kg	4.5E-06	6.8E-05	9.9E-05	Calculated in Table 22. Speciation of oil and grease according to Table 2
COD	kg	0.003	0.018	0.0005	Calculated in Table 22
Ammonium	kg	0.002	0.0108	0.012	Calculated in Table 22
Emissions to seawater:					
Refinery sludge disposal, INTEGROIL scenario	kg	0.29	0.29	0.29	LCI data in Table 25

6. Inventories for supporting activities

6.1. Acid cleaner

The inventory refers to the product DIVOS 35 VM30, used for cleaning in place (CIP) operations. This product contains (in mass) 20% to 30% citric acid and 3% to 10% glycolic acid, as reported in the safety data sheet provided by Diversey. We assumed a content of 25% and 6.5% for these two chemicals, respectively, and the rest was assumed to be pure water. The LCI includes the production of the three components, however for glycolic acid we take the generic ecoinvent data set for organic chemicals, since this specific product is not covered by the database. We also added average transport services considered in the ecoinvent data base for the distribution of chemical products. It must be highlighted that the manufacturing of the product (blending, packaging, etc.) as well as the packaging materials are not included.

Table 34. LCI for production of the acid cleaner DIVOS 35 VM30.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Acid cleaner	kg	1	
Inputs of products and services:			
Citric acid	kg	0.25	Citric acid {GLO}| market for | Conseq
Glycolic acid	kg	0.065	Chemical, organic {GLO}| production | Conseq
Ultrapure water	kg	0.685	Water, ultrapure {GLO}| market for | Conseq
Transport, inland water	kgkm	0.0246	Transport, freight, inland waterways, barge {GLO}| market for | Conseq
Transport, train	kgkm	0.3091	Transport, freight train {GLO}| market group for | Conseq
Transport, road	kgkm	0.2088	Transport, freight, lorry, unspecified {GLO}| market for | Conseq
Transport, sea	kgkm	0.599	Transport, freight, sea, transoceanic ship {GLO}| market for | Conseq

6.2. Actuator valve

The LCI for an automated valve, on a per kg valve basis, is taken from an environmental product declaration by Life Cycle Engineering Experts (2013), in which a broad material composition is given as 15% steel, 15% copper, 15% brass, 44% aluminium and 12% plastics. Our LCI includes the production of these materials, however the manufacturing process itself as well as packaging materials and distribution, are excluded.

Table 35. LCI for production of an actuator valve.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Actuator valve	kg	1	
Inputs of products and services:			
Steel parts	kg	0.15	Steel product (LCI data in this section 6)
Copper parts	kg	0.15	Copper product (LCI data in this section 6)
Brass parts	kg	0.15	Brass product (LCI data in this section 6)
Aluminium parts	kg	0.44	Aluminium product (LCI data in this section 6)
Polyvinylchloride parts	kg	0.12	PVC product (LCI data in this section 6)

6.3. Air compressor, screw-type compressor, 300kW

The LCI for a 300 kW compressor is used to model the compressors used by the DAF and MBR modules. The original ecoinvent data set for this product has a reference flow of one unit of compressor, which has a weight of 4,600 kg. We modified the data set to express the reference flow as 4,600 kg instead of one unit. In this way, we can scale the data set to the desired weight according to the INTEGROIL plant compressors. The LCI is shown below.

Table 36. LCI for production of an air compressor, screw-type compressor, 300kW.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Compressor, screw-type compressor, 300kW	kg	4,600 kg	
Inputs of products and services:			
Compressor, screw-type compressor, 300kW (EU)	Unit	0.33	Air compressor, screw-type compressor, 300kW {RER}| production | Conseq
Compressor, screw-type compressor, 300kW (RoW)	Unit	0.67	Air compressor, screw-type compressor, 300kW {RoW}| production | Conseq

6.4. Air compressor, screw-type compressor, 4kW

The LCI for a 4 kW compressor is used to model the compressors used by the AOP modules. The original ecoinvent data set for this product has a reference flow of one unit of compressor, which has a weight of 140 kg. We modified the data set to express the reference flow as 140 kg instead of one unit. In this way, we can scale the data set to the desired weight according to the INTEGROIL plant compressors. The LCI is shown below.

Table 37. LCI for production of an air compressor, screw-type compressor, 4kW.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Compressor, screw-type compressor, 4kW	kg	140 kg	
Inputs of products and services:			
Compressor, screw-type compressor, 4W (EU)	Unit	0.33	Air compressor, screw-type compressor, 4kW {RER}| production | Conseq
Compressor, screw-type compressor, 4kW (RoW)	Unit	0.67	Air compressor, screw-type compressor, 4kW {RoW}| production | Conseq

6.5. Air filter

This data set is created to represent the production of the particle filters used in the AOP modules. The original ecoinvent data set for an air filter refers to a unit weighting 84 g and the reference flow for this data set is one unit. We changed the reference flow from one unit of filter to 84 g of filter, in order to scale the data set to the weight of the actual filter used in the INTEGROIL plant. The LCI is shown below.

Table 38. LCI for production of an air filter.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Air filter	kg	0.084	
Inputs of products and services:			
Product distribution, rail	Tkm	0.000724	Transport, freight train {GLO}| market group for | Conseq
Product distribution, urban	Tkm	0.000392	Transport, freight, light commercial vehicle {GLO}| market for | Conseq
Product distribution, road	Tkm	0.01262	Transport, freight, lorry, unspecified {GLO}| market for | Conseq
Product distribution, inland waters	Tkm	0.000048	Transport, freight, inland waterways, barge {GLO}| market for | Conseq
Product distribution, sea	tkm	0.029472	Transport, freight, sea, transoceanic ship {GLO}| market for | Conseq
Air filter production (EU)	unit	0.331	Air filter, in exhaust air valve {RER}| production | Conseq
Air filter production (RoW)	unit	0.669	Air filter, in exhaust air valve {RoW}| production | Conseq

6.6. Alkaline cleaner

The inventory for the alkaline cleaner used for cleaning-in-place (CIP) operations in the UF and MBR modules has been created based on the approximate composition declared by Diversey for the product Divos 120 CL VM9 in its safety data sheet. This product contains 10-20% potassium hydroxide and 1-3% sodium hydroxide. We took the average concentration and assumed the remaining mass to be ultrapure water. We also added transport services, in order to account for an average distribution of the product to the point of use. This was done with ecoinvent data on transport services for chemicals. The LCI is shown below.

Table 39. LCI for production of the alkaline cleaner used for ceramic membranes.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Alkaline cleaner	kg	1	
Inputs of products and services:			
Water for solution	kg	0.83	Water, ultrapure {GLO}| market for | Conseq
Potassium hydroxide	kg	0.15	Potassium hydroxide {GLO}| market for | Conseq
Sodium hypochlorite	kg	0.02	Sodium hypochlorite, without water, in 15% solution state {GLO}| market for | Conseq
Product distribution, inland waters	Tkm	0.0246	Transport, freight, inland waterways, barge {GLO}| market for | Conseq
Product distribution, rail	Tkm	0.3091	Transport, freight train {GLO}| market group for | Conseq
Product distribution, road	Tkm	0.2088	Transport, freight, lorry, unspecified {GLO}| market for | Conseq
Product distribution, sea	Tkm	0.599	Transport, freight, sea, transoceanic ship {GLO}| market for | Conseq

6.7. Aluminium product

This data set was created to represent the production of a finished aluminium product. The reference flow is 1 kg product. It includes the production of 1kg aluminium, an average finishing process for 1 kg aluminium product and an output of of 0.154 kg scrap aluminium to manage as waste. The amount of waste scrap is obtained from the metal working data set. The LCI is shown below.

Table 40. LCI for production of an average aluminium product

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Aluminium product	kg	1	
Inputs of products and services:			
Aluminium production	kg	1	Aluminium, wrought alloy {GLO}| market for | Conseq
Product manufacturing	kg	1	Aluminium, wrought alloy {GLO}| market for | Conseq
Waste treatment:			
Aluminium scrap recycling	kg	0.154	Aluminium scrap, new {RER}| market for | Conseq

6.8. Antiscalant DP5053

The inventory for the antiscalant used in the RO modules has been created based on the approximate composition provided by BWA, according to which this product contains 35% polycarboxylic acid. The rest is assumed to be ultrapure water. Polycarboxylic acid production was approximated by means of the average organic chemical data set in ecoinvent. We also added transport services, in order to account for an average distribution of the product to the point of use. This was done with ecoinvent data on transport services for chemicals. The LCI is shown below.

Table 41. LCI for production of the antiscalant DP5053.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Antiscalant DP5053	kg	1	
Inputs of products and services:			
Water for solution	kg	0.65	Water, ultrapure {GLO}| market for | Conseq
Polycarboxylic acid	kg	0.35	Chemical, organic {GLO}| production | Conseq
Product distribution, inland waters	Tkm	0.0246	Transport, freight, inland waterways, barge {GLO}| market for | Conseq
Product distribution, rail	Tkm	0.3091	Transport, freight train {GLO}| market group for | Conseq
Product distribution, road	Tkm	0.2088	Transport, freight, lorry, unspecified {GLO}| market for | Conseq
Product distribution, sea	Tkm	0.599	Transport, freight, sea, transoceanic ship {GLO}| market for | Conseq

6.9. Bactirep 2007

The inventory for the biocide Bactirep 2007 used in the RO modules has been created based on the composition declared by REP. This product contains, by volume, 45% mono ethylene glycol (MEG), 8% 2,2-dibromo-3-nitrilopropionamide (DBNPA), 15% butyl glycol (BG) and 32% water. The concentration in kg/L was obtained by means of the corresponding densities, of 1.11, 2.40, 0.9 kg/L and 1 kg/L for MEG, DBNPA, BG and water, respectively. The resulting density of the formulation is 1.15 kg/L. In the ecoinvent database there are no data sets for production of either DBNPA or BG; for this reason they have been modelled with the generic data set for organic chemicals. Also, we added transport services, in order to account for an average distribution of the product to the point of use. This was done with ecoinvent data on transport services for chemicals. The LCI is shown below.

Table 42. LCI for production of the biocide Bactirep 2007.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Bactirep 2007	kg	1	
Inputs of products and services:			
Water for solution	kg	0.28	Water, ultrapure {GLO}| market for | Conseq
MEG	kg	0.44	Ethylene glycol {GLO}| market for | Conseq
DBNPA, BG	kg	0.29	Chemical, organic {GLO}| production | Conseq
Product distribution, inland waters	Tkm	0.0246	Transport, freight, inland waterways, barge {GLO}| market for | Conseq
Product distribution, rail	Tkm	0.3091	Transport, freight train {GLO}| market group for | Conseq
Product distribution, road	Tkm	0.2088	Transport, freight, lorry, unspecified {GLO}| market for | Conseq
Product distribution, sea	Tkm	0.599	Transport, freight, sea, transoceanic ship {GLO}| market for | Conseq

6.10. Concrete

The data set for concrete used in this study corresponds to the original ecoinvent data set for normal concrete, produced in the RoW region. The only change we introduced was to change the reference flow, from 1 m3 to its equivalent weight, namely 2,200 kg (Frischknecht et al. 2007). The LCI is shown below.

Table 43. LCI for production of concrete.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Concrete	kg	2,2200	Equals 1 m^3 concrete
Inputs of products and services:			
Product distribution, rail	Tkm	32.368	Transport, freight train {GLO}| market group for | Conseq, U
Product distribution, urban	Tkm	4.284	Transport, freight, light commercial vehicle {GLO}| market for | Conseq, U
Product distribution, road	Tkm	138.754	Transport, freight, lorry, unspecified {GLO}| market for | Conseq, U
Concrete production, RoW	m^3	0.85	Concrete, normal {RoW}| unreinforced concrete production, with cement CEM II/A | Conseq, U
Concrete production, RoW	m^3	0.15	Concrete, normal {RoW}| unreinforced concrete production, with cement CEM II/B | Conseq, U

6.11. CWAO catalyst incineration

Incineration of the spent catalyst has been included using the hazardous waste incinerator model developed by Doka (2007) for ecoinvent v2, describing a modern facility in Switzerland. The inventory addresses not only the mass and energy balance of the incinerator, but also the disposal of the ash in a controlled landfill after inertization with cement.

This model was programmed in Excel and requires the user to enter the elementary waste composition. The spent catalyst composition was approximated by that of a bituminous coal, containing 10% moisture and a dry weight content of 80% carbon, 5% hydrogen and 15% oxygen. This material composition results in a net calorific value of 27 MJ/kg, which produces an excess energy in the incinerator. According to the incinerator model, the average waste burned in this plant requires 23 MJ of external fuel (light fuel oil), thus a net excess of around 4 MJ/kg catalyst is obtained, which substitutes light fuel oil. Also, the plant produces heat and electricity by means of cogeneration, which in turn substitutes heat and electricity produced from other sources. We adapted the original model by Doka (2007) in two ways:

- The original model was developed for ecoinvent v2. In order to use it in ecoinvent v3.2 we replaced the v2 background system with the equivalent v3.2 data sets.
- The original model was designed to work with a cut-off approach to multifunctionality, whereby energy by-products did not lead to substitutions. We modified this aspect in the spreadsheet in order to account for these by-product substitutions in the incineration inventory. This was possible given that the model keeps the mass and energy balance in its intermediate calculations, where the amounts of by-products are quantified.

The resulting inventory was then imported to SimaPro, as shown in the table below.

Table 44. LCI for incineration of the spent CWAO catalyst.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
CWAO catalyst incineration	kg	1	
Inputs of products and services:			
Transports, road	tkm	0.00057	Transport, freight, lorry, unspecified {GLO}| market for | Conseq
Incineration plant construction	Unit	1.25E-09	Hazardous waste incineration facility {GLO}| market for | Conseq
Generic incineration plant inputs and emissions	kg	1	Process-specific burdens, hazardous waste incineration plant {GLO}| market for | Conseq
Ash landfill construction	Unit	1.65E-11	Residual material landfill {GLO}| market for | Conseq
Generic ash landfill operation inputs and emissions	kg	0.00792	Process-specific burdens, residual material landfill {GLO}| market for | Conseq
Chemical reagent for incineration process	kg	3.65E-05	Hydrochloric acid, without water, in 30% solution state {RER}| market for | Conseq
Chemical reagent for incineration process	kg	6.08E-05	Chemical, inorganic {GLO}| market for chemicals, inorganic | Conseq
Cement for ash inertization	kg	0.00317	Cement, unspecified {GLO}| market for | Conseq
Transports, rail	tkm	0.00092	Transport, freight train {GLO}| market group for | Conseq
Excess heat in catalyst	MJ	-3.7	Heat, district or industrial, other than natural gas {RoW}| heat production, light fuel oil, at industrial furnace 1MW | Conseq
Energy recovery, heat	MJ	-17.1	Heat, for reuse in municipal waste incineration only {TR}| market for | Conseq
Energy recovery, electriity	MJ	-1.3	Electricity, high voltage {TR}| market for | Conseq
Emissions to air:			
Carbon monoxide, fossil	kg	1.2E-05	Combustion emissions
Carbon dioxide, fossil	kg	2.61	Combustion emissions
Emissions to river water:			
BOD5, Biological Oxygen Demand	kg	3.6E-05	Emission from incinerator and landfill
COD, Chemical Oxygen Demand	kg	3.6E-05	Emission from incinerator and landfill
TOC, Total Organic Carbon	kg	1.6E-05	Emission from incinerator and landfill
DOC, Dissolved Organic Carbon	kg	1.6E-05	Emission from incinerator and landfill
BOD5, Biological Oxygen Demand	kg	3.6E-05	Emission from incinerator and landfill
Emissions to groundwater, long-term:			
BOD5, Biological Oxygen Demand	kg	0.0117	Emission from landfill
COD, Chemical Oxygen Demand	kg	0.0117	Emission from landfill
TOC, Total Organic Carbon	kg	0.0051	Emission from landfill
DOC, Dissolved Organic Carbon	kg	0.0051	Emission from landfill
Waste treatment:			
Cement waste	kg	0.0079	Waste cement, hydrated {GLO}| market for | Conseq

6.12. Display, liquid crystal, 17 inches

This data set is created to represent the production of screens/displays used in the INTEGROIL plant. The original ecoinvent data set refers to a unit weighting 5.1 kg and the reference flow for this data set is one unit. We changed the reference flow from one unit of liquid crystal display to 5.1 kg, in order to scale the data set to the weight of the actual devices used in the INTEGROIL plant.

Table 45. LCI for production of a display, liquid crystal, 17 inches.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Display, liquid crystal, 17 inches	kg	5.6	
Inputs of products and services:			
Product distribution, urban	Tkm	0.0816	Transport, freight, light commercial vehicle {GLO}| market for | Conseq
Product distribution, road	Tkm	2.63058	Transport, freight, lorry, unspecified {GLO}| market for | Conseq
Product distribution, rail	Tkm	0.13005	Transport, freight train {GLO}| market group for | Conseq
Product distribution, sea	Tkm	5.6712	Transport, freight, sea, transoceanic ship {GLO}| market for | Conseq
Display production	Unit	1	Display, liquid crystal, 17 inches {GLO}| production | Conseq

6.13. Electricity from biomass

The ecoinvent database does not contain data sets for production of electricity from biomass. This was solved by adapting a RoW data set for heat production from biomass (heat production from hardwodd chips at forest, at furnace 1000 kW), assuming the calorific value of the biomass can be transformed to electricity with 30% efficiency. The resulting LCI is shown in the table below.

Table 46. LCI for production of electricity from biomass.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Electricity from biomass, RoW	kWh	0.113	Calculated based on the mass input of biomass, a calorific value for this biomass of 18.9 MJ/kg in the original ecoivent data set, an electric conversion efficiency of 30% and 3.6 MJ/kWh.
Inputs of products and services:			
Biomass, EU	kg	0.00068	Wood chips, wet, measured as dry mass {Europe without Switzerland}| market for | Conseq
Biomass, RoW	kg	0.072	Wood chips, wet, measured as dry mass {RoW}| market for | Conseq
Electricity, GLO	kWh	0.00556	Electricity, low voltage {GLO}| market group for | Conseq
Emissions to air:			
Bromine	kg	8.0E-08	Combustion emission
Arsenic	kg	1.3E-09	Combustion emission
Benzene, ethyl-	kg	4.0E-08	Combustion emission
NMVOC	kg	9.3E-06	Combustion emission
Acetaldehyde	kg	8.1E-08	Combustion emission
Nitrogen oxides	kg	2.4E-04	Combustion emission
Sulfur dioxide	kg	3.3E-06	Combustion emission
Chlorine	kg	2.4E-07	Combustion emission
Copper	kg	2.9E-08	Combustion emission
Calcium	kg	7.8E-06	Combustion emission
Hydrocarbons, aliphatic, unsaturated	kg	4.1E-06	Combustion emission
Dinitrogen monoxide	kg	3.1E-06	Combustion emission
Hydrocarbons, aliphatic, alkanes, unspecified	kg	1.2E-06	Combustion emission
Particulates, < 2.5 um	kg	6.0E-05	Combustion emission

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Toluene	kg	4.0E-07	Combustion emission
Chromium	kg	5.3E-09	Combustion emission
Carbon monoxide, biogenic	kg	4.0E-04	Combustion emission
Lead	kg	3.3E-08	Combustion emission
Phenol, pentachloro-	kg	1.1E-11	Combustion emission
Chromium VI	kg	5.3E-11	Combustion emission
Manganese	kg	2.3E-07	Combustion emission
Benzo(a)pyrene	kg	6.7E-10	Combustion emission
m-Xylene	kg	1.6E-07	Combustion emission
Potassium	kg	3.1E-05	Combustion emission
Dioxin, 2,3,7,8 Tetrachlorodibenzo-p-	kg	4.1E-14	Combustion emission
Mercury	kg	4.0E-10	Combustion emission
Zinc	kg	4.0E-07	Combustion emission
PAH	kg	1.5E-08	Combustion emission
Benzene	kg	1.2E-06	Combustion emission
Carbon dioxide, biogenic	kg	1.4E-01	Combustion emission
Fluorine	kg	6.7E-08	Combustion emission
Formaldehyde	kg	1.7E-07	Combustion emission
Particulates, > 2.5 um, and < 10um	kg	3.3E-06	Combustion emission
Magnesium	kg	4.8E-07	Combustion emission
Water	m^3	6.0E-05	Combustion emission
Ammonia	kg	2.3E-06	Combustion emission
Sodium	kg	1.7E-06	Combustion emission
Cadmium	kg	9.3E-10	Combustion emission
Nickel	kg	8.0E-09	Combustion emission
Phosphorus	kg	4.0E-07	Combustion emission
Methane, biogenic	kg	4.0E-06	Combustion emission
Benzene, hexachloro-	kg	9.6E-15	Combustion emission
Waste to treament:			Combustion emission
Ash for disposal	kg	0.00067	Wood ash mixture, pure {GLO}| market for | Conseq

6.14. Fuels for clinker production

Consumption of conventional fuels by the cement industry has been modelled taking into account the inputs to the cement industry in Europe according to the ecoinvent database, in particular with the data set for clinker production in Europe without Switzerland. The LCI is shown below.

Table 47. LCI for production and consumption of fuels for clinker production.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Fuels for clinker production	MJ	2.23	The reference flow is the calorific value of fuel required to produce 1 kg clinker according to the ecoinvent data set Clinker {Europe without Switzerland}| production | Conseq. This calorific value is calculated using the following net calorific values: 35 MJ/kg for coke, 42.6 MJ/kg for light fuel oil, 28.9 MJ/kg for coal, 36.3 MJ/m^3 for natural gas, 41.2 MJ/kg for heavy fuel oil.
Inputs of products and services:			
Petroleum coke	Kg	0.00391	Ecoinvent data set Petroleum coke {GLO}| market for | Conseq
Light fuel oil	Kg	0.000374	Ecoinvent data set Light fuel oil {Europe without Switzerland}| market for | Conseq
Hard coal	Kg	0.0354	Hard coal {PL}| market for | Conseq, U
Natural gas	m^3	0.000175	Ecoinvent data set Natural gas, high pressure {Europe without Switzerland}| market group for | Conseq
Heavy fuel oil	kg	0.0255	Ecoinvent data set Heavy fuel oil {Europe without Switzerland}| market for | Conseq
Emissions to air [a]:			
CO_2, fossil	kg	0.315	Overall CO_2 emissions per kg clinker in the ecoinvent data set are 0.839 kg, but part of this is not fuel-dependent, but rather from calcination of raw materials. We have subtracted calcination emissions as follows: Lime is 100% $CaCO_3$ and calcareous marl in the ecoinvent database is constituted by 75% $CaCO_3$. The quantities of marl and lime in the clinker production process are 0.466 and 0.841 kg per kg clinker, respectively. Thus, the CO_2 emission attributable to calcination is 0.524 kg CO_2/kg clinker. The CO_2 emission attributable to fuels is 0.839 - 0.524 = 0.315 kg CO_2/kg clinker.

[a] Emissions to air other than CO_2 are neglected, since we assume they remain constant in the cement kiln regardless of the use of sludge as fuel.

6.15. Raw meal for clinker production

Consumption of minerals (raw meal) by the cement industry for clinker production has been modelled taking into account the inputs to the cement industry in Europe according to the ecoinvent database, in particular with the data set for clinker production in Europe without Switzerland. The LCI is shown below.

Table 48. LCI for production and consumption of raw meal for clinker production.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Raw meal for clinker production	kg	1.638	The reference flow is the amount of raw materials required to produce 1 kg clinker according to the ecoinvent data set Clinker {Europe without Switzerland}| production | Conseq
Inputs of products and services:			
Clay	Kg	0.331	Ecoinvent data set Clay {GLO}| market for | Conseq
Calcareous marl	Kg	0.466	Ecoinvent data set Calcareous marl {GLO}| market for | Conseq
Lime	Kg	0.841	Ecoinvent data set Lime {GLO}| market for | Conseq
Emissions to air:			
CO_2, fossil	kg	0.524	Overall CO_2 emissions per kg clinker in the ecoinvent data set are 0.839 kg, but only part of this is related to calcination of raw materials. Calcination emissions are calculated as follows: Lime is 100% $CaCO_3$ and calcareous marl in the ecoinvent database is constituted by 75% $CaCO_3$. The quantities of marl and lime in the clinker production process are 0.466 and 0.841 kg per kg clinker, respectively, as reported in this table. Thus, the CO_2 emission attributable to calcination is 0.524 kg CO_2/kg clinker.

6.16. Hydrogen peroxide, 30%

The inventory for the hydrogen peroxide solution used in the AOP modules has been created based on the a concentration of 30% in weight. We modelled this product with the hydrogen peroxide data set in ecoinvent, assuming the remaining 70% is ultrapure water. Also, we added transport services, in order to account for an average distribution of the product to the point of use. This was done with ecoinvent data on transport services for chemicals. The LCI is shown below.

Table 49. LCI for production of hydrogen peroxide solution.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Hydrogen peroxide, 30%	kg	1	
Inputs of products and services:			
Hydrogen peroxide	kg	0.3	Hydrogen peroxide, without water, in 50% solution state {GLO}| market for | Conseq
Ultrapure water	kg	0.7	Water, ultrapure {GLO}| market for | Conseq
Product distribution, inland waters	Tkm	0.0246	Transport, freight, inland waterways, barge {GLO}| market for | Conseq
Product distribution, rail	Tkm	0.3091	Transport, freight train {GLO}| market group for | Conseq
Product distribution, road	Tkm	0.2088	Transport, freight, lorry, unspecified {GLO}| market for | Conseq
Product distribution, sea	Tkm	0.599	Transport, freight, sea, transoceanic ship {GLO}| market for | Conseq

6.17. IBC

The inventory for an Intermediate Bulk Container (IBC) of 1,000 L capacity was established with primary data from Manuilova (2003, p. 10), where this product is stated to weight 75.81 kg, constituted by 39,88 kg steel, 19.93 kg high-density polyethylene (HDPE) and 16 kg wood, the latter referring to a pallet. We modelled these materials with existing ecoinvent data sets. In the case of wood, this was modelled by means of the EUR-flat pallet available in the database. Also, the moulding of the HDPE body was modelled by means of an existing blow moulding process. Finally, we added transport services, in order to account for an average distribution of the product to the point of use. This was done with ecoinvent data on transport services for chemicals. The LCI is shown below.

Table 50. LCI for production of an Intermediate Bulk Container.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
IBC	kg	75.81	
Inputs of products and services:			
Wooden pallet	unit	1	EUR-flat pallet {GLO}| market for | Conseq
Steel	kg	39.88	Steel, low-alloyed {GLO}| market for | Conseq
High-density polyethylene	kg	19.93	Polyethylene, high density, granulate {GLO}| market for | Conseq
Plastic moulding	kg	19.93	Blow moulding {GLO}| market for | Conseq
Product distribution, inland waters	Tkm	0.0246	Transport, freight, inland waterways, barge {GLO}| market for | Conseq
Product distribution, rail	Tkm	0.3091	Transport, freight train {GLO}| market group for | Conseq
Product distribution, road	Tkm	0.2088	Transport, freight, lorry, unspecified {GLO}| market for | Conseq
Product distribution, sea	Tkm	0.599	Transport, freight, sea, transoceanic ship {GLO}| market for | Conseq

6.18. Klingersil

The inventory for Klingersil sealing material has been built based on the material safety data sheet for Klingersil C4430 (KLINGER 1996), where it is declared that it contains 30-60% calcined aluminia silicate, 30-60% glass fibre, 10-30% nitrile butadiene rubber, 10-30% rock wool, 10-30% calcium metasilicate and less than 10% precipitated silica. We modelled these materials with existing ecoinvent data sets. The manufacturing of Klingersil was approximated with the ecoinvent data set for aluminium-polyethylene sealing tape available in ecoinvent. In this data set, the reference flow is 1 m sealing tape weighting 0.057 kg. We scaled up the different flows (capital equipment, energy use, etc.) from this weight to 1 kg, which is the reference flow we used for Klingersil. Finally, we added transport services, in order to account for an average distribution of the product to the point of use. This was done with ecoinvent data on transport services for chemicals. The LCI is shown below.

Table 51. LCI for production of Klingersil.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Klingersil	kg	1	
Inputs of products and services:			
Glass fibre	kg	0.3	Glass fibre {GLO}| market for | Conseq
Rubber	kg	0.1	Synthetic rubber {GLO}| market for | Conseq
Calcined aluminia silicate and calcium metasilicate	kg	0.4	Chemical, inorganic {GLO}| market for chemicals, inorganic | Conseq
Rock wool	kg	0.1	Rock wool {GLO}| market for | Conseq
Precipitated silica	kg	0.1	Activated silica {GLO}| market for | Conseq
Klingersil factory	kg	4.0E-09	Ventilation components factory {GLO}| market for | Conseq
Packaging	kg	0.0275	Packaging film, low density polyethylene {GLO}| market for | Conseq
Manufacturing energy	MJ	1.983	Heat, district or industrial, other than natural gas {RER}| market group for | Conseq
Manufacturing energy	MJ	1.983	Heat, district or industrial, natural gas {RER}| market group for | Conseq
Manufacturing energy	kWh	0.120	Electricity, medium voltage {RER}| market group for | Conseq
Product distribution, inland waters	Tkm	0.0246	Transport, freight, inland waterways, barge {GLO}| market for | Conseq
Product distribution, rail	Tkm	0.3091	Transport, freight train {GLO}| market group for | Conseq
Product distribution, road	Tkm	0.2088	Transport, freight, lorry, unspecified {GLO}| market for | Conseq
Product distribution, sea	Tkm	0.599	Transport, freight, sea, transoceanic ship {GLO}| market for | Conseq

6.19. Machinery disposal

This data set was created to represent the disposal of machinery such as compressors and pumps. The inventory is based on the material composition by the 40W-pumps in ecoinvent. These pumps are composed on a weight basis by 87% steel, 10% copper, 0.8% aluminium and 1.5% plastics. We model the disposal of these materials with existing ecoinvent data sets. The LCI is shown below.

Table 52. LCI for production of an inventory for an Intermediate Bulk Container.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Machinery disposal	kg	2.43	
Waste treatment:			
Steel waste	kg	2.12	Steel scrap recovery (LCI data in this Section 6)
Plastic waste	kg	0.037	Waste plastic, mixture {GLO}| market for | Conseq
Copper waste	kg	0.25	Copper scrap, sorted, pressed {GLO}| market for | Conseq
Aluminium waste	kg	0.02	Aluminium scrap, post-consumer {GLO}| market for | Conseq

6.20. Sodium hypochlorite solution

The inventory for the sodium hypochlorite solution used for cleaning the UF and MBR modules has been created considering a solution with 161 g Cl/L. Such a solution is estimated to have a density of 1.074 kg/L and a concentration of 0.072 kg NaOCl/L or 7.2% in mass. We modelled the remaining mass as ultrapure water. We also added transport services, in order to account for an average distribution of the product to the point of use. This was done with ecoinvent data on transport services for chemicals. The LCI is shown below.

Table 53. LCI for production of sodium hypochlorite solution.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Sodium hypochlorite solution	kg	1	
Inputs of products and services:			
Water for solution	kg	0.928	Water, ultrapure {GLO}| market for | Conseq
Sodium hypochlorite	kg	0.072	Sodium hydroxide, without water, in 50% solution state {GLO}| market for | Conseq
Product distribution, inland waters	Tkm	0.0246	Transport, freight, inland waterways, barge {GLO}| market for | Conseq
Product distribution, rail	Tkm	0.3091	Transport, freight train {GLO}| market group for | Conseq
Product distribution, road	Tkm	0.2088	Transport, freight, lorry, unspecified {GLO}| market for | Conseq
Product distribution, sea	Tkm	0.599	Transport, freight, sea, transoceanic ship {GLO}| market for | Conseq

6.21. Polyethylene product

This data set was created to represent the production of an average polyethylene product and is based on an existing ecoinvent data set for production of a polyethylene pipe, weighting 3 kg. We changed the reference flow from one m of pipe to 3 kg, in order to scale the data set to the desired weight of the different polyethylene products inventoried in the study. Also, we used the global data set for production of electricity. All the remaining flows in the original data set remain the same. The LCI is shown below.

Table 54. LCI for production of a polyethylene product.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Polyethylene product	kg	1	
Inputs of products and services:			
Polyethylene production	kg	3.15	Polyethylene, high density, granulate {GLO}| market for | Conseq
Polyethylene product moulding	kg	3.15	Extrusion, plastic pipes {GLO}| market for | Conseq
Polyethylene products factory	unit	2.22E-09	Plastic processing factory {GLO}| market for | Conseq
Electricity	kWh	0.33	Electricity, medium voltage {GLO}| market group for | Conseq
Heat, natural gas	MJ	4.1325	Heat, district or industrial, natural gas {RER}| market group for | Conseq
Heat, other fuels	MJ	4.1325	Heat, district or industrial, other than natural gas {RER}| market group for | Conseq
Waste treatment:			
Waste polyethylene	kg	0.15	Waste polyethylene {GLO}| market for | Conseq

6.22. Polypropylene product

This data set was created to represent the production of an average polypropylene product and is based on an existing ecoinvent data set for production of a polyethylene pipe, weighting 3 kg. We changed the reference flow from one m of pipe to 3 kg, in order to scale the data set to the desired weight of the different polypropylene products inventoried in the study, as well as the plastic material, from polyethylene to polypropylene. Also, we used the global data set for production of electricity. The LCI is shown below.

Table 55. LCI for production of a polypropylene product.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Polypropylene product	kg	1	
Inputs of products and services:			
Polypropylene production	kg	3.15	Polypropylene, granulate {GLO}| market for | Conseq
Polypropylene product moulding	kg	3.15	Extrusion, plastic pipes {GLO}| market for | Conseq
Polypropylene products factory	unit	2.22E-09	Plastic processing factory {GLO}| market for | Conseq
Electricity	kWh	0.33	Electricity, medium voltage {GLO}| market group for | Conseq
Heat, natural gas	MJ	4.1325	Heat, district or industrial, natural gas {RER}| market group for | Conseq
Heat, other fuels	MJ	4.1325	Heat, district or industrial, other than natural gas {RER}| market group for | Conseq
Waste treatment:			
Waste Polypropylene	kg	0.15	Waste polypropylene {GLO}| market for | Conseq

6.23. Ion exchange plant

The data set for equipment of an ion exchange plant is based on the ecoinvent data set for an ion exchanger, in which we removed the input of cationic and anionic exchange resins, as this is included in our study as part of the operation inventory. Also, we added the dismantling of the materials at the end-of-life stage. The LCI is shown below.

Table 56. LCI for production of water treatment equipment for an ion-exchange plant.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Ion-exchange plant	unit	1	
Inputs of natural resources:			
Transformation, from unknown	m2	100	
Transformation, to industrial area	m2	100	
Occupation, industrial area	m2a	1,500	
Inputs of products and services:			
Polypropylene parts	kg	1,000	Polypropylene, granulate {GLO}| market for | Conseq
Steel parts	kg	3,000	Steel, low-alloyed, hot rolled {GLO}| market for | Conseq
Stainless steel parts	kg	5,900	Steel, chromium steel 18/8, hot rolled {GLO}| market for | Conseq
Waste treatment:			
Waste Polypropylene	kg	1,000	Waste polypropylene {GLO}| market for | Conseq
Waste steel	kg	8,900	Steel scrap recovery (LCI data in this Section 6)

6.24. Phosphoric acid, 54%

The inventory for the phosphoric acid solution in a concentration of 54% by weight, used in biological treatment, is modelled with existing ecoinvent data sets. We also added transport services, in order to account for an average distribution of the product to the point of use. This was done with ecoinvent data on transport services for chemicals. The LCI is shown below.

Table 57. LCI for production of phosphoric acid solution.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Phosphoric acid, 54%	kg	1	
Inputs of products and services:			
Water for solution	kg	0.46	Water, ultrapure {GLO}| market for | Conseq
Phosphoric acid	kg	0.54	Phosphoric acid, industrial grade, without water, in 85% solution state {GLO}| market for | Conseq
Product distribution, inland waters	Tkm	0.0246	Transport, freight, inland waterways, barge {GLO}| market for | Conseq
Product distribution, rail	Tkm	0.3091	Transport, freight train {GLO}| market group for | Conseq
Product distribution, road	Tkm	0.2088	Transport, freight, lorry, unspecified {GLO}| market for | Conseq
Product distribution, sea	Tkm	0.599	Transport, freight, sea, transoceanic ship {GLO}| market for | Conseq

6.25. Pump

This data set is created to represent the production of the pumps installed in the INTEGROIL plant. The original ecoinvent data set for a 40-W pump refers to a unit weighting 2.42 kg and the reference flow for this data set is one unit. We changed the reference flow from one unit of pump to 2.42 kg, in order to scale the data set to the weight of the actual pumps installed in the plant.

Table 58. LCI for production of a pump.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Pump	kg	2.42	
Inputs of products and services:			
Pump production (CH)	unit	0.008	Pump, 40W {CH}| production | Conseq, U
Pump production (RoW)	unit	0.992	Pump, 40W {RoW}| production | Conseq, U

6.26. PVC product

This data set was created to represent the production of an average polyvinylchloride (PVC) product and is based on an existing ecoinvent data set for production of a polyethylene pipe, weighting 3 kg. We changed the reference flow from one m of pipe to 3 kg, in order to scale the data set to the desired weight of the different polypropylene products inventoried in the study, as well as the plastic material, from polyethylene to PVC. Also, we used the global data set for production of electricity. The LCI is shown below.

Table 59. LCI for production of a PVC product.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
PVC product	kg	1	
Inputs of products and services:			
PVC production	kg	3.15	Polyvinylchloride, bulk polymerised {GLO}| market for | Conseq
PVC product moulding	kg	3.15	Extrusion, plastic pipes {GLO}| market for | Conseq
PVC products factory	unit	2.22E-09	Plastic processing factory {GLO}| market for | Conseq
Electricity	kWh	0.33	Electricity, medium voltage {GLO}| market group for | Conseq
Heat, natural gas	MJ	4.1325	Heat, district or industrial, natural gas {RER}| market group for | Conseq
Heat, other fuels	MJ	4.1325	Heat, district or industrial, other than natural gas {RER}| market group for | Conseq
Waste treatment:			
Waste PVC	kg	0.15	Waste polyvinylchloride {GLO}| market for | Conseq

6.27. Refrigeration machine, R134a as refrigerant

The inventory for production of the air drier used in the AOP module is based on the original ecoinvent data set for a refrigeration machine using R134a as refrigerant. The data set refers to a unit weighting 326.5 kg and the reference flow for this data set is one unit. We changed the reference flow from one unit of machine to 326.5 kg, in order to scale the data set to the weight of the actual equipment installed in the plant.

Table 60. LCI for production of a refrigeration machine.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Refrigeration machine, R134a as refrigerant	kg	326.5	
Inputs of products and services:			
Refrigeration machine production	unit	1	Refrigeration machine, R134a as refrigerant {GLO}| production | Conseq

6.28. Router

The inventory for production of a router is based on the original ecoinvent market data set for a router. The data set refers to a unit weighting 1.89 kg and the reference flow for this data set is one unit. We changed the reference flow from one unit of machine to 1.89 kg, in order to scale the data set to the weight of the actual equipment installed in the plant.

Table 61. LCI for production of a router.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Router	kg	1.89	
Inputs of products and services:			
Router production (CH)	unit	0.008	Refrigeration machine, R134a as refrigerant {GLO}| production | Conseq
Router production (RoW)	unit	0.992	

6.29. Steel product

This data set was created to represent the production of an average finished steel product. The reference flow is 1 kg product. It includes the production of 1 kg steel, an average finishing process for 1 kg steel product and an output of 0.227 kg scrap steel to manage as waste. The amount of waste scrap is obtained from the metal working data set. The LCI is shown below.

Table 62. LCI for production of a steel product.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Steel product	kg	1	
Inputs of products and services:			
Steel production	kg	1	Steel, low-alloyed, hot rolled {GLO}| market for | Conseq
Steel product manufacture	kg	1	Metal working, average for steel product manufacturing {GLO}| market for | Conseq
Waste treatment:			
Steel waste	kg	1	Steel scrap recovery (LCI data in this Section 6)

6.30. Steel product, chromium steel

This data set was created to represent the production of an average finished stainless steel product. The reference flow is 1 kg product. It includes the production of 1 kg steel, an average finishing process for 1 kg steel product and an output of 0.227 kg scrap steel to manage as waste. The amount of waste scrap is obtained from the metal working data set. The LCI is shown below.

Table 63. LCI for production of a stainless steel product.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Steel product, chromium steel	kg	1	
Inputs of products and services:			
Stainless steel production	kg	1	Steel, chromium steel 18/8 {GLO}| market for | Conseq
Stainless steel product manufacture	kg	1	Metal working, average for steel product manufacturing {GLO}| market for | Conseq
Waste treatment:			
Stainless steel waste	kg	1	Steel scrap recovery (LCI data in this Section 6)

6.31. Steel scrap recovery

The data set for steel scrap is based on the ecoinvent data set for sorted and pressed iron scrap, to which we add a credit for the obtained scrap, which substitutes primary iron scrap. The LCI is shown below.

Table 64. LCI for scrap steel recovery.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Steel scrap recovery	kg	1	
Inputs of products and services:			
Sorting plant	unit	1.0E-9	Scrap preparation facility {GLO}| market for | Conseq
Electricity	kWh	0.01	Electricity, medium voltage {GLO}| market group for | Conseq
Heat, diesel	MJ	0.1	Diesel, burned in building machine {GLO}| market for | Conseq
Scrap to recycling	kg	-1	Pig iron {GLO}| market for | Conseq

6.32. Waste actuator valve

The LCI for managing an automated valve as waste, on a per kg valve basis, is based on the material composition for this product (see LCI for Actuator valve in this Section 6), which is taken from an environmental product declaration by Life Cycle Engineering Experts (2013), in which a broad material composition is given as 15% steel, 15% copper, 15% brass, 44% aluminium and 12% plastics. We modelled the disposal of these materials with generic ecoinvent data sets, with exception of steel, for which we used the Steel scrap recovery data set presented in this Section 6. Given that ecoinvent lacks a data set for brass waste, this was modelled as copper waste. The LCI is shown below.

Table 65. LCI for disposal of an actuator valve.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Waste actuator valve	kg	1	
Waste treatment:			
Steel waste	kg	0.15	Steel scrap recovery (LCI data in this Section 6)
Copper and brass waste	kg	0.30	Copper scrap, sorted, pressed {GLO}| market for | Conseq
Aluminium waste	kg	0.44	Aluminium scrap, post-consumer {GLO}| market for | Conseq
Polyvinylchloride waste	kg	0.12	Waste polyvinylchloride {GLO}| market for | Conseq

6.33. Waste air filter

This data set was created to represent the disposal of the particle filters used in the AOP modules. The original ecoinvent data set for disposal of an air filter refers to a unit weighting 84 g and the reference flow for this data set is one unit. We changed the reference flow from one unit of filter to 84 g of filter, in order to scale the data set to the weight of the actual filters used in the INTEGROIL plant. The LCI is shown below.

Table 66. LCI for disposal of an air filter.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Waste air filter	kg	0.084	
Inputs of products and services:			
Product distribution, rail	Tkm	0.00448	Transport, freight train {GLO}| market group for | Conseq
Product distribution, road	Tkm	0.007728	Transport, freight, lorry, unspecified {GLO}| market for | Conseq
Product distribution, inland waters	Tkm	0.000796	Transport, freight, inland waterways, barge {GLO}| market for | Conseq
Product distribution, sea	tkm	0.00846	Transport, freight, sea, transoceanic ship {GLO}| market for | Conseq
Air filter disposal (CH)	Unit	0.008	Used air filter in exhaust air valve {CH}| treatment of used air filter, in exhaust air valve | Conseq
Air filter disposal (RoW)	Unit	0.992	Used air filter in exhaust air valve {RoW}| treatment of used air filter, in exhaust air valve | Conseq

6.34. Waste glass fibre reinforced plastic

This data set was created to represent the disposal of glass fibre reinforced plastic, given that a data set for this activity is not available in the ecoinvent database. The data set assumes the material is composed of 40% plastic, namely polyethylene and 60% glass fibre. Generic data sets were used to model the disposal of the two materials. The LCI is shown below.

Table 67. LCI for disposal of glass fibre reinforced plastic.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Waste glass fibre reinforced plastic	kg	1	
Inputs of products and services:			
Polyethylene waste	kg	0.4	Waste polyethylene terephtalate {GLO}| market for | Conseq
Glass fibre waste	kg	0.6	Waste glass {GLO}| market for | Conseq

6.35. Waste IBC

The inventory for disposal of an IBC of 1,000 L capacity was established with primary data from Manuilova (2003, p. 10), where this product is stated to weight 75.81 kg, constituted by 39,88 kg steel, 19.93 kg HDPE and 16 kg wood, the latter referring to a pallet. We modelled these materials with existing ecoinvent data sets for material disposal, with the exception of steel, which was modelled with the data set for steel scrap recovery presented in this Section 6. The LCI is shown below.

Table 68. LCI for disposal of an Intermediate Bulk Container.

Exchanges	Unit	Amount	Ecoinvent data sets/comments
Reference flow:			
Waste IBC	kg	75.81	
Inputs of products and services:			
Wood waste	kg	16	Waste wood, untreated {GLO}| market for | Conseq
Steel waste	kg	39.88	Steel scrap recovery (LCI data in this Section 6)
High-density polyethylene waste	kg	19.93	Waste polyethylene {GLO}| market for | Conseq

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