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Abbreviations and acronyms

CAPEX	Capital expenditures
DMC	Direct manufacturing costs
E.O.	Essential oil
FCI	Fixed capital investment
FMC	Fixed manufacturing costs
GE	General expenses
ISBL	Inside battery limits
LCA	Life Cycle Assessment
MC	mixed culture
MDO	Multidisciplinary Design Optimization
OPEX	Operating expenditures
OSBL	Outside Battery Limits
CPC	Partition Chromatography technique
PHA	Polyhydroxyalkanoate
P3HB	Poly(3-hydroxybutyrate)
RO	Reverse osmosis
SDS	Sodium dodecyl sulphate
TEE	Techno-economic evaluation
TFCI	Total fixed capital investment
UF	Ultra - filtration
VFA	volatile fatty acids
WW	Wastewater
WCI	Working capital investment

1 Executive summary

The AFTERLIFE project proposes a flexible, cost- and resource-efficient process for recovering and valorising the relevant fractions from wastewater (WW). The AFTERLIFE process will separate out the different components of value using a series of membrane filtration units that will separate all the solids in the wastewater. These will then be treated to obtain high-pure extracts and metabolites or, alternatively, to be converted into value-added biopolymers, polyhydroxyalkanoates (PHAs). In addition to the value extracted from the solids, the remaining outflow of the water will be ultrapure and ready for re-use. Therefore, the overarching objective of the AFTERLIFE project is to demonstrate an innovative wastewater treatment that simultaneously recovers compounds of interest while converting the remaining organic matter into a high-volume added value biopolymer. The project is funded by the European Commission via Horizon 2020 (https://afterlife-project.eu).

As part of the project a hotspot techno-economic evaluation (TEE) has been carried out by nova-Institut GmbH to identify techno-economic hotspots at an early stage of the development in order to guide the process design optimization, using a feedback loop approach.

The analysis is based on the current developments of each work package and uses the mass and energy flows provided by the responsible project partners.

The following outcomes and issues to be mentioned:

- The results of this TEE give an early understanding of the techno-economic performance of the AFTERLIFE PHA namely P3HB, essential oils, amino acids and polyphenols production at their current *status quo* of development.
- At the moment wastewater from sweet and candies manufacturing (Jake WW line) seems to be the most promising feedstock to produced PHA compared to wastewater from cheese and juice and other products from citric fruits manufacturing.
- For Jake wastewater (WW) line, which at base scenario displays positive economic results, the price at which the P3HB will be sold on the market plays a large role on the economic performance of the process.
- The foreground AFTERLIFE processes are based on primary mainly experimental lab scale data from the project partners and are subject to optimization in the course of the project.
- The AFTERLIFE process at this stage do not yet include heat integration. Further improvements in the TEE will be achieved when this is included.
- The main limitations of this TEE study are due to the data quality of the inventories. Some inputs are based on secondary data (literature), are based on lab scale processes (lab experiments or simulation models (calculated or estimated data) or estimated data), therefore scoring badly in completeness.
- Given that some uncertainty is present at the data inventory level the potential techno-economic assessment is to be considered informative and is expected to change during the research development and with increasing knowledge.

To conclude, this TEE will be updated in a final report (deliverable D7.4 "Final techno-economic assessment" due at M46, at the end of the project,) including optimization, feedback loops and a more detailed assessment of the AFTERLIFE-process with the most promising wastewater as feedstock. The

full TEE will be based on measured data from the pilot plant, which is been set up at the facilities of BBEU.

2 Introduction

The overarching objective of the AFTERLIFE project is to demonstrate, at TRL-5, an innovative wastewater treatment that simultaneously recovers compounds of interest while converting the remaining organic matter into a high-volume added value biopolymer. Specifically, it sets out to:

- Develop the filtration system for recovering suspended and soluble solids in wastewater by using membrane filtration units.
- Develop the process for recovering and purifying valuable compounds in the concentrates extracted in the filtration step.
- Develop an anaerobic/aerobic process for converting the low value-added organic matter into PHAs.
- Optimize the resources in the process, following a circular economy approach
- Design and optimize the AFTERLIFE process from a holistic perspective following a Multidisciplinary Design Optimization (MDO) approach
- Conduct a demonstration, at a pilot scale, using real industrial wastewater to generate the end products
- Prove the economic and industrial feasibility for AFTERLIFE process along with a comprehensive Lifecycle Analysis (LCA) and cost assessment.
- Promote exploitation of the project’s results and expand its impact.

Techno-economic evaluation (TEE) is the economic counterpart of the environmental life cycle assessment aiming at analysing the economic dimension of sustainability from cradle-to-grave or -gate. This task will provide a breakdown in processes via TEE aiming to provide economic key figures for decision making.

The goal of the economic evaluation within the AFTERLIFE project is the evaluation of innovative technologies from wastewater streams. It aims at assessing the economic performance of a PHA production process from different wastewaters.

The focus of the assessment is on identifying techno-economic hotspots, in order to determine, at an early stage of the development, approaches to guide further optimization within the project’s technology development work packages, using a feedback loop approach.

Summing up, this report aims principally at identifying techno-economic hotspots in order to guide the process design optimization. The following sections describe the techno-economic assessments conducted as part of WP7 and are structured as follows:

- TEE methodology;
- Goal and scope definition;
- TEE data inventory analysis;
- Results and discussion of TEE;
- Conclusions and further work.
- In the appendix supporting information can be found.

3 Techno-economic evaluation methodology

For the techno-economic evaluation of innovative industrial processes often only limited data is available. The chosen methodology for the implementation of TEEs was developed for cases where energy and material flows from process simulation models are available. For the evaluation of techno-economic parameters, a model is required that leads to satisfactory results even when limited data is available.

The costing methodology outlined below has been developed and first applied in the FP7 project BIOCORE S. Piotrowski, M. Carus et al. (2014).

The techno-economic analysis of the investment for an industrial process includes the evaluation of capital costs (CAPEX), annual operating expenses (OPEX), revenues and profits. Table 1 shows the detailed cost structure of the CAPEX and OPEX components.

Table 1 Cost structure based on the study by Turton, Bailie et al. (2012)

	Capital expenditures (CAPEX)	Operating expenditures (OPEX)
Fix costs	**FCI - Fixed capital investment (*costs associated with ISBL: inside battery limits*)**	**Fixed manufacturing costs (FMC)**
	Costs of utilities (C_{UT})	C_D - Depreciation
	Contingency charges (C_{CC})	C_{LT} - Local taxes and insurances
	Engineering costs (C_{ENG})	C_{PO} - Plant overhead costs
	Investments related to Outside Battery Limits (OSBL)	**General expenses (GE)**
	Total fixed capital investment (TFCI) = $C_{UT} + C_{CC} + C_{ENG}$ + OSBL	C_{AD} - Administration costs
	Working capital investment (WCI 10% of FCI)	C_{DI} - Distribution and selling costs
	Capital expenditures (CAPEX) = TFCI + WCI	C_{RD} - Research and development
Variable costs		**Direct manufacturing costs (DMC)**
		C_{WF} - Wastewater as feedstock
		C_{RM} - Other raw materials
		C_{UL} - Utilities
		C_{OL} - Operating labour
		C_{DS} - Direct supervisory and clerical labour
		C_{MR} - Maintenance and repairs
		C_{OS} - Operating supplies
		C_{LC} - Laboratory charges
		C_{PR} - Patents and royalties
		Operating expenditures (OPEX) = FMC + DMC + GE

3.1 Outline of the CAPEX

The total investment needed for a project, also called Capital Expenditures (CAPEX), can be roughly divided into the sum of the fixed capital investment (FCI) and working capital investment (WCI).

According to (Sinnott 1999) (p. 243) the FCI is the total cost of the plant ready for start-up. It includes the cost of:

1. Design, and other engineering and construction supervision,
2. All items of equipment and their installation,
3. All piping, instrumentation and control systems,
4. Buildings and structures,
5. Auxiliary facilities, such as utilities, land and civil engineering work.

The FCI is a once-only cost that is not recovered at the end of the project life, other than the scrap value. The FCI includes the complete construction cost of the plant with all its processing and handling equipment as well as its ground preparation and non-process structures and equipment. FCI would also include the investment for purchasing land to build the plant on. However, this investment is left out of the analysis of the AFTERLIFE project for two reasons: First, the surface area needed for the plant is unknown. Second, the sustainability assessment should be location independent and the cost for land varies widely between locations. Land is the only part of the FCI that is not depreciable so that the remainder constitutes the depreciable FCI.

The WCI includes the initial cost of resources, such as feedstock and catalyst, as well as money required for labour and services required to start operation of the plant. WCI is the additional investment needed, over and above the fixed capital, to start up the plant and operate it to the point when income is earned. It includes the cost of:

1. Start-up.
2. Initial catalyst charges.
3. Raw materials and intermediates in the process.
4. Finished product inventories.
5. Funds to cover outstanding accounts from customers.

According to Peters and Timmerhaus (1991) typical values for the WCI are between 15-20% of the FCI. However, this estimate has been made for conventional chemical plants. A study by (Fernando D. Ramos 2019), which however considers working capital to be 10% of the fixed capital for PHA production plants. This value for WCI is therefore used for the following calculations.

Due to the early design stage of the AFTERLIFE processes, it is not possible to calculate CAPEX directly from the plant design. However, there are several methods to rapidly estimate total investments costs (see e.g. (Sinnott 1999) p. 248).

Additional to such methods, Lange (2001) showed that the "power loss" of a process, defined as the difference between the Lower Heating Values (LHV) of the plant intake (including feed and fuel streams) and that of the product stream leaving the plant, is a good indicator for plant investment costs. Therefore, the energy balance, known from the process flow sheets, can be used as a first approximation of investment costs. However, Lange (2001) also showed that this relation is less reliable for small-scale, heat-neutral reactions and in the case of batch processes used for manufacturing fine and specialty chemicals.

Lange (2001) also presented a second correlation approach for estimating the fixed capital investment (FCI), based on the sum of energy transfer duties of all process segments, roughly equivalent to the total rated power of the process equipment (Figure 1).

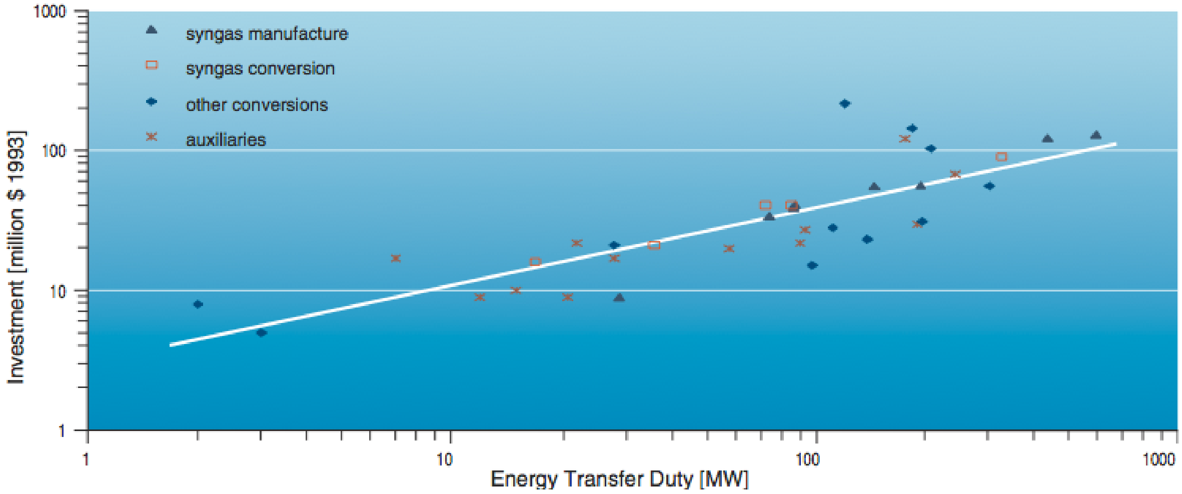

Figure 1 Correlation between energy transfer duty and investment costs (Source: Lange (2001))

For the AFTERLIFE CAPEX estimation, this last approach appears to be most suitable, given the limited level of process data available. As will be shown below, estimates of the total rated power can be derived from the dataset provided by the project partners.

The original equation that Lange 2001 [21] found was:

$$FCI\ [\text{Mill. USD 1993}] = 2.9 * \text{Rated Power}\ [MW]^{0.55.}$$

The conversion of this formula into Euro in 2019 results in the following formula:

$$FCI\ [\text{Mill. EUR 2019}] = 4.7 * \text{Rated Power}\ [MW]^{0.55}$$

This conversion was achieved by first adjusting for inflation (using the CPI inflation adjustment, 1 USD in 1993 is equivalent to 1.80 USD in 2019) and then converting USD into EUR (1 USD in 2010 being equivalent to about 0.90 EUR in 2015) (Bureau of Labour Statistics (2019), OFX (2019)).

The FCI calculated using the correlation proposed by Lange (2001) does not include investments related to Outside Battery Limits (OSBL) nor contingency charges (Lange 2013).

These are all costs that are not related to investments in the facility itself, i.e. infrastructure such as roads, pipes, energy supply etc. The investments related only to the specific facility are called Inside Battery Limits (ISBL). In principle, the choice of whether to assess ISBL or OSBL depends on whether a “green field” plant is assumed or one integrated in an already existing chemical park.

Cheuvel, Foumier et al. (2003) provide some guidance on how approximate OSBL, engineering costs and contingency charges.

Outside Battery Limits

According to Cheuvel, Foumier et al. (2003), OSBL can be estimated as a percentage of the ISBL costs. As a rule of thumb, they propose 40% of the ISBL costs as an estimate for OSBL.

Engineering costs

The costs for designing equipment and structures of a chemical plant are called engineering costs and they constitute extra costs usually outside the scope of chemical process design. Cheuvel, Foumier et al. (2003) propose that engineering costs may amount to 10-30% of ISBL, depending on the size and complexity of the project.

Contingency charges

Contingency charges are included to account for unexpected events such as unanticipated prices increases or delays in construction. Cheuvel, Foumier et al. (2003) state that "an absolute minimum for contingency charges is 10% of the ISBL and OSBL, with a more realistic value being closer to 20 %".

3.2 Outline of the OPEX

According to Turton et al. 2012[33], the annual operating expenditures (OPEX) can be grouped into direct or variable manufacturing costs (DMC), fixed manufacturing costs (FMC) and general expenses (GE). The Table 1 shows the types of cost items as grouped into these categories following Turton, Bailie et al. (2012). Ideally, all cost items listed in Table 1 under OPEX would be calculated directly even if some estimations are necessary. According to Turton, Bailie et al. (2012) OPEX can be determined when the following costs are known or can be estimated:

1. Fixed capital investment (FCI)
2. Cost of operating labour (C_{OL})
3. Cost of utilities (C_{UT})
4. Cost of raw materials (C_{RM})

This result follows from the assumption, as described in Turton, Bailie et al. (2012) (p. 206), that all other cost items are fixed factors of these four cost components shown above. The procedure for estimating FCI has been explained in section 3.1, as well as a detailed description of the costs of utilities, operating labour and raw materials (feedstock and operating materials), which can be directly calculated from the AFTERLIFE process data. The model therefore provides a robust and transparent means of estimating both CAPEX and OPEX with limited data.

Turton, Bailie et al. (2012) present typical corresponding multiplication factors for each of the OPEX components shown in Table 1, combined from several literature sources. In the following, we are discussing each of these multiplication factors.

3.2.1 Direct manufacturing costs

Variable or direct manufacturing costs (DMC) represent operating expenses that vary with production rate. In the following, each position in the total DMC and their calculation are explained.

Raw materials

This includes the wastewaters from Jake, Heritage and Citromil (both essential oil and juice lines) as feedstock as well as other operating materials and auxiliaries needed in the process. Due to the importance of the biomass feedstock for the whole process, we split total raw material costs into wastewater as feedstock costs (C_{WF}) and other operating material costs (C_{RM}). The quantities of the other operating materials (C_{RM}) needed for the processes can be obtained from the flowsheets and prices of each material from market research.

Utilities

According to Towler and Sinnott (2013) the word “utilities” is used for the ancillary services needed in the operation of any production process. These typically include (Towler and Sinnott (2013), p. 104):

1. Electricity
2. Fuel for fired heaters
3. Fluids for process heating
    a. Steam
    b. Hot oil or specialized heat transfer fluids
4. Fluids for process cooling
    a. Cooling water
    b. Chilled water
    c. Refrigeration systems
5. Process water
    a. Water for general use
    b. Demineralized water
6. Compressed air
7. Inert-gas supplies (usually nitrogen)

The quantities required can be obtained from the energy balances and the flowsheets and prices are obtained from market research.

Operating labour

The assessment of operating labour costs (C_{OL}) also requires an estimation as at this point of research it is not possible to assess the time needed for the labour in the facility.

In the AFTERLIFE project an assumption is made that the facility for PHA production for all wastewaters will take place in the factories, where individual three industry partners (Jake, Heritage and Citromil) operate. Therefore, while making assumptions about the employees needed for the PHA production, it is assumed that the complete infrastructure in the factory will be already set up and maintained by the employees that are already working, and the additional employees will be hired only for the maintenance of the PHA plant. In this study, we assume that three full time employees (FTE) will be required to run and maintain the PHA plant at industrial level.

The average labour cost in the EU in 2018 amounted to about 27.4 EUR/h (EUROSTAT 2018). This labour cost will be used for this evaluation.

Direct supervisory and clerical labour

These are costs of administrative, engineering and support personnel. Turton, Bailie et al. (2012) link the costs for direct supervisory and clerical labour to the costs of operating labour (C_{OL}) with a factor of 0.10-0.25. For the base case, we are therefore using the average factor of 0.18 * C_{OL}.

Maintenance and repairs

These are costs of labour and materials associated with maintenance. Turton, Bailie et al. (2012) are proposing a factor of 0.02-0.10 linked to FCI. According to Cheuvel, Foumier et al. (2003) it is customary

in the heavy industry sectors (refining, petrochemical, major intermediates, inorganic chemistry, metalworking etc., to estimate maintenance expenses at an average of 4% of the cost of the plant, i.e. of the battery limits investments, as well as for general services and storage (Cheuvel, Foumier et al. (2003), p. 152). However, this percentage is very dependent on the kind of products that are processed and the type of equipment. Concrete constructions, which are both static and corrosion resistant, require only minimal maintenance. Therefore, the maintenance cost may be lower, e.g. 3%, for general services and storage, while being higher, e.g. 4% for the production units. When the products are very aggressive, and special equipments may be required, costs may reach as much as 10% per year of the battery limits investments. Overall, to treat maintenance cost as a fixed percentage of investments is a simplification because expenses may diminish substantially, if not entirely, if the units are shut down for a longer time period.
For the base case, a value of 2% of FCI will be used, so one at the lower end of the estimations given above.

Operating supplies
According to Turton, Bailie et al. (2012) these are “costs of miscellaneous supplies that support daily operation not considered to be raw materials. Examples include chart paper, lubricants, miscellaneous chemicals, filters, respirators and protective clothing for operators etc.” (Turton, Bailie et al. (2012), p. 204).
For this cost item, Turton, Bailie et al. (2012) propose to use 10-20% of maintenance and repairs or, equivalently, on average 0.003 * FCI.

Laboratory charges
The annual cost of the laboratory analyses required for process monitoring and quality control is a significant item in most modern chemical plants. Sinnott (1999) propose as a rough estimate of laboratory charges 20-30% of operating labour cost or 2-4% of the total production cost. Turton, Bailie et al. (2012) use a factor of (0.1-0.2)*C_{OL} or on average 0.15 * C_{OL}. The latter value has been considered in this analysis.

Patents and royalties
These are costs of using patented and licenced technology. Turton, Bailie et al. (2012) use for these a multiplication factor of (0-0.06) * OPEX, or on average 0.03 * OPEX, which will be used for the base case.

3.2.2 Fixed manufacturing costs
Fixed manufacturing costs are independent from the production rate. The main cost items subsumed under this heading include depreciation, local taxes and insurance and plant overhead costs. These are shortly explained below.

Depreciation

The investment required for the project is recovered as a charge on the project. Capital is often recovered as a depreciation charge, which sets aside a given sum each year to repay the cost of the plant. The plant is not necessarily replaced at the end of the depreciation period. The depreciation sum is really an internal transfer to the organisation's fund for future investment.

If the plant is considered to "depreciate" at a fixed rate over its predicted operating life (so-called straight-line method), the annual sum to be included in the operating cost can be easily calculated. The period over which a plant may be depreciated has fiscal implications and therefore there are national rules for the depreciation of a chemical plant and parts thereof. In Germany, for example, the depreciation period for movable equipment such as pumps, distillation columns or coolers is 10 years while it is 40 years for factory buildings.

Due to fact that total investment is not available in such detail, an average depreciation period of 15 year is used for the FCI. The FCI is therefore depreciated over 15 years so that 1/15 (0.067 *FCI) of the initial FCI accrue each year of operation.

Local taxes and insurance

A plant usually has to pay various taxes (local and regional taxes, property taxes, licence and other payments, environmental protection) and insurances against damages to the production units and also for materials and products tied up in this equipment and also against damages caused to third parties and the environment. These costs are periodic in nature and have to be paid at about the same amount every year unless significant changes have been made to the manufacturing complex being insured.

Turton, Bailie et al. (2012) propose a factor of (0.014-0.05)*FCI or on average 0.032*FCI for both local taxes and insurances. For the base case of the AFTERLIFE assessment, 2% of FCI will be assumed.

Plant overhead costs

Overhead costs are costs incurred by non-productive components or its ancillary services and have to be carried by all productive activities. These typically include general management, plant security, medical, canteen, general clerical staff and safety and plant technical personnel not directly associated with and charged to a particular operating area. Alternatively, some of these costs could be attributed to supervision costs (Sinnott (1999), p. 264). Overhead costs can be expected to rise with the scale of the manufacturing facilities. Here, it is customary to take a fixed percentage of about 1% of the investment costs (Cheuvel, Foumier et al. (2003)) or 50-100% of labour costs (Sinnott (1999), p. 264).

(Turton, Bailie et al. 2012) propose a factor related to both operation labour costs and FCI. Following their proposal, we are estimating plant overhead costs in the base case as $0.708*C_{OL} + 0.036*FCI$.

3.2.3 General expenses

General expenses account for additional overhead necessary for carrying out business. The main items subsumed under this heading include administration costs, distribution and selling costs and research and development costs.

Administration costs

This heading covers the direct operating supervision: the management directly associated with running the plant. These costs will depend on the size of the plant and the nature of the process.

Turton, Bailie et al. (2012) estimate administration costs to be 15% of the sum of operating labour costs, direct supervisory and clerical labour costs and maintenance and repairs. By making use of the estimates shown above, this equates to 0.177*C_{OL}+ 0.003*FCI. This estimate will be used for the base case.

Distribution and selling costs

On top of actual production costs, there are sales expenses, general overheads and costs for research and development to consider. These costs are estimated by Turton, Bailie et al. (2012) as lying between 2-20% of OPEX. For the base case we will therefore use the average of 0.11*OPEX.

Research and development

These are all costs of research activities related to the process and products and include salaries and funds for research-related equipment and supplies etc. (Turton, Bailie et al. (2012), p. 205). Turton, Bailie et al. (2012) estimate these costs as 0.05*OPEX, i.e. 5% of annual manufacturing costs.

3.2.4 Formula for the estimation of OPEX

From applying all of the multiplication factors discussed above, the final estimation procedure for DMC, FMC and GE is as follows:

DMC:

Raw materials: Actual prices

Utilities: Actual prices

Operating labour: For Jake wastewater: 12,600 h/year; for Heritage wastewater: 3,600 h/year; for Citromil wastewater 5,600 h/year

Direct supervisory and clerical labour: 0.18*C_{OL}

Maintenance and repairs: 0.02*FCI

Operating supplies: 0.003*FCI

Laboratory charges: 0.15*C_{OL}

Patents and royalties: 0.03*OPEX

FMC:

Depreciation: 0.067*FCI

Local taxes and insurance: 0.02*FCI

Plant overhead costs: 0.708*C_{OL}+ 0.036*FCI

GE:

Administration costs: 0.177*C_{OL}+ 0.003*FCI

Distribution and selling costs: 0.11*OPEX

Research and development: 0.05*OPEX

Summing up all of the above and solving for OPEX leads to the following equation:
$OPEX = 0.184*FCI + 2.735*C_{OL} + 1.235*(C_{UT} + C_{RM})$
The annual manufacturing costs can therefore be estimated using figures for FCI, C_{OL}, C_{UT} and C_{RM}. All of the necessary data can be derived from the dataset provided by the AFTERLIFE project partners.

4 Goal and scope definition

The study intends to support decisions on a strategic level such as raw material strategies, technology scenarios, biorefinery scenarios. The assessment answers the following interrelated questions:

- What is the overall economic performance of the different processing routes?
- Which hotspots are driving the costs of the production process?
- What is the economic performance of a specific product and is it competitive with existing products?
- Is the overall PHA production concept of AFTERLIFE competitive and under which conditions?

4.1 Goal

The techno-economic assessment will provide insights into the general cost structure and competitiveness of the AFTERLIFE process to guide decisions improving the economic feasibility of the production processes.

4.2 Scope

The TEE hotspot will be conducted based on the inventory of material and energy flows (inputs and outputs) of the process used in the life cycle, based on market prices of these flows. The study focuses on P3HB production as a main output (for wastewaters from Jake, Heritage and Citromil) and other by-products from Citromil's essential oil (E.O.) line.

4.2.1 Targeted audience

The results and inventory data of this TEE have a public dissemination level. Targeted audience are within the project partners and externally all interested stakeholders.

4.2.2 Geographical and time representativeness

The individual process steps of the AFTERLIFE process were developed and tested at the labs and facilities of the responsible project partners. For example, the pretreatment of the different wastewater was developed at Lurederra in Spain, filtration at VTT in Finland, VFA- and biogas production at Innoven in Italy, PHA-production at Nova ID in Portugal and CSIC in Spain and PHA-recovery at BBEU in Belgium. At the current status of the project each process step was developed in a different location and therefore the goal of the study is to reflect the European situation. Later the pilot plant will be located in Belgium at the facilities of BBEUP.

Primary data reflects the current status of the process designs for the AFTERLIFE process. As such, this is a preliminary assessment which will be updated and completed at the end of the project (deliverable D7.4, due in M46).

4.2.3 Function and functional unit

The functional unit provides a reference to which the inputs and outputs are related. (Klöpffer and Grahl 2009). It defines qualitative and quantitative aspects of the good or service under study along the questions: "what", "how much", "how well", and "for how long". Further the role of the functional

unit definition in TEE is to ensure that the techno-economic factors of products or processes are based on a fair comparison.
The functional unit in this assessment is defined as one ton of PHA polymer granulate (namely poly(3-hydroxybutyrate) (P3HB)) with a purity of 99.2 %.

4.2.4 Product system, system boundaries and cut-off criteria

The assessment includes all life cycle stages (production steps) from cradle-to-gate, that is,

(1) Acquisition of raw materials, utilities and auxiliaries including transports
(2) AFTERLIFE production process

as described exemplarily in Figure 2 for the AFTERLIFE process with Jake wastewater input.

4.2.4.1 Feedstock

The starting material called feedstock is wastewater from several origins. Three different profiles of food processing industries were evaluated as wastewater suppliers:

- Sweet and candies manufacturing (represented by the company JAKE, Spain)
- Cheese manufacturing (represented by the company HERITAGE, Belgium)
- Juice and other products from citric fruits (represented by the company CITROMIL, Spain)

Jake

Jake SA uses water for human consumption for its entire activity and consumes between 40,000 and 50,000 m^3/year, including the process water plus the one used for cleaning and staff use. The volume of concentrated wastewater generated by Jake is between 6000 and 8000 m^3/year (between 22,000 and 24,000 m^3/year without concentrating). Considering that of every 1000 L of wastewater entering into the evaporator tank 650 L are evaporated and 350 L of condensate are generated. Therefore, the evaporation ratio is 65%. Jake products incorporate as an ingredient between 30-40% of the water that enters the line. Part of this water evaporates in the drying process of the product. The most relevant stage in relation to the generation of wastewater is the washing phase of the supplying and mixing of ingredients tanks and the cleaning of equipment and facilities. Gums & Jellies line produces 2/3 of wastewater. Jake uses these concentrated wastewaters for the production of biogas through an anaerobic fermentation with excellent results due to its high content of sugars. These tanks continuously supply waste water to a concentrator through evaporation that concentrates between 60 and 65% of the residual water. The concentrate goes to an expedition deposit from which every day a concentrate cistern is sent to a biomethanization plant where it is valued for the production of biogas. Qualitatively the characteristics of Jake SA wastewater are similar throughout the year as a result of a more or less similar daily activity. The high content of sugars (mainly sucrose and glucose, but also relevant amounts of fructose and maltotriose) (this content varies between 3.25 and 11.13%). It causes high COD values (see Table 2), and according to the information received by the company, causes high viscosity that makes later membrane filtration difficult.

Heritage

The activity of HERITAGE 1466 is focused on the production of Herve cheeses which comprises two different production lines or processes involving the production of: cheeses “a Pate Demi Dure” (PDD line) and cheeses “a Pate Molle” (PM line), as the main products delivered by this milk processing and cheese manufacturing company. Belgian cow milk is the only raw material used in both production lines, and rennet plus distinct ferments are used as additives.

The wastewater generated by HERITAGE derives exclusively from the cleaning operations of the facilities and equipment. Such wastewater contains milk and cheese residues and small amounts of milk whey. Therefore, they can contain remains of fat, proteins, peptides and amino acids. Sugars, mainly lactose, may appear too.

Citromil

Citromil consumes between 20,000 and 30,000 m^3/y of public supply water. Citromil's consumption of water includes water for the manufacturing processes as well as the equipment and facilities cleaning water. Approximately 90% of the total consumed water is discharged to the public sewerage network after being properly treated. So, both lines of Citromil generates between 18,000 and 27,000 m^3 of wastewater per year. Both lines of work have tanks for collecting and distributing the generated wastewater. These tanks have sufficient capacity to homogenize the wastewater that they collect in one day and are situated before the primary treatment carried out by the company. Then, these wastewaters are sent to the active sludge treatment plant where these waters are treated.

In the extraction process, the oil is separated from the rest of the products. While the juice is extracted, the fruit's crust is scraped and pressed, dragging the obtained products with small showers of water. The scrape dragged by the water is pressed against the sieves of the finishers in two successive stages: separating the sieved and dried solids by pressure on the one hand and the emulsion of oil and water on the other hand.

This oil-water emulsion is fed constantly to the centrifuges, obtaining an oil-water emulsion richer in oil (cream), and water with solids. The cream is again centrifuged (polishers) to remove all the remaining water and solids from the essential oil. The obtained essential oil is introduced into stainless steel decanting tanks with a conical bottom, to decant the waxes by gravity and to obtain a clean oil.

The water with solids obtained in the centrifuges go through a decanter where they are pressed, eliminating a large part of the solids and obtaining water that contains small quantities of oil that has been dragged from the centrifugation stage. This water is distilled to obtain distilled essential oil. After distillation, the distillated oil is decanted, filtered and packed and the water resulting from the process is considered wastewater from the oil line.

In the juice line, about 100 m^3 of wastewater per day is generated in the months of production. There are three stages that generate waste water, reception, transport and washing of the fruit, cleaning of equipment and cleaning of facilities. Wastewater is collected in two tanks with 25 m^3 capacity each before being sent to the pre-treatment and to the treatment plant.

In the line of essential oils, the wastewater passes through steps to extract essential oils and finally they are collected in a tank of 9 m^3 of capacity. This production line generates approximately 10 m^3 of wastewater per day.

Essential Oil Line

Wastewaters generated by the line of essential oils extraction are much more interesting for the purposes of this project than those generated in the juice line. In the case of the Essential Oils Line, the main issue detected for the processing of this wastewater is the presence of an important amount of pulp. This suspended mater clogs easily membrane filters and, thus, should be removed prior to membrane filtration processes. However, the pulp can contain valuable compounds to be utilized. Among the compounds of interest present in this stream are Hesperidin and Limonene, and Hesperidin is poorly soluble in water. For this reason, another issue to be tackled in pretreatment operations is to determine the fraction in which Hesperidin is enriched after pretreatment.

Juice Line

Wastewater from the Juice Line is poor in compounds of interest, but the high volume of wastewater produced in the process (approx. 90% of total wastewater of Citromil) makes necessary a treatment plan. The removal of suspended solids in this stream is the main issue for pretreatment operations in order to proceed with further processes within the AFTERLIFE project (ultrafiltration, RO, etc.).

Table 2: Characterization of wastewater and volatile fatty acids (VFA) and PHA conversion rates

	gCOD / L WW	gVFA / gCOD	gPHA / gVFA
Jake	135	0.36	0.67
Heritage	3.01	0.3	0.67
Citromil E.O.	46.2	0.2	0.67

Table 3 states the annual production yields according to the starting material, the annual generated wastewater and yields of Table 2.

Table 3: Annual production yields related to starting material

WW origin	WW	PHA (mixed cultures)	Essential Oils (pure)	Polyphenols (pure)	Total amino acids (pure)
	m3	ton			
Jake	23 000	586			
Heritage	15 000	7			
Citromil E.O.	1 800	8.73	1.53	0.73	
Citromil E.O.	1 800	8.73	1.53	0.58	1.39

4.2.4.2 Production from Jake wastewater

For Jake wastewater tests resulted that a direct use in the VFA-production is most suitable. Therefore, no filtration is considered. The process scheme is described in Figure 2.

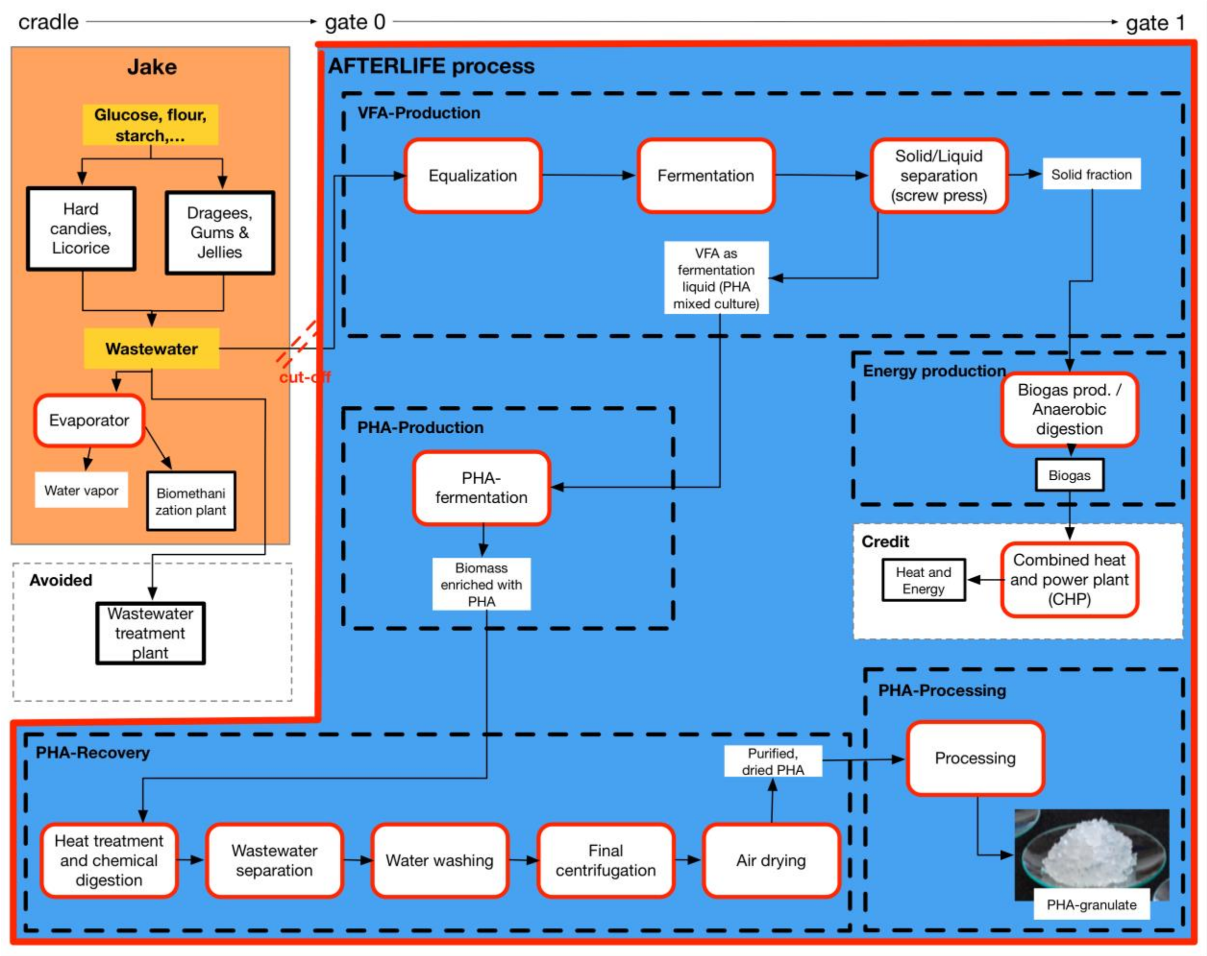

Figure 2: AFTERLIFE process scheme of Jake WW

VFA-production

The purpose of the anaerobic fermentation process implemented in AFTERLIFE is the production of volatile fatty acids (VFAs) from the organic compounds. In a first step the wastewater is equalized with Calcium carbonate ($CaCO_3$) and mixed for the further processing. The fermentation is done under heating and mixing in a bioreactor, which produces the fermentation liquid, which consists the VFAs. The fermentation liquid is further purified via a screw press adding polyelectrolite which separates solid from liquids. The solid fraction is sent to the anaerobic digester for biogas production, while the purified liquid containing VFAs is sent to the PHA production.

PHA-production

Interest is currently focused on the use of mixed microbial cultures coming from wastewater and waste treatment plants, with the aim of turning waste materials into resources. The merits of mixed culture (MC) fermentation are the utilization of organic wastes as the substrate and the absence of a requirement for septic processing. Moreover, a mixed culture may be more robust than a pure culture in the context of an open culture because it can grow on various organic compounds and adapts easily to the variable substrate composition of the wastes and to the variable environments. As seen previously, the type of VFAs used to feed an MC greatly influences the PHA composition and thus determines the mechanical and thermal properties of the polymer extracted. Hence, only the VFA-production via MC was assessed.

The production of the PHA biopolymer is performed from the VFAs produced during the anaerobic fermentation process. A mixed culture two stage process, consisting in a selection reactor and accumulation reactor, will be implemented and operated. The culture selection will be performed under feast and famine regime, aiming at selecting a high and stable PHA-storage capacity microbial culture and producing the biomass required in the subsequent stage (accumulation reactor) where the PHA-production occurs (maximize PHA cell content). Such a strategy allows the selection of the PHA producing bacteria since the accumulated PHA is a source of carbon during the scarcity periods. The VFAs from the VFA-production are supplemented in the selection reactor with micronutrients. The accumulation reactor is fed with the VFA-stream directly to maximize PHA production.

PHA-recovery

Once produced, the polymer should be separated from the cellular biomass. Different strategies are developed during the project for polymer recovery. In this case, the parameters of recovery (percentage of initial polymer recovery after extraction) and purity (percentage of PHA in the recovered solid) are for modelling the extraction process. It is known that recovery and purification of the polymer account for a huge part of the PHA total production cost and environmental impacts. Consequently, PHA-recovery is a key issue to make the global process economically and environmentally acceptable. The method to be chosen must lead to high extraction yield and high polymer purity, and PHA degradation must be minimized or nullified during extraction.

PHA-processing

The purified, dried PHB is continuously feed into a plastic extruder. A rotating screw forces the plastic into the heated barrel were the material is melted. Melted material is pressed through a round die, which gives the material the final form. The material is usually cooled down and cut into granulates or pellets, which later can be compounded with additives such as colourant and UV inhibitors.

4.2.4.3 Production from Heritage wastewater

For Heritage wastewater tests resulted that a pre-treatment of several filtration steps would be more suitable than a direct use in the VFA-production. A FOG adsorption with elastomeric material was tested but neglected in this assessment. The process scheme is described in Figure 3.

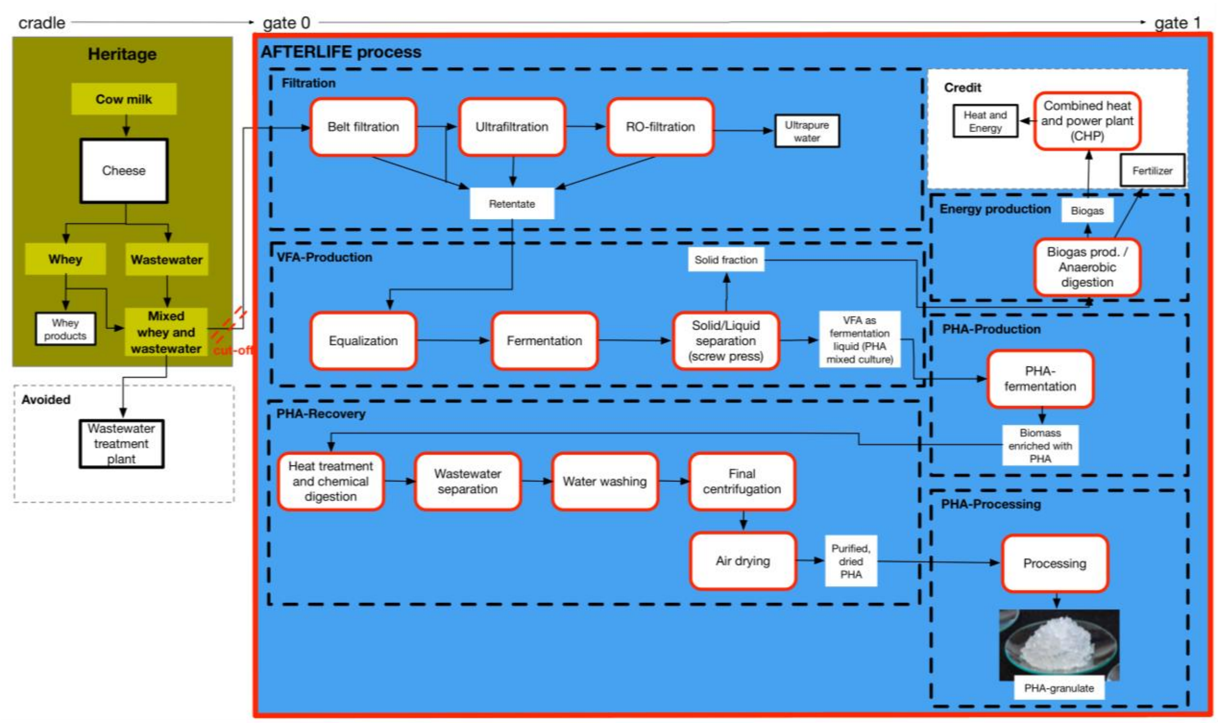

Figure 3: AFTERLIFE process scheme of Heritage WW

Filtration

The wastewater is filtered through cascaded membrane filtration steps. The wastewater enters the filtration unit which is processed through belt-, ultrafiltration and reverse osmosis. The retentate of each filtration step is further processed into the VFA-production process. The water obtained after the last filtration step is suitable for reuse in the AFTERLIFE-process. VFA-production, PHA-production and PHA-recovery steps are described under 4.2.4.2 as process are assumed to be similar except yields which are described in Table 2.

4.2.4.4 Production from Citromil E.O. line WW

The difference between the Citromil E.O. WW and Jake are the additional filtration steps and the purification of valuable compounds. The full AFTERLIFE process of Citromil E.O. WW can be seen in Figure 4.

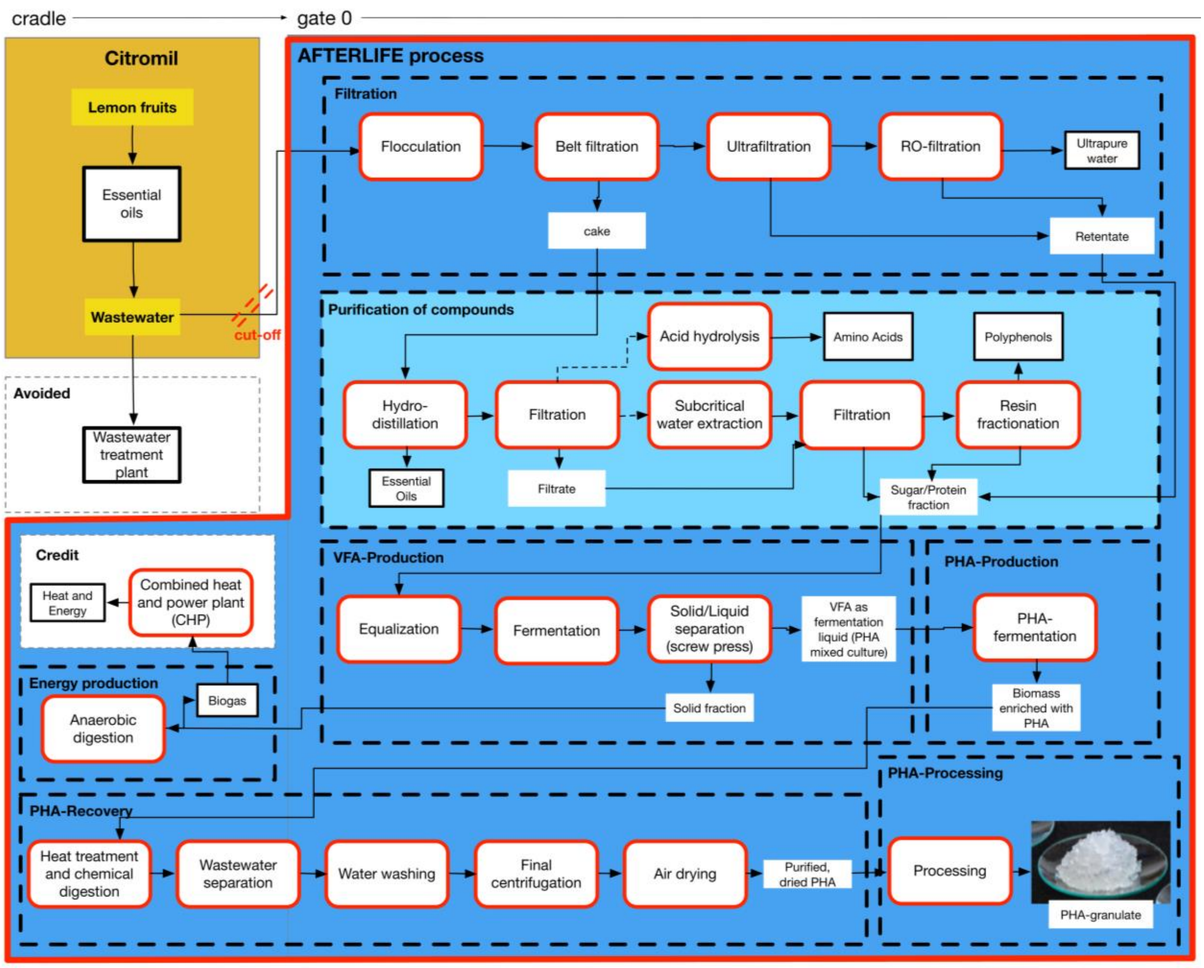

Figure 4: AFTERLIFE process scheme of Citromil E.O. line WW

The starting material is treated in a flocculation step and a filter cake is obtained after the belt filtration. The cake is can be treated with hydro- or steam-distillation to obtain essential oils.

Essential oil distillation

Two techniques need to be distinguished: hydro-distillation and steam-distillation.

Hydro-distillation, also known as water distillation, is a technique were the raw material is immerged in water and the solution is heated until vapor formation. Celabor produced in their trials 46 ml of essential oils per kg wet cake.

Steam-distillation is carried out by BBEU passing dry steam through the raw material whereby the steam volatile compounds are volatilized. Tests resulted in 8 ml essential oils per kg wet cake (see Deliverable 2.3).

Filtration after E.O. distillation

After the distillation the first step of the process consists in the filtration of the wet cake in order to separate the particles in suspension after the hydro- or steam-distillation step. The residue is treated in subcritical water extraction. As most of the actives remains in the residue after the filtration step (81%) especially for Hesperidin and Diosmin while Limonin and Eriocitrin are distributed in both.

Subcritical water extraction is a promising green-oriented and cost-effective process for the recovery of polar and slightly apolar compounds. Its main advantage is the use of water as solvent and represents an alternative to conventional extraction with solvents such as ethanol, acetone. Residue is extracted with water under subcritical conditions. The major issue is the high wet content of the wet cake which lead to some leaks from the cells. The use of subcritical water allows the destruction of hydrogens bonds, ions interaction and Van der Waals forces that could non-covalently link secondary metabolites to carbohydrates or proteins.

Combination

The final step of the extraction process consists in the combination of the extract obtained after the subcritical water extraction with the filtrate obtained at the filtration step.

Resin fractionation

The fractionation process was carried out on the filtered wet cake. A purity of 22.71% polyphenols could be retrieved. The polyphenols can be further purified to around 69% with centrifugal Partition Chromatography technique (CPC). This step was not included in the assessment.
The retentate of ultra- and RO-filtration could be utilized for the valorisation steps as described in Figure 4, but were considered to be used directly in the VFA-production. Further all other sugar/protein fraction that result during the purification of compounds are considered to be used in the VFA-production as feedstock as described in Figure 4.

Acid hydrolysis

The residue that can be treated in subcritical water extraction can optionally utilized in an acid hydrolysis to obtain amino acids. Experiments showed that per kg residue of filtration after distillation 0.5 kg total AA can be retained with oxalic acid in a thermoreactor.

Further processing

VFA-production, PHA-production, PHA-recovery and PHA-processing steps are described under 4.2.4.2 as processes are assumed to be similar except yields which are described in Table 2.

Biogas/Energy production

The anaerobic digestion converts the organic matter into carbon dioxide and methane, which can be used as a source of energy for the process. The anaerobic digestion of the solid fraction of the VFA-production as well as other biomass waste to produce methane and later energy e.g. for internal use in the AFTERLIFE process is tested by Innoven and was not considered in this analysis, but could be considered in a future analysis.

5 TEE data Inventory analysis

The TEE data Inventory consists of detailed tracking of all flows into and outside of the product system, including raw resources or materials, energy by type, water, etc. Prices of all these inputs and outputs are estimated based on the market prices of the materials, energy or other materials used in the process.

The in- and outputs of all necessary processes were collected during the data collection phase from the project partners and literature. The prices of all materials and energy used has been obtained from various credible internet sources, or by estimations based on market knowledge.

5.1 General considerations

An important part of a TEE case study report is to state data sources, data gaps, taken assumptions and identified limitations that have to be considered when interpreting and concluding the results. In the context of this case study, the following should be considered.

5.1.1 Sources of TEE Inventory data

Foreground data for wastewater to PHA-granulate processes were provided by the responsible project partners throughout email, conference calls, and/or in person-meetings. Further data of each process step were gathered through an excel data collection sheet, which was send to the involved project partners.

5.2 Inventory data

- **Primary data**
  - Filtration (VTT)
  - VFA-production (Innoven)
  - PHA-production (nova ID)
  - PHA-recovery (BBEU)
  - Purification of compounds from (Celabor, CTC and Lurederra)

Table 4 shows mass and energy balances used from the LCA model with the used LCA datasets.

Table 4 LCA data of AFTERLIFE process per kg of output

ecoinvent dataset	Unit	JAKE	Heritage	Citromil E.O.			
Output							
purified PHB from PHA recovery and purification JAKE (EU) AFTERLIFE	kg	1	1	1			
pure flavonoids (EU) AFTERLIFE	kg				1		
Essential oils from steamdistillation (EU) AFTERLIFE	kg						1
amino acids from acid hydrolysis (EU) AFTERLIFE	kg					1	
Input							
Jake wastewater (EU) AFTERLIFE	m3	0.040					
Heritage wastewater (EU) AFTERLIFE	m3		2.123				
Citromil wastewater (EU) AFTERLIFE	m3			0.169	0.244	0.51	0.009
Boric acid, anhydrous, powder (GLO)	kg	1.15641E-13	1.63E-12	1.38181E-13			
Calcium carbonate, precipitated (RER)	kg	0.199	2.65	0.238			
Copper sulfate (GLO)	kg	2.31215E-14	3.26E-13	2.76283E-14			
Electricity, medium voltage (RER)	MJ	3.01	4.62E+01	7.18	1.56	2.01	0.032
Ethanol, without water, in 99.7% solution state, from fermentation (CH)	kg	1,00	1,00	1,67	1,53		
Iron(III) chloride, without water, in a 12% iron solution state (GLO)	kg	1.15641E-12	1.63E-11	1.38181E-12			
Manganese dioxide (GLO)	kg	9.24862E-14	1.30E-12	1.10513E-13			
Polyacrylamide (GLO)	kg	0.095	1.26	0.123	0.0136	0.0283	0.000527
Potassium hydroxide (GLO)	kg	2.31215E-14	3.26E-13	2.76283E-14			

Sodium sulfate, anhydrite (RER)	kg	0.211	0.211	0.211			
Steam, in chemical industry (RER)	kg	0.441	6.21	0.318			
Sulfuric acid (GLO)	kg	4.08	4.08	4.08			
Wastewater, average (Europe without Switzerland)	m3	0.104	0.248	0.127	0.049		
Water, deionised, from tap water, at user (Europe without Switzerland)	kg	103.10	241.28	719.51	875.88	1826.01	34.00
Zinc monosulfate (GLO)	kg	9.24862E-14	1.30E-12	1.10513E-13			
steam produced by BBEUP AFTERLIFE (EU)	kg			53.70	77.78	162.14	3.02
Heat, district or industrial, natural gas (Europe without Switzerland)	MJ			197.19	285.59	595.40	11.08
High impact polystyrene resin, at plant/RNA	kg			0.005	0.011		
Electricity, medium voltage (BE)	MJ				1.85	3.87	0.072
Citric acid (RER)	kg					8.04	

5.2.1 Market prices of in and outputs used in TEE

In order to carry out a TEE, parallel to the mass balance of inputs and outputs, market prices of energy, materials, labour costs are additionally required. Different sources have been used to retrieve information concerning the market prices. For energy and gas (needed for the production of steam), market prices have been retrieved from EUROSTAT. For market prices of materials used in the process the commodity prices of the chemicals were taken from the Zauba.com website. For PHA granulate the price ranges from 4,000 €/t to 5,000 €/t. In this study the target price is considered 4,900€/t, which is an estimate by the nova-Institut regarding the future trends of market needs for biodegradable polymers.

The prices given in Table 5 have been used for the OPEX and CAPEX calculations for Jake, Heritage and Citromil E.O. line processes.

Table 5 Market price of inputs and outputs that have been used in this TEE

In/Outputs	Price per unit €/t	Source
Utilities		
Electricity	0.11	(EUROSTAT 2018)
Gas (for production of steam)	0.05	(EUROSTAT 2018)
Demineralised water	0.80	nova-Institut estimation
Operating labour		
Average hourly wage in EU	27.40	(EUROSTAT 2018)
Used materials		
SDS Sodium dodecyl sulfate ($NaC_{12}H_{25}SO_4$)	250.00	Zauba.com
Calcium carbonate ($CaCO_3$)	140.00	Zauba.com
Polyacrylamide ($(C_3H_5NO)_n$)	2,700.00	Zauba.com
Sulfuric acid (H_2SO_4)	85.00	Zauba.com
Ethanol (C_2H_5OH)	650.00	Zauba.com
Polystyrene resin	265,000.00	Sigmaaldrich.com
Output		
PHA granulate	4,900.00 (target price)	nova-Institut estimation
Amino acids (application as a food additive)	48,000.00	(Amazon.com 2019)
Polyphenols	48,000.00	nova-Institut estimation

Essential oil	7,500	nova-Institut estimation
Wastewater for disposal in municipal wastewater treatment plant	0.20	(Mulder 2015)

5.2.2 Assumptions

Due to the fact that some process information, mass and energy flows are not available the following assumptions at inventory level were made in order to perform TEE:

- Retentate of UF- and RO-filtration of CItromil E.O. line to be used directly in the VFA-production steps instead of the purification of compounds steps.
- Only mixed culture PHA-production is considered
- A ethanol recovery of 95% in the PHA-recovery was assumed based BBEU, by that only the lost amount (5%) were considered in the assessment. The same assumption was made for the used ethanol for the desorption of the resin.
- A recovery of 95% of the resin was considered
- The purification step of the essential oil from 22,71% to 69% by CPC was neglected
- A purity of 100% of amino acids, essential oils and polyphenols were assumed
- For the PHA processing:
    - Additives and other materials needed for the compounding are neglected
    - Only the electricity of the compounding is included
    - Materials losses during compounding are neglected
- Electricity is supplied by medium voltage grid based on the average transformation technology and the average electricity loss during transmission in EU.
- The use of process waste such as the solids of the VFA-production into biogas-production may increase the revenues, or by heat integration reduce the needs for energy. As according to preliminary calculations, the methane produced converts into low amounts of electricity and heat at the moment. The biogas-production will be therefore neglected in this assessment, but will be included with the latest developments in a final TEE.

- In the calculation of TEE, no costs have been allocated to the Jake, Citromil E.O. and Heritage wastewaters as feedstock, by considering that PHA production facility will be built in the industrial park where these companies are operating. Hence the WW will be directed to the **P3HB** production facility. No transportation costs for the wastewater transport have been considered.
- Yearly operational hours for all three WW processes are estimates based on information that partners have provided on duration of each processing step, as well as the volume that runs through each processing step. The operational hours for the base scenario are:
  - Jake WW: 4,200 h/year
  - Heritage WW: 1,200 h/year
  - Citromil E.O.: 1,400 h/year
- Estimation has been done on the necessary work force to run the facility. The assumptions are done based on the volume of the processing material as well as the complexity of the system.

5.2.3 Data quality assessment and limitations

Since TEE is a tool founded on quantification, uncertainty is present at the data inventory level. Incorrect estimations or modelling assumptions, outdated data and data gaps are sources of uncertainty.

This data quality assessment has been carried out for the hot spot LCA analysis, which is published in deliverable 7.1. However, since the same data were used for the LCA and TEE studies, this assessment describes the data quality of the TEE as well.

A qualitative analysis of the uncertainty of the inventory data was carried out, to validate the TEE results (see Table 6). Indications on the quality of data include the evaluation of the reliability and completeness of the data itself, combined with the evaluation of the representativeness (temporal, geographical and technological) of the processes used to model it. The inventory data quality assessment is assessed according to (Weidema and Wesnæs 1996). The indicators are explained in the Annex Chapter 8.1,

Table 6: Data quality assessment of AFTERLIFE process steps

Processes	Source	Importance	Reliability	Completeness	Temporal correlation	Geographical correlation	Further technological correlation
1 primary; 2 literature		Low, medium, high	Indicator score (1, 2, 3, 4, 5)				
Filtration	1	Low	2	4	1	1	1
Purificatio of compounds	1, 2	Medium	2/3	4	1	1	1
VFA-production	1	High	2	3	1	1	1
PHA-recovery	1, 2	High	3	3	1	1	1
PHA-processing	2	Low	2	2	3	2	2

The main limitations of this environmental study are due to the data quality of the inventories. On the one hand, the purification of compounds and PHA-production are based on experimental and lab scale data as well as assumptions based on literature. On the other hand, for the filtration steps and VFA-production steps upscaled scaled data was provided by VTT and Innoven. Further the PHA processing is fully based on literature. All in all, the data quality is low due to incomplete data, estimated and calculated data and low TRL processes, mostly lab or experimental data. Therefore, high uncertainties of the results are expected.

5.2.4 Scenario discussion

Jake WW

In the base scenario for all three processes, the target price of P3HB is considered around 4,900 €/t. An alternative scenario has been presented, where an average price of 4,500 €/t P3HB has been considered, to evaluate the effects of the market price of the produced product on financial indicators.

Table 7 Jake WW differences of scenarios considered

	Base scenario	Jake – alternative scenario
P3HB market price (€/t)	4,900	4,500

Heritage WW

Since the yields of Heritage WW process are low to cover the operational expenditures, an alternative scenario is presented to show the rate of yield increase required to reach profitable economic outcomes in the process. Additionally, to evaluate how costs associated with operating labour can effect on the overall performance of the process, in the alternative scenario less working hours (2,400 h/year, instead of the 3,600 h/year) have been considered.

Table 8 Heritage WW differences of scenarios considered

	Base scenario	Alternative scenario
Operating labour (h/year)	3,600	2,400

Citromil WW

For Citromil E.O. WW line two alternative scenarios are presented, to understand the conditions at which the process will become economically profitable.

In the first alternative model, the rate of reductions of material and energy inputs (while FCI remains same as in the base scenario) to reach positive economic results is presented.

In the second model the yields of all four outputs of Citromill E.O. WW line are gradually increased, to determine the rate of yields which will provide positive economic outcome of the process. In this model, while the yields of the outputs are increased, all other all other factors remain the same, as considered in base scenario.

Table 9 Citromil E.O. WW differences of scenarios considered

	Base scenario	Alternative scenario 1	Alternative scenario 2
Operating labour (h/year)	5,600	4,200	5,600
Achieving profitability through reduction of materials and energy	Material and energy inputs based on process data obtained from project partners.	Modelling a gradual reduction of material and energy inputs to determine the rate of reduction which will result in positive economic outcome	Amount of material and energy inputs remain as in base scenario
Achieving profitability through increasing yields	Rate of yields as given in Table 3	Amount of yields as given in Table 3	Modelling a gradual increase of yields to determine the rate of yields necessary for achieving positive economic outcome.

6 Results and discussion

For the implementation of the TEE, the expenses and costs for materials, energy and labour were calculated as indicated in Chapter 6.2.1. Based on the material and energy flows, CAPEX and OPEX are calculated as described in chapter 3. In the following paragraphs the results of the TEE for the AFTERLIFE project are presented and discussed in detail.

In the calculation of TEE, no costs have been allocated to the Jake, Citromil E.O. and Heritage wastewaters as feedstock, by considering that PHA production facility will be built in the industrial park where these companies are operating. Hence the water will be directed to the **P3HB** production facility. No transportation costs for the wastewater transport have been considered.

6.1 Overview

Figure 5 gives an overview of the annual financial indicators for all three processes and Figure 6 describes the costs per ton of P3HB. Looking at both figures it is clear that with current conditions Heritage WW line and Citromil E.O. WW line are unprofitable, while the process of Jake WW line is profitable under base scenario conditions. For each of the processes, under paragraphs 6.2, 6.4 and 6.3 there are alternative scenarios suggested to show how at changing conditions the results of financial indicators can change.

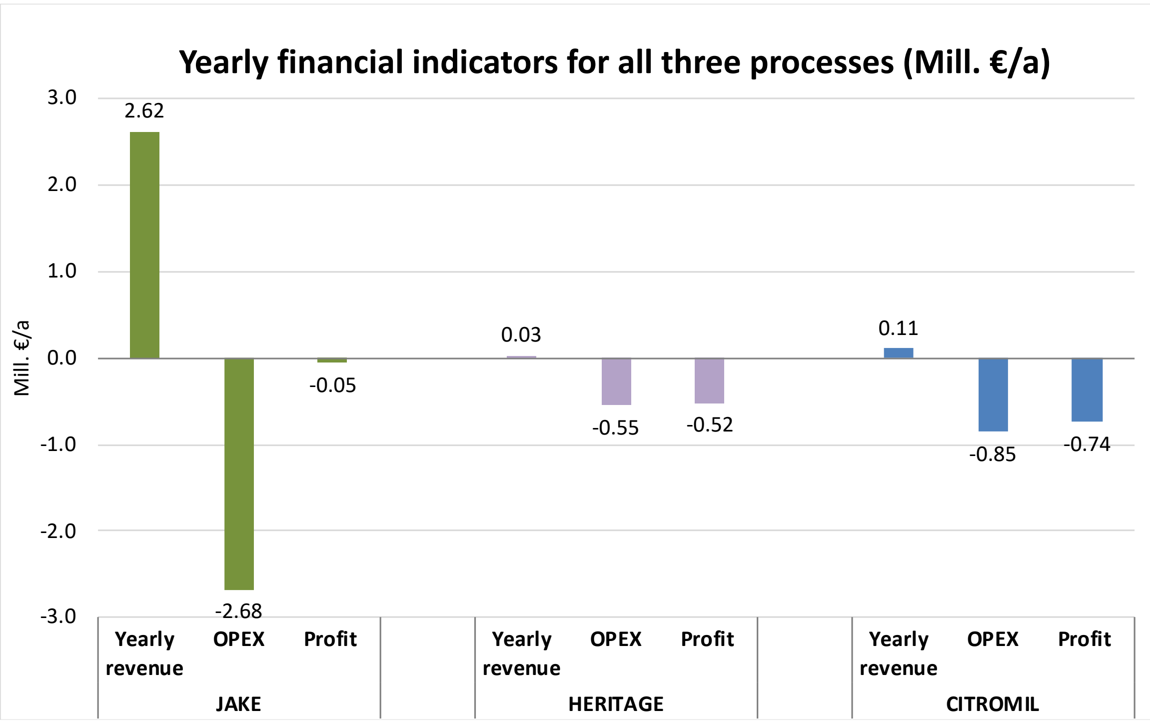

Figure 5 Yearly financial indicators for all three processes

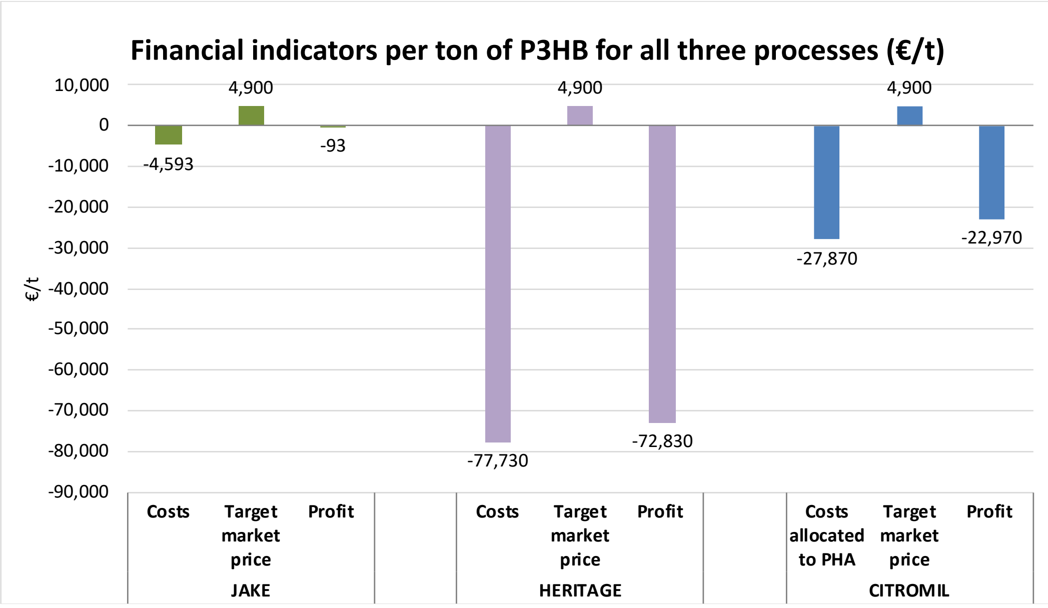

Figure 6 Financial indicators per ton of P3HB production for all three processes

More detailed description of the TEE is described in the next paragraphs.

6.2 Hotspot TEE for Jake wastewater

6.2.1 Costs associated with inputs

Input of raw material: The yearly capacity for Jake wastewater has been considered 23.300 m^3 and the required inputs of energy, materials and personal have been appropriately upscaled for this capacity. In this scenario, 4,200 h / year of operational time has been considered. During the planned operational hours 3 employees are planned to operate / maintain the facility.

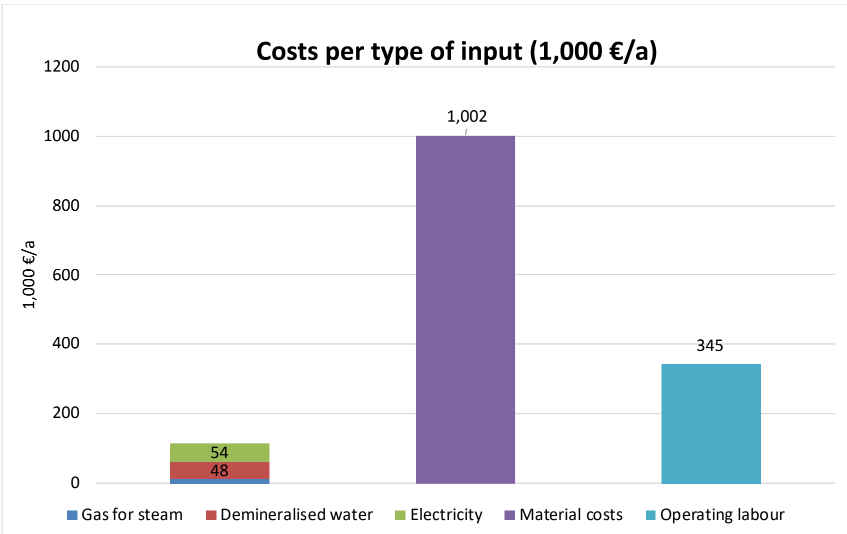

Figure 7 Costs per type of input for Jake WW

Figure 7 illustrates the costs per type of input. It is obvious that material costs are far higher than the energy costs and the costs associated with operating labour. However, it is important to note, that this is largely influenced by the data which were generated in laboratory tests. In the next paragraph more details will be given concerning the materials that constitute these costs.

6.2.1.1 Material costs

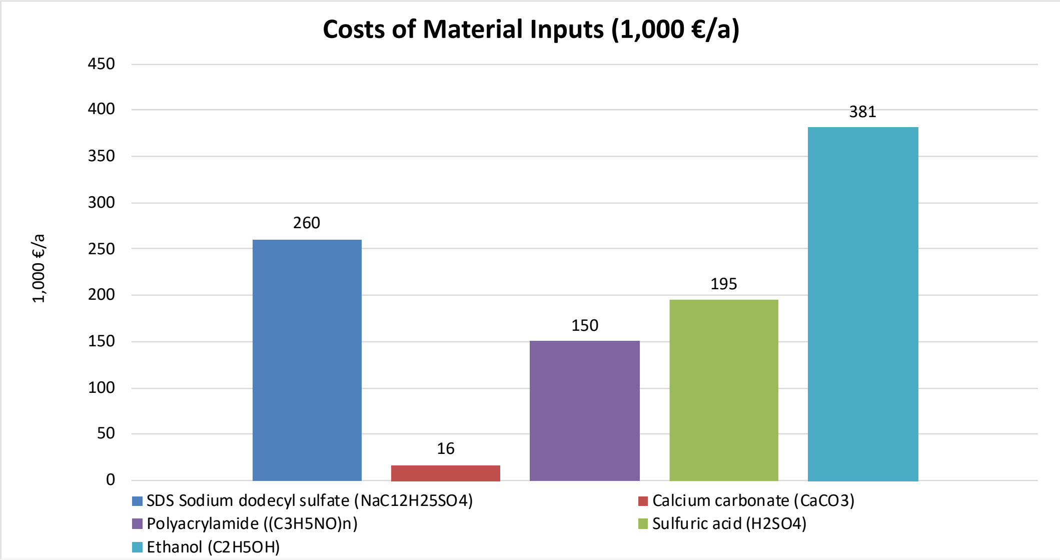

Figure 8 Costs associated with material inputs for Jake WW process

As figure Figure 8 shows the main contributors to the costs of material inputs are ethanol, SDS and sulfuric acid. Ethanol is used in P3HB recovery phase, where via ethanol wash the remaining protein impurities are removed to reach a high degree of P3HB purity (Mitra Mohammadi 2011). In this evaluation it is considered that 95% of the ethanol will be possible to recycle. Thus, the amount of ethanol showed in Figure 8 is needed for Jake WW process is to cover the 5% losses.

The next contributor to the material costs is SDS (Sodium dodecyl sulfate). The high costs are associated with both, the high consumption rate that has been used in the laboratory tests as well as its high market price (around 2.700 €/t). SDS is used for P3HB recovery and usually shows a high efficiency for a high rate of P3HB recovery (Yung-Hun Yang 2010).

Sulfuric acid is similarly used in P3HB recovery phase. Although it's not an expensive chemical (85 €/t), its relatively high rate of application during the laboratory tests have resulted in large amounts of sulfuric acid in the upscaled model.

At industrial scales it is expected that the system will be highly optimized, thus the rate of chemicals used during the laboratory tests is expected to drop.

6.2.1.2 Utility costs

The energy demand of the facility is the cumulative energy demand of the various processes described in Figure 2.

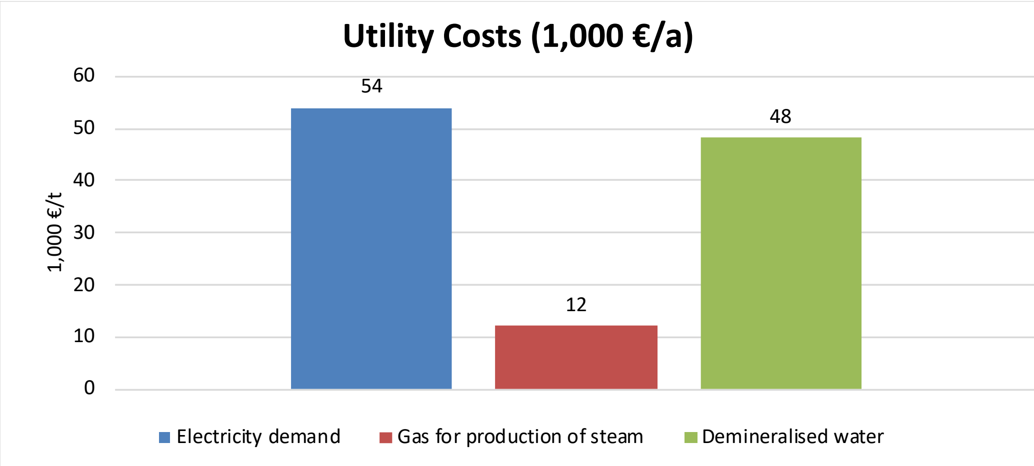

Figure 9 Utility costs for Jake WW

The contributors to the electricity costs are mainly the P3HB processing and recovery phases.
The costs associated with demineralised water are considerably high, which is used in PHA recovery phase. Distilled water along with ethanol is used for washing and separating PHA from impurities. An assumption can be done that certain percentage of distilled water will be recycled at the industrial scale production, however in this model, the recycling of demineralised water is not considered.
In this TEE model, all energy-based utilities are expressed in kWh, hence the amount of steam needed has been converted into gas that will be necessary for the production of needed steam. The following conversion factors have been used to convert steam into gas. These factors have been taken from Ecoinvent v.3.4: 1 kg stem needs 0,09 m^3 gas is necessary to produce 1 kg steam. 1 m^3 gas converts into energy that is equal to 10,5 kWh electricity.
Since gas is cheaper than electricity and the amount used for production of steam is not as high as the electricity use, the costs associated with gas are lower.
Apart from the possibility of recycling distilled water, here again applies the rationale of possible cost reductions for electricity and gas demand at industrial production scale.

6.2.1.3 Personnel costs

While planning personnel for the operational costs, it is important to note that not all production steps will need to run full time at industrial scale. During data collection, the project partners have provided information on duration of some production steps, in other cases assumptions have been made based on the volumes that will be running through these particular process steps. Overall, yearly 4,200 operational hours have been considered for running Jake wastewater facility. In this scenario it is considered that 3 employees will be necessary for the operation of the complete facility during its operational hours (more employees could be hired, but during facility operation 3 employees will be present). Thus, the costs associated with operating labour will equal to 12,600 working hours according to European average salary rate of 27,4 €/hour (EUROSTAT 2018).

Table 10 Yearly operating labour for Jake WW

Operating labour		
Total hours worked per year (3 employees each working 4,200 h/year	Hours	12,600.0
Hourly wage	€/hour	27.4
Total yearly costs for operating labour	€/year	**345,240.0**

6.2.2 Outputs

The main outputs of PHA production processes are P3HB granulate and wastewater generated during the production processes. It is considered, that the wastewater as an outcome of the process can be sent to the municipal wastewater treatment, since a large amount of the organic matter of Jake wastewater will be extracted during PHA production. Figure 10 shows the revenue associated with P3HB production and the costs associated with the wastewater which will be sent to the municipal wastewater treatment facility.

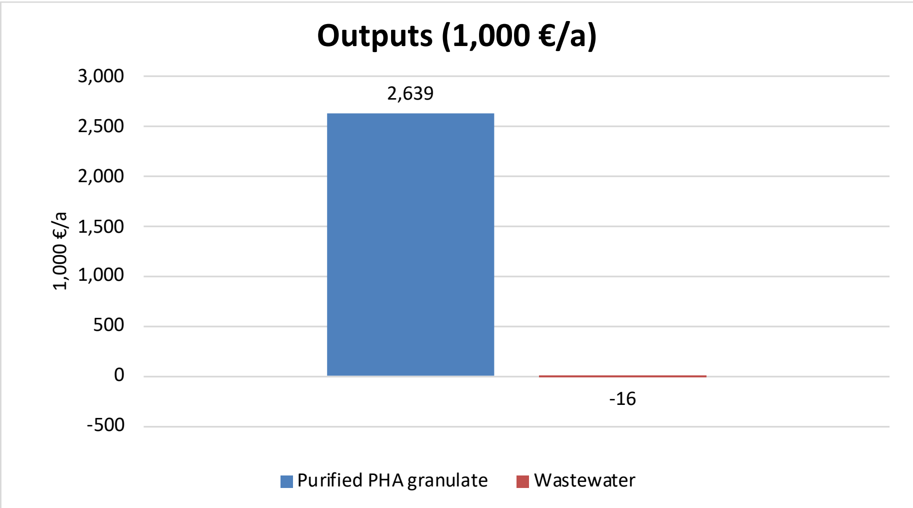

Figure 10 Yearly outputs of the process for Jake WW

6.2.3 Capital expenditures (CAPEX)

Calculations for CAPEX have been carried out as described in paragraph 3.1. Table 11 shows the results of CAPEX for Jake WW process.

The rated power of this process has been calculated to be around 180.6 kW. This estimation is based on the calculated energy use for Jake WW and the average operating hours that has been considered in base scenario in Table 7.

*Engineering costs (C_{ENG}) = 0.1 * FCI (10 % of FCI)*

*Contingency charges (C_{CC}) = 0.1 * FCI (10 % of FCI)*

Total FCI (TFCI) = FCI + C_{ENG} + C_{CC}

*Working capital investment (WCI; 10 % of FCI) = 0.1 * TFCI (10 % of FCI)*

CAPEX = WCI + TFCI = 2.90 Mill. Euro

Table 11 Capital expenditures for Jake WW process

Capital expenditures (CAPEX):	Value (Mill. €)
Fixed capital investment (FCI), **ISBL**	1.93
Engineering costs (C_{ENG})	0.39
Contingency charges (C_{CC})	0.39
Total FCI (TFCI)	2.71
Working capital investment (WCI; 10 % of FCI)	0.19
Total Capital Investment TCI = TFCI + WCI	**2.90**

6.2.4 Operating expenditures (OPEX)

$$OPEX = DMC + FMC + GE$$

DMC, FMC and GE consist of different cost elements. The cost elements contained in each of these costs as well as the method of OPEX calculation are listed in paragraph 3.2.

The overall picture of OPEX for Jake wastewater is shown in Figure 11.

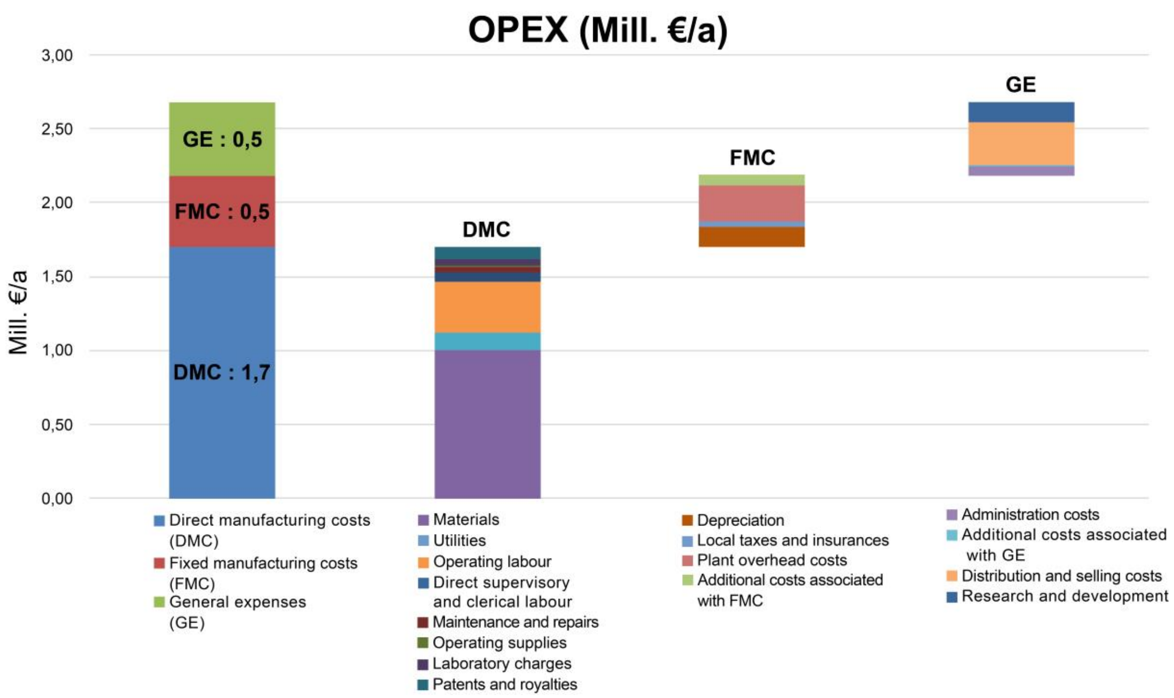

Figure 11 Overall picture of OPEX for Jake WW process

6.2.5 Economic indicators

The yearly economic indicators for Jake wastewater show that the process is profitable based on current assumptions that have been made in this study (see Figure 12). With 2.7 Mill. €/year operating expenses and 2.9 Mill. €/year revenue, the profit for this process is around 0.2 Mill. €/year.

The disposal of wastewater at Jake facility is currently costing around 0.3 Mill €/year. AFTERLIFE process will thus bring value to the wastewater that is currently creating costs for Jake.

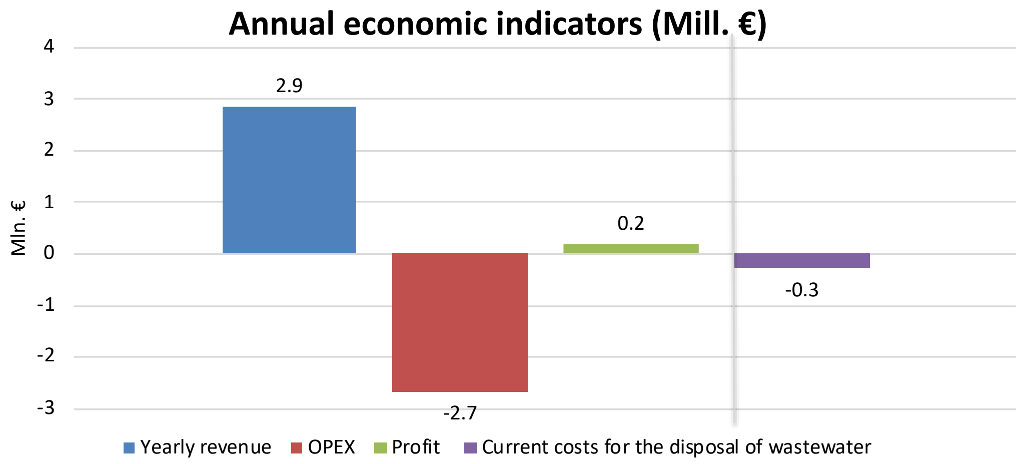

Figure 12 Yearly economic indicators for Jake WW process

Figure 13 shows the financial indicators for a ton of PHA. The costs associated with a ton of P3HB production are around 4,600 €. With a target cost of 4,900 €, the process is profitable. However, it is important to mention, that the average price of PHA lies between 4,500 €/t – 5,000 €/t. As the target price considered in the base scenario plays a big role in these results, below in chapter 6.2.6 a scenario will be presented to show the economic results for P3HB production at its market price of 4,500 €/t.

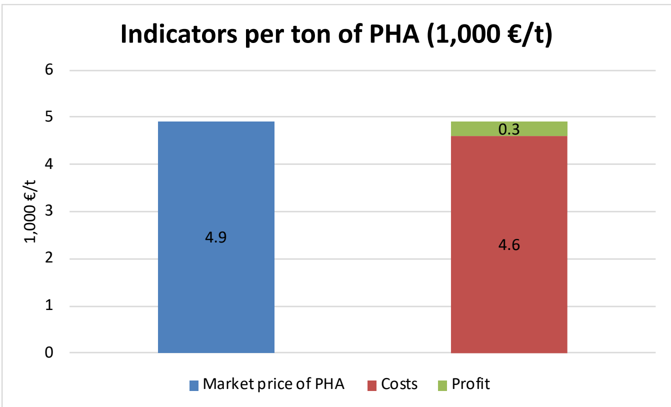

Figure 13 Financial indicators for a ton of PHA for Jake WW (PHA = 4,900 €/t)

6.2.6 Scenario with lower PHA target price

As mentioned above in paragraph 6.2.5 the results are highly dependent on the PHA target price. The PHA market price varies between 4,000 €/t to 5,000 €/t.

In this scenario an average market price of 4,500 €/t for PHA is considered, to evaluate its effects on the results. As Figure 14 shows, with the average market price of 4,500 €/t the process is economically not profitable and generates around 90 € losses per ton of P3BH. However, since currently the costs for wastewater disposal are around 480 € for the amount of wastewater corresponding to 1t of P3HB production, the AFTERLIFE process creates overall value by reducing the costs for wastewater disposal (according to this scenario).

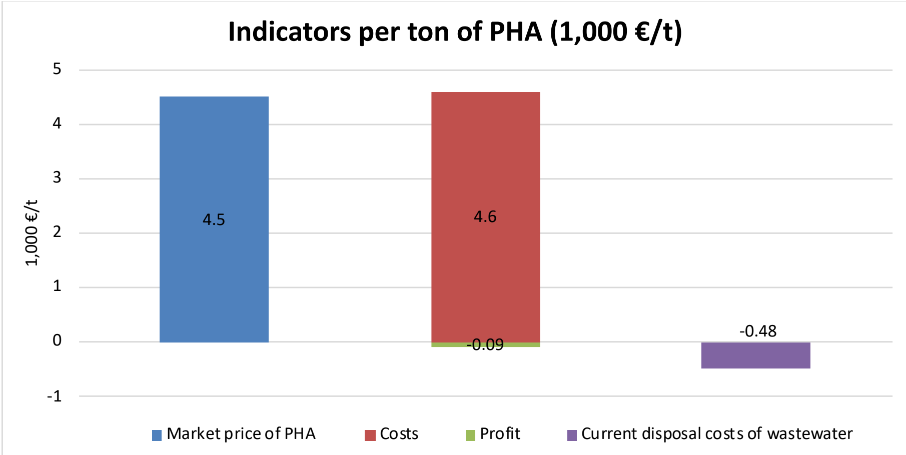

Figure 14 Financial indicators for a ton of PHA for Jake WW (PHA = 4,500 €/t)

6.3 Hotspot TEE for Heritage wastewater

Since both Jake and Heritage WW have as an output only the P3HB granulate and the P3HB production processes are mainly the same for these two processes, (apart from the ultrafiltration and reverse osmosis filtration processes that have been carried out in Heritage WW process and have not been included in Jake WW PHA production process). Hence the TEE evaluation has been carried out similarly to the one for Jake wastewater.

6.3.1 Inputs and associated costs

The yearly capacity of the Heritage line has been considered around 15.000 m^3, as mentioned in Table 3. The chemicals used for the production of P3HB from Heritage wastewater are the same as it has been used during tests of Jake WW line. However, compared to the PHA production costs from Jake wastewater, in Heritage after the ultrafiltration and reverse osmosis filtration the material sent to the downstream processes is considerably reduced, which requires less input of chemicals and energy for the process. As Figure 15 illustrates, the largest costs are associated with operating labour. Three employees have been considered each working yearly around 1,200h by taking into the account that the processing volumes are noticeably lower in comparison to Jake WW line.

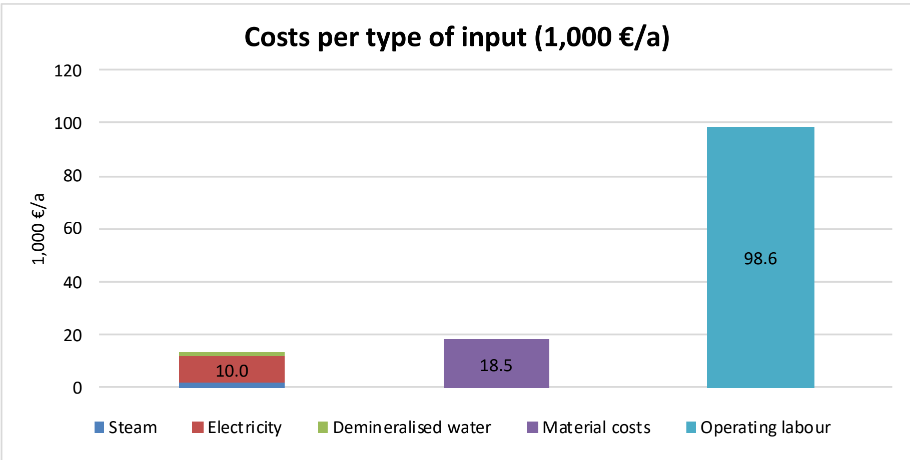

Figure 15 Costs per type of input for Heritage wastewater

6.3.1.1 Material costs

As Figure 16 shows, polyacrylamide, which is used in VFA separation phase is the biggest contributor to material costs.

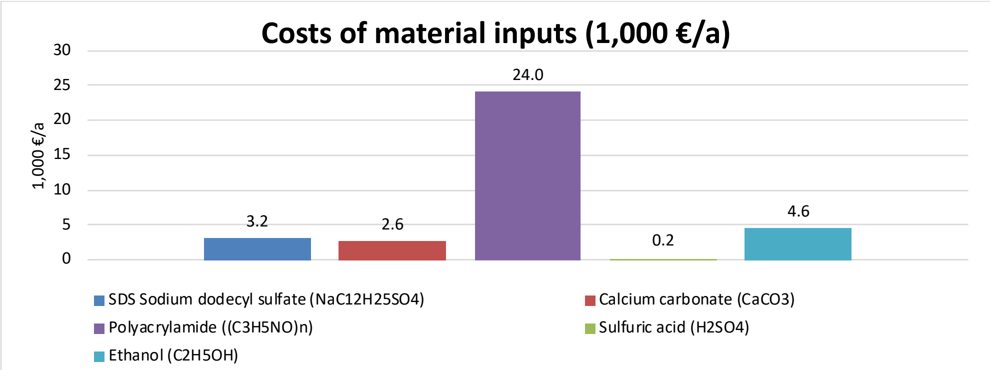

Figure 16 Material inputs for Heritage WW process

6.3.1.2 Utility costs

Electricity is as expected the highest contributor to the overall utility costs as shown in the Figure 17.

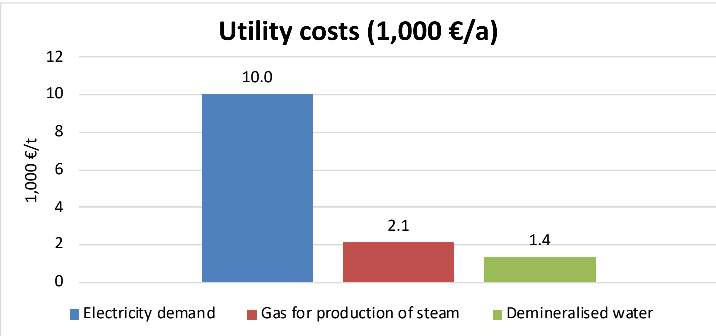

Figure 17 Utility costs for Heritage WW process

6.3.1.3 Personnel costs

As mentioned in paragraph 6.3.1, for Heritage WW line, 3 employees have been considered, each working yearly around 1,200h due to low scale production process in comparison to Jake WW line.

Table 12 Costs for operating labour for Heritage WW

Operating labour		
Total hours worked per year (3 employees, each working 1,200 h/year)	Hours	3,600.0
Hourly wage	€/hour	27.4
Total yearly costs for operating labour	€/annum	**98,640.0**

6.3.2 Outputs

Heritage WW line similar to the Jake WW line, has two outputs of the process, which are the purified P3HB granulate and the wastewater generated in PHA production process. The disposal of this wastewater is considered to be at the municipal wastewater treatment. The Figure 18 shows the components of revenues and costs associated with the outputs of the process.

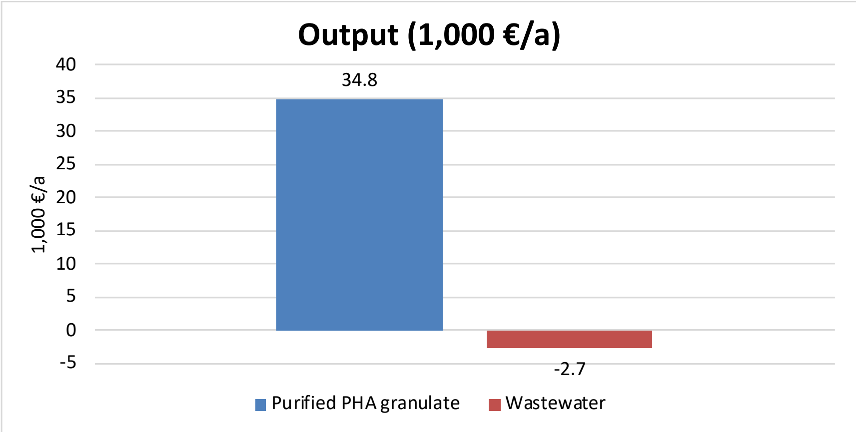

Figure 18 Yearly outputs for Heritage WW

6.3.3 Capital expenditures (CAPEX)

Calculations for CAPEX have been carried out as described in paragraph 3.1. Table 13 shows the results of CAPEX for Heritage WW process.

The rated power of this process has been calculated to be around 76.20 kW. This estimation is based on the calculated energy use for Jake WW and the average operating hours that has been considered in base scenario in Table 8.

*Engineering costs (C_{ENG}) = 0.1 * FCI (10 % of FCI)*

*Contingency charges (C_{CC}) = 0.1 * FCI (10 % of FCI)*

Total FCI (TFCI) = FCI + C_{ENG} + C_{CC}

*Working capital investment (WCI; 10 % of FCI) = 0.1 * TFCI (10 % of FCI)*

CAPEX = WCI + TFCI = 1.74 Mill. Euro

Table 13 Capital expenditures for Heritage WW process

Capital expenditures (CAPEX):	Value (Mill. €)
Fixed capital investment (FCI), **ISBL**	1.20
Engineering costs (C_{ENG})	0.24
Contingency charges (C_{CC})	0.24
Total FCI (TFCI)	1.68
Working capital investment (WCI; 10 % of FCI)	0.06
Total Capital Investment TCI = TFCI + WCI	**1.74**

6.3.4 Operating expenditures (OPEX)

Figure 19 illustrates the overall operational expenditures for Heritage WW line.

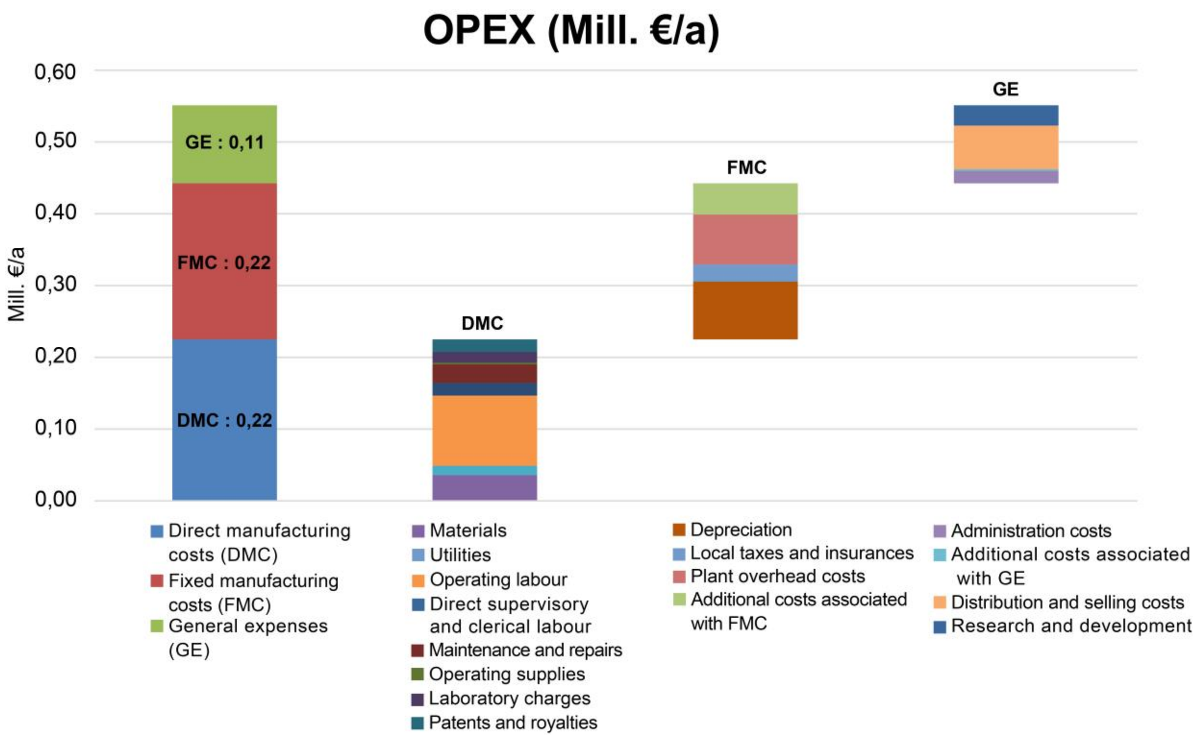

Figure 19 OPEX for Heritage WW process

6.3.5 Economic indicators: Base scenario

Figure 20 shows that even though the OPEX is not too high (due to lower processing volume in production processes), the revenue of the process is too low, in order to cover the operational expenditures. Low yields of P3HB in Heritage WW process, result in considerably higher price for a ton of P3HB (Figure 21), making the process unprofitable.

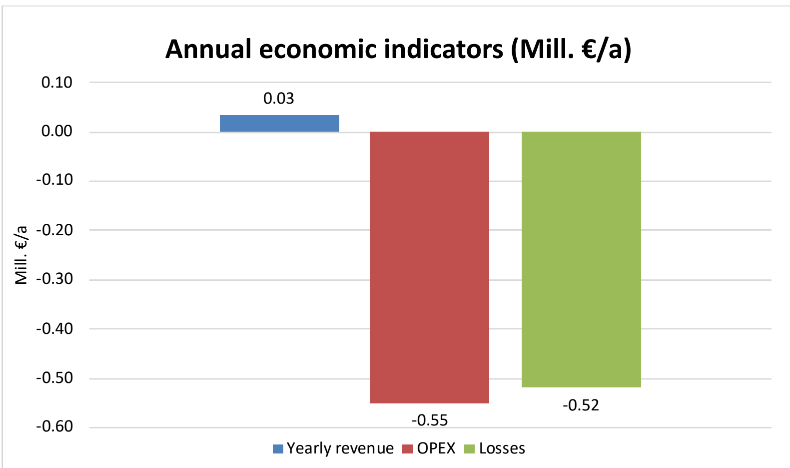

Figure 20 Annual economic indicators for Heritage WW process

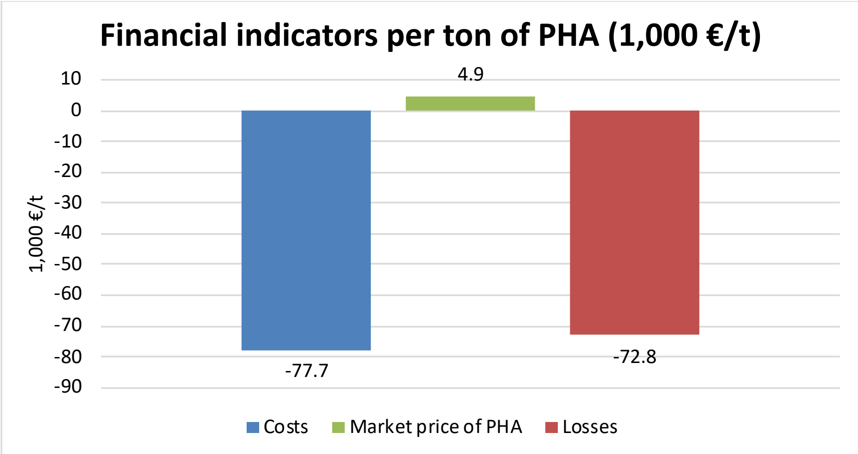

Figure 21 Financial indicators per ton of PHA (1,000 €/t) for Heritage WW process

6.3.6 Alternative model with higher yields

As mentioned in paragraph 6.3.5, the low yields of the process in Heritage WW, play a big role in the economic negative results. Figure 22 shows that the yields need to be increased at least 16 times, in order to achieve a positive economic outcome at conditions considered for this process.

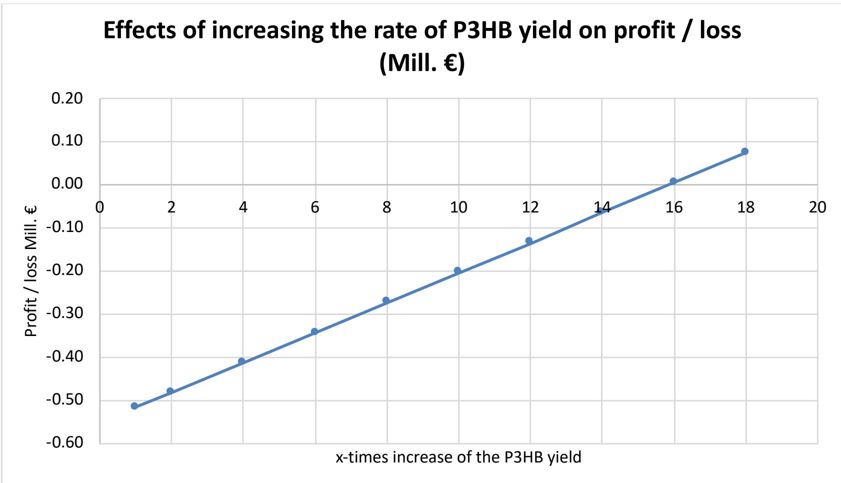

Figure 22 Effects of increasing the rate of P3HB yield on profit / loss for Heritage WW process

6.4 Hotspot TEE for Citromil E.O. wastewater

Citromil E.O. WW process differs from Jake and Heritage processes, since from this process a number of by-products, that have a market value are produced along with P3HB. This paragraph will investigate if the additional value created by the by-products added to the revenue created by P3HB production. As mentioned in Table 3 the volume of Citromil E.O. WW to be operated in a year is considered to be around 1,800 m3.

6.4.1 Costs associated with inputs

The yearly operational capacity for Citromil E.O. process is relatively low, therefore the costs associated with material inputs and electricity is are not too high.

As Figure 23 shows, the costs associated with operating labour are the highest, since the value chain (as shown in Figure 4) has additional processing steps for producing the by-products and therefore requires more employees to run the facility. In this evaluation yearly 1,400 h/year operational time has been considered for Citromil E.O. WW process. In this scenario four employees are planned to be parallelly working during those 1,400 operational hours.

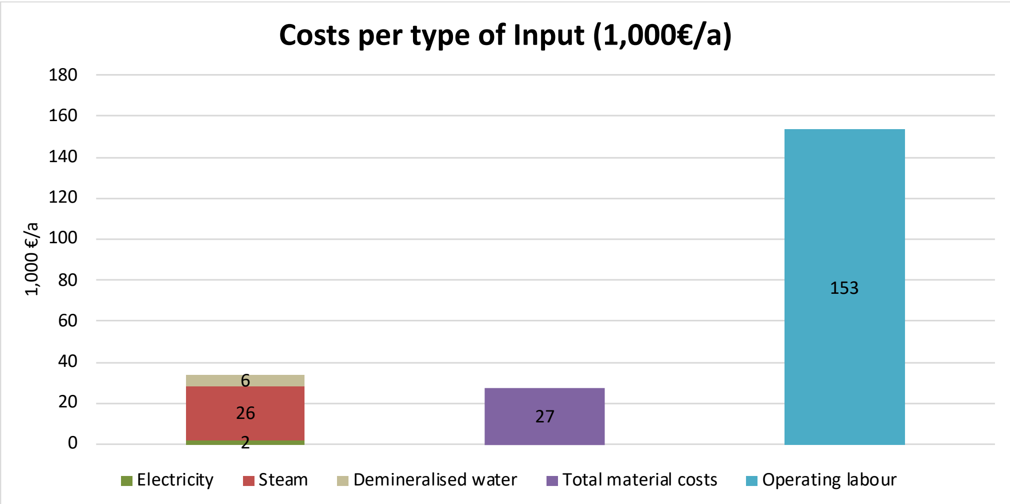

Figure 23 Costs per type of input for Citromil E.O. WW line

6.4.1.1 Material costs

Figure 24 illustrates the contributors of the material costs. Ethanol, similar to Jake WW process, is in the case of Citromil E.O. as well the main contributor to the material costs. In the case of Citromil E.O. as well a 95% recycling rate of ethanol has been considered, which means that the amount of ethanol shown in Figure 24 comprises the 5% addition which is fed into the process to balance the losses. The next contributor to the material costs is the polystyrene resin, which is used in resin fractionation step. The type of polystyrene resin used is quiet high in price (see Table 5), therefore at lower consumption rate of the chemical, it still remains expensive.

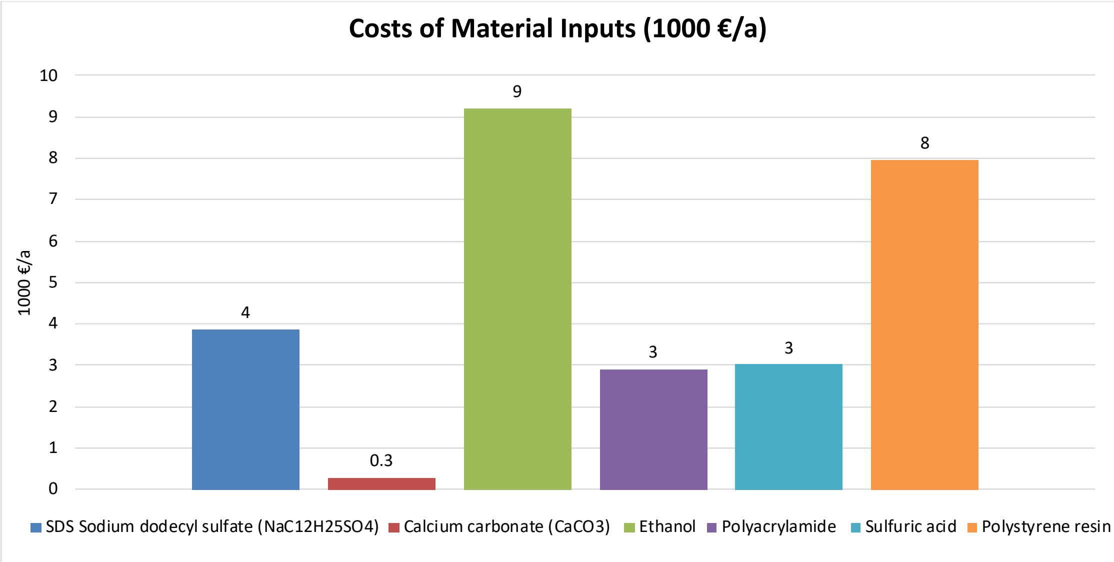

Figure 24 Material costs of Citromil WW process

6.4.1.2 Utility costs

The main costs are associated with steam, which is largely used in steam distillation phase for extraction of essential oils.

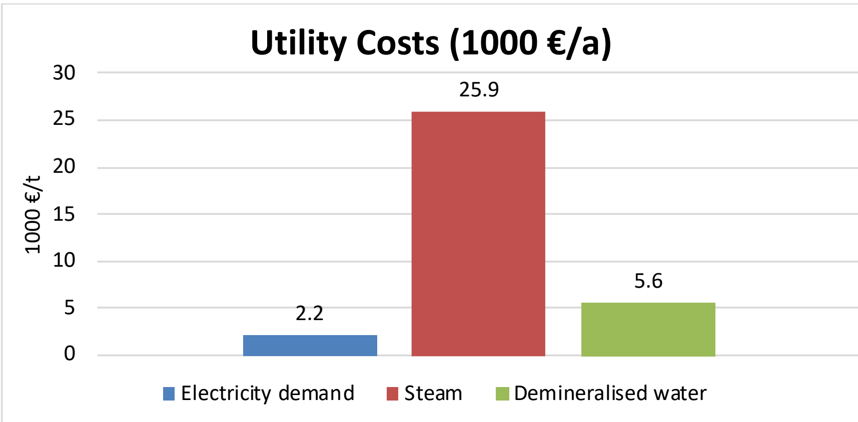

Figure 25 Utility costs of Citromil WW process

6.4.1.3 Personal costs

As already mentioned in paragraph 6.4.1 for Citromil E.O. WW process yearly 1,400 operational hours have been considered, due to the low volume of WW to be processed. However, compared to Jake and Heritage WW processes, Citromil E.O. WW process comprises additional processing steps for the production of by-products (amino acids, polyphenols, essential oils). Therefore, in this scenario four employees working parallelly during the planned 1,400 yearly operational hours is considered.

Table 14 Personnel costs for Citromil WW process

Operating labour		
Total hours worked per year (4 employees, each working 1,400 h/year)	Hours	5,600.0
Hourly wage	€/hour	27.4
Total costs for operating labour	€/year	153,440.0

At the hourly wage of 27.4 €/h, the yearly costs associated with the personnel are equal to 153,440 €/year. Below, in paragraph 6.4.6 another scenario will be presented, where the economic results of the process will be estimated while considering 3 employees working each 1,400h/year.

6.4.2 Outputs

Figure 26 represents the revenues generated by the different outputs of Citromil WW process.
Amino acids provide with the highest revenue due to their high rate and relatively high recovery rate from the process. It is important to note, that the market price for high quality amino acids in food applications has been considered (see Table 5). At this phase of the project it is however unclear whether the amino acids produced in the process will need extra processing steps in order to have the quality necessary for food applications.
For polyphenols produced in the process as well a price for high value applications has been considered.
Essential oils have number of applications in food too. The price in food application has been considered.

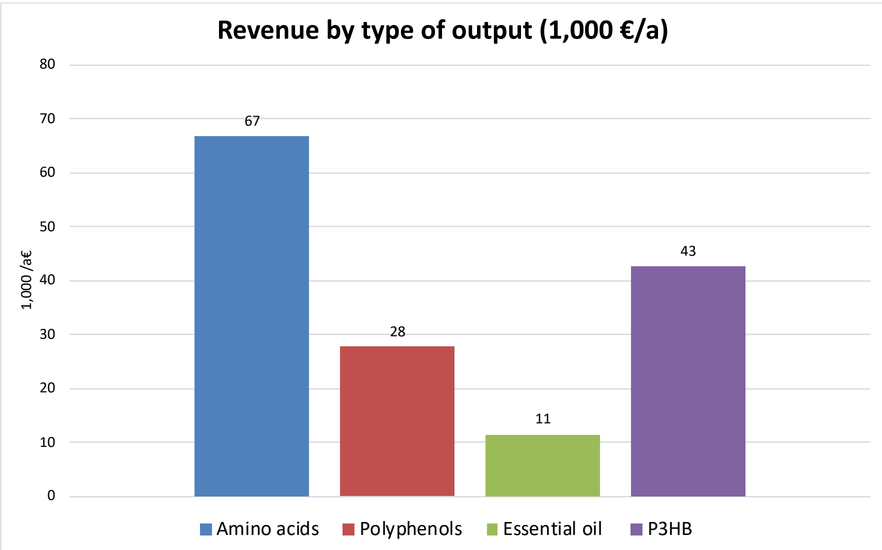

Figure 26 Yearly revenue by type of output for Citromil E.O. WW process

6.4.3 Capital expenditures (CAPEX)

Calculations for CAPEX have been carried out as described in paragraph 3.1. Table 15 shows the results of CAPEX for Jake WW process.
The rated power of this process has been calculated to be around 285.8 kW. This estimation is based on the calculated energy use for Jake WW and the average operating hours that has been considered in base scenario in Table 9.

$$\textit{Engineering costs } (C_{ENG}) = 0.1 * FCI \textit{ (10 \% of FCI)}$$

$$\textit{Contingency charges } (C_{CC}) = 0.1 * FCI \textit{ (10 \% of FCI)}$$

$$\textit{Total FCI (TFCI)} = FCI + C_{ENG} + C_{CC}$$

$$\textit{Working capital investment (WCI; 10 \% of FCI)} = 0.1 * TFCI \textit{ (10 \% of FCI)}$$

CAPEX = WCI + TFCI = 3.73 Mill. Euro

Table 15 Capital expenditures for Citromil E.O. WW process

Capital expenditures (CAPEX):	Value (Mill. €)
Fixed capital investment (FCI), **ISBL**	2.49
Engineering costs (C_{ENG})	0.50
Contingency charges (C_{CC})	0.50
Total FCI (TFCI)	3.48
Working capital investment (WCI; 10 % of FCI)	0.25
Total Capital Investment TCI = TFCI + WCI	**3.73**

6.4.4 Operating expenditures (OPEX): Base scenario

The calculation of OPEX as shown in paragraph 3.2 was carried out for Citromil E.O. WW process.

As already mentioned in paragraph 6.4.1 the costs associated with operating labour are large contributors to the overall costs. Under FMC, depreciation and plant overhead costs are large contributors. Both of these are calculated based on fixed factors of FCI. In paragraph 3.2 the literature sources of these factors are given. Under GE costs associated with distribution and selling are the main contributor. These costs are similarly calculated as a factor of OPEX. More details about the factors considered is to be found in paragraph 3.2.

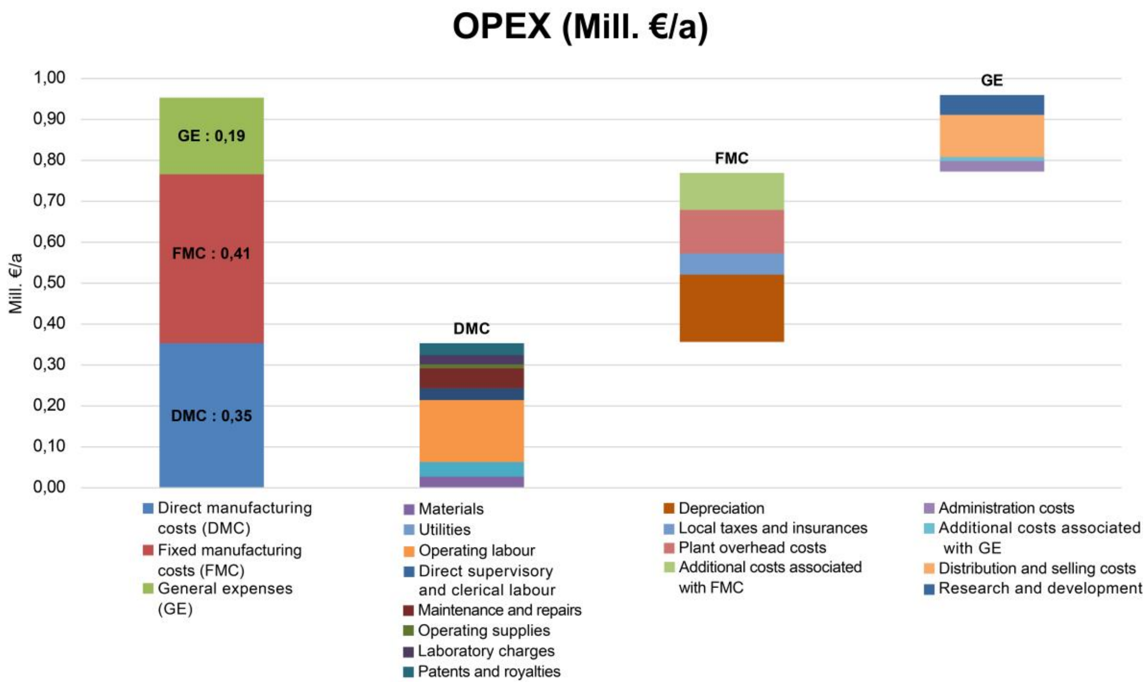

Figure 27 OPEX for Citromil E.O. WW process

6.4.5 Economic indicators: Base scenario

The yearly economic indicators show that the operating expenditures are much higher compared to revenues generated. Thus, as a result yearly 0.8 Mill € losses are generated in Citromil E.O. WW line.

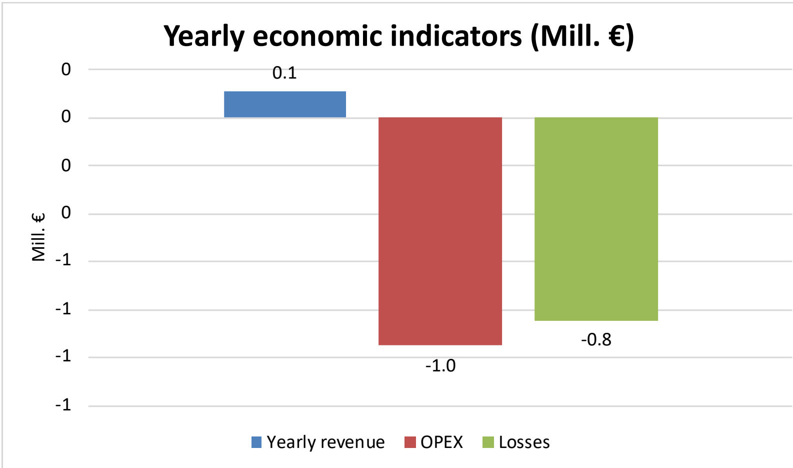

Figure 28 yearly economic indicators for Citromil WW process

6.4.6 Costs reduction effects on losses: Alternative scenario 1

Figure 29 illustrated how OPEX is reduced dependent on the reduction of material and energy costs. In paragraph 3.2 the calculation of OPEX is explained, which states that the various costs listed under OPEX are calculated as factors of the following costs:

1. Fixed capital investment (FCI)
2. Cost of operating labour (C_{OL})
3. Cost of utilities (C_{UT})
4. Cost of raw materials (CRM)

In the scenario, which is depicted in Figure 29

- FCI: remains constant and is the same estimate as it has been considered in base scenario.
- Operating labour: Figure 23 shows, the contribution of operating labour is large on overall costs of Citromil. Therefore, in this scenario 3 employees, each working yearly 1,400h have been considered.
- Costs of utilities: percentage of reduction is shown in Figure 29
- Cost of raw materials: percentage of reduction is shown in Figure 29

Figure 29 shows that at 90% reduction of material and energy costs, while 3 employees are working yearly 1,400 h, the losses are around 0.68 Mill €.

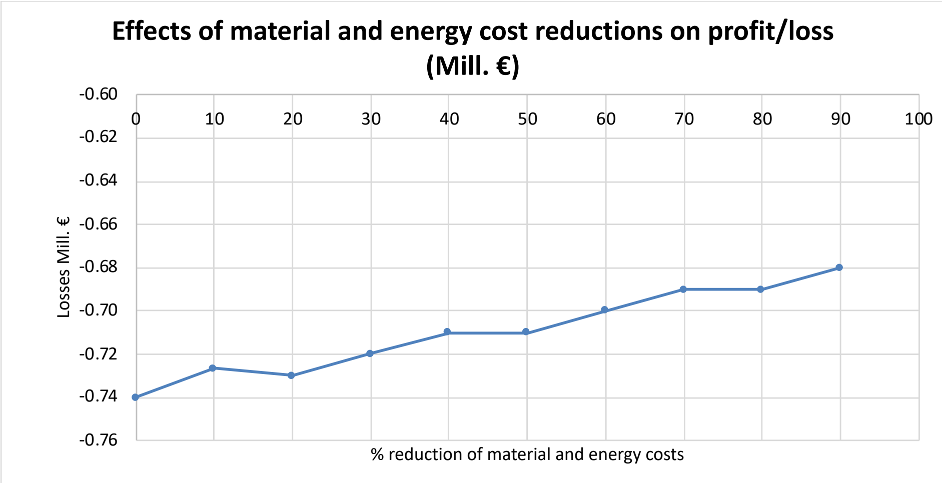

Figure 29 Effects of material and energy cost reductions on OPEX for Citromil WW process

6.4.7 Increasing the rate of outputs: Alternative scenario 2

Figure 29 illustrates, that the reduction of material and energy costs will not lead to positive economic outcomes, since the yields of the produced products are too low. Therefore, another possibility for carrying out further research on, is the prospect of increasing the rate of the outputs produced in the process. In this scenario, all the assumptions and considerations that were made in base scenario are kept, apart from considering higher yields of recovered products. The Figure 30 shows that at conditions when the yields from all four outputs (P3HB, amino acids, essential oils, polyphenols) are more than eight times higher than the current yields, the process will be economically positive.

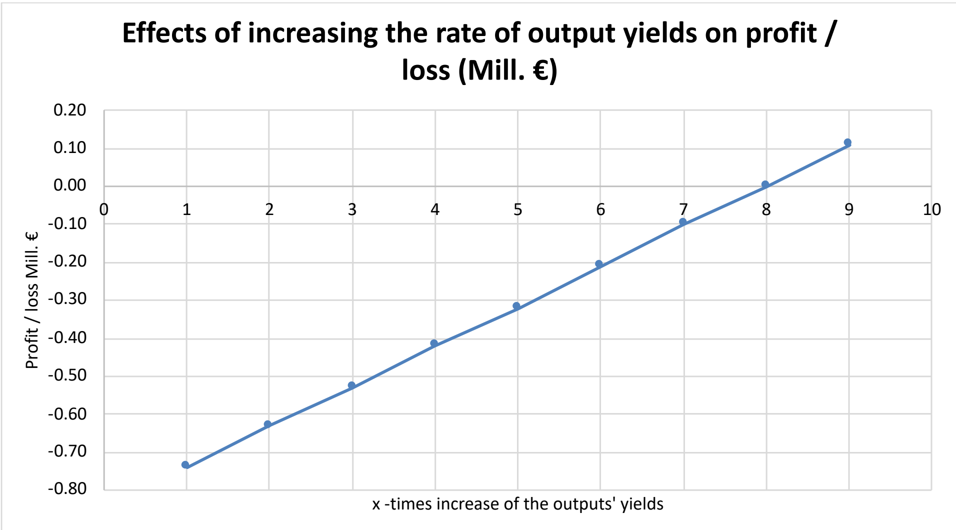

Figure 30 Effects of increasing the rate of outputs on profit / loss of Citromil WW process

7 Conclusions and further work

Based on the analyses in previous chapters, the following conclusions are drawn up for this hotspot TEE study:

The results of this hotspot TEE give an early understanding of the techno-economics of the AFTERLIFE P3HB, essential oils, amino acids and polyphenols production at their current *status quo* of development. The identification of hotspots at this stage of the project can lead to identification of approaches to improve the hot spots of the AFTERLIFE process.

The foreground AFTERLIFE processes are based on primary mainly experimental lab scale data from the project partners and are subject to optimization in the course of the project. The AFTERLIFE processes at this stage do not yet include heat integration. Further improvements in the TEE will be achieved when this is included. The main limitations of this techno-economic study are due to the data quality of the inventories. On the one hand, some inputs are based on secondary data (literature), are based on lab scale processes (lab experiments or simulation models (no measured data) or estimated data), therefore scoring badly in completeness.

The following conclusions can be drawn from this hotspot analyses:

- At the moment PHA produced from Jake WW seems to be the most promising feedstock to achieve positive economic outcome.
- The market price at which the P3HB will be sold on the market plays a big role in the profitability of the model. In this model, if P3HB is sold at price of 4,900 €/t, the process is economic, while at the P3HB market price of 4,500 €/t the process is not creating profit, however it reduces the costs of wastewater disposal (which an assumption that the wastewater after PHA production will be sent to a municipal wastewater treatment facility).
- Material inputs of Jake WW process are a large contributor to the overall process, based on the data collected from lab scale tests. These costs are expected to sink at industrial scale production.
- The Heritage WW process does not create economic value, due to low P3HB yields. The alternative model illustrates, that the process would achieve profitability, if P3HB yields would be 16 times higher compared to the current yield rates.
- The yearly capacity of Citromil E.O. WW line is considerably low which provides low yields and high operational costs.
- The alternative model 1 of Citromil E. O. process shows that reduction of energy and material inputs, even at the rate of 95%, will not help to make the process profitable.
- The alternative model 2 of Citromil E.O. process shows that the increase of all four yields at the rate of 8 will result in positive economic outcomes for the model.
- The rate at which the energy and material costs, as well as the yields affect the process will be different at higher yearly capacity.

TEE is a tool founded on quantification. The TEE carried out in this study take place during the experimental and modelling stage of development. Given that some uncertainty is present at the data inventory level the potential economic results are to be considered informative and expected to become more precise along the development path with increasing knowledge and decreasing uncertainty.

To conclude, this TEE will be updated in a final report (deliverable 7.4 Final techno-economic assessment" due at M46, at the end of the project,) including optimization, feedback loops and a more detailed assessment of the AFTERLIFE-process with the most promising wastewater as feedstock. The full TEE will be based on measured data from the pilot plant, which is being set up at the facilities of BBEU.

8 Appendix

8.1 Inventory data quality assessment

Figure 31 Indicator of Inventory data quality assessment adapted from (Weidema and Wesnæs 1996)

Indicator score	1	2	3	4	5
Reliability	Verified data based on measurements	Verified data partly based on assumptions or non-verified data based on measurements	Non-verified data partly based on assumptions	Qualified estimate (e.g. by industrial expert)	Non-qualified estimate
Completeness	Representative data from a sufficient sample of sites over an adequate period to even out normal fluctuations	Representative data from a smaller number of sites over adequate periods	Representative data from an adequate number of sites over shorter periods	Representative data from a smaller number of sites and shorter perios or incomplete data from an adequate number of sites and periods	Representativeness unknown or incomplete data from a smaller number of sites and/or over shorter periods
Temporal correlation	Less than 3 years difference to year of study	Less than 6 years difference	Less than 10 years difference	Less than 15 years difference	Age of data unknown or more than 15 years difference
Geographic correlation	Data from study area	Average data from larger area that includes the studied area	Data from areas with similar production conditions	Data from areas with slightly similar production conditions	Data from unknown areas or areas with very different production conditions
Further technological correlation	Data from studied businesses, processes and materials	Data from studied processes and materials from different businessess	Data on studied processes and materials from a different technology	Data on related processes or materials with the same technology	Data on related processes or materials with different technology

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