AFTERLIFE

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1 Executive summary

The AFTERLIFE project proposes an innovative process for recovering and valorising relevant fractions from food industrial wastewater (WW). The AFTERLIFE process is able to separate the different components of value present in WW by means of technologies specifically designed for the purpose. These fractions will then be treated to obtain value-added biopolymers, Polyhydroxyalkanoates (PHAs). In addition to the value extracted from the solid fraction, the remaining outflow of the water will be ultrapure and ready for re-use. Finally, what remains as waste from the developed process is used as a useful raw material for biogas production through anaerobic fermentation. The project is funded by the European Commission via Horizon 2020 (https://afterlife-project.eu).

As part of the project, nova-Institute conducted a techno-economic evaluation (TEE) to examine the economic viability of the process. A first hotspot TEE was carried out at an early stage of development, assessing the lab-scale process design and identifying the largest cost factors. This study can be found in D7.1 "Hot spot LCA analysis for further optimization" (delivered on January the 31st, 2020). The present study, D7.4 "Final Techno-Economic Assessment", assessed the pilot scale operation, which in turn served as a basis for further assumptions with regard to industrial-scale operation. It is based on the latest information from upscaled experiments. In contrast to the first study, which examined the AFTERLIFE processes for four different wastewaters, this study is based only on the results of the pilot-scale process with Jake wastewater (wastewater from the confectionery manufacturer Jake). This decision was taken because the experimental data describing the latter process is the one with the highest quality and the fewest data gaps, and therefore best reflects the pilot plant operations. Moreover, as far as PHA production is concerned, this production line showed the best results among the others. Two different PHA fermentation processes were assessed, pure and mixed culture fermentation.

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 key outcomes could be obtained:

- Neither the mixed nor the pure culture system prove profitable in the current process scheme. However, the pure route is shown to yield more profit due to higher production yields and lower costs for fermentation medium and pH control agent.
- The integration of 99% ethanol recovery through distillation could lead to significant cost reductions.
- Operating costs were significantly reduced compared to the hotspot analysis because recycled water (RO water) from the water purification stage was used instead of demineralised water.
- In both processes, the revenue and energy reduction potential of the biogas produced was shown to be low. By-products from this process such as digestate seem to show a higher turnover potential.

2 Introduction

In this study, nova-Institute (from here on referred to as "nova") conducted a techno-economic evaluation (TEE) or techno-economic assessment (TEA), which is a method for analysing the economic performance of an industrial process, product or service. This report will provide a breakdown of processes via TEE in order to deliver economic key figures for decision making. The goal of the economic evaluation within the AFTERLIFE project is to explore innovative technologies for wastewater streams. For this, a first hotspot TEE was carried out at an early stage of development, assessing the lab-scale process design and identifying cost factors. This study can be found in D7.1 "Hot spot LCA analysis for further optimization" (delivered on January the 31st, 2020). The present study, D7.4 "Final Techno-Economic Assessment", assessed the economic performance of PHA production processes from different wastewaters, based on pilot scale results provided by BBEPP (Bio Based European Pilot Plant). This study only examines the pilot scale process with the Jake WW (WW from the sweet and candies manufacturer Jake) among the different tested WW streams, because the experimental data describing the Jake process is the one with the highest quality and the fewest data gaps, and therefore best reflects the pilot plant operations. Moreover, as far as PHA production is concerned, this production line showed the best results among the others. The focus of the evaluation is on identifying techno-economic hotspots and cost factors that could provide approaches to potential optimisations. Based on these results, an economic evaluation of the process on an industrial level was also attempted.

Nova also explored the environmental sustainability of the processes developed in the AFTERLIFE project, these studies can be found in D7.2 and D7.3.

The following sections describe the environmental assessment conducted as part of WP7 and are structured as follows:

- TEE methodology
- Goal and scope definition
- Life Cycle Inventory analysis
- TEE
- Conclusions
- Appendix

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 are available from process simulation models or from medium or small-scale experiments (laboratory or pilot scale). For the evaluation of the techno-economic parameters, a model is needed that can make the most realistic assumptions possible for usable results, given the limited data available in the early stages. However, such modelling leads to a level of uncertainty in the results. The costing methodology outlined below has been developed and first applied in the FP7 project BIOCORE (Piotrowski 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.

	Capital expenditures (CAPEX)	Operating expenditures (OPEX)
	FCI - Fixed capital investment (<i>costs</i> 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
S	Working capital investment (WCI 10% of FCI)	C _{DI} - Distribution and selling costs
Fix costs	Capital expenditures (CAPEX) = TFCI + WCI	C _{RD} - Research and development
<u>.</u>		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
sts		Cos - Operating supplies
e co		C _{LC} - Laboratory charges
Variable costs		C _{PR} - Patents and royalties
Var		Operating expenditures (OPEX) = FMC + DMC + GE

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

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 and only available pilot scale data 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 (**¡Error! No se encuentra el origen de la referencia.**).

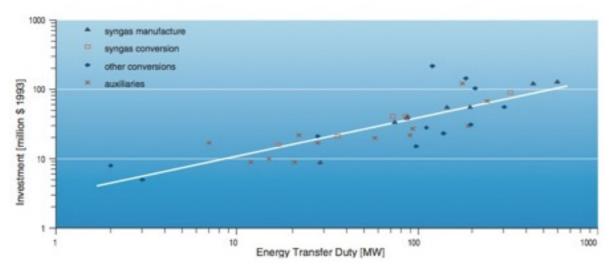


Figure 1 Correlation between energy transfer duty and investment costs (Lange 2001)

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 found was:

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

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

FCI [Mill. EUR 2021] = 4.9 * Rated Power [MW]^{0.55}

This conversion was achieved by first adjusting for inflation and then converting USD into EUR (Bureau of Labour Statistics 2019; OFX 2021)

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

Outside Battery Limits

According to Cheuvel 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 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 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, 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**¡Error! No se encuentra el origen de la referencia.** shows the types of cost items as grouped into these categories following Turton et al. (2012). Ideally, all cost items listed in **¡Error! No se encuentra el origen de la referencia.** under OPEX would be calculated directly even if some estimations are necessary. According to Turton 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 (CUT)
- 4. Cost of raw materials (C_{RM})

This result follows from the assumption, as described in Turton 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 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 wastewater from Jake 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 from Jake wastewater will take place in the factory, where Jake also operates. 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 consider that four full-time employees (FTE) are required to operate and maintain the PHA plant 24 hours a day at pilot level. For industrial scale, we assume 7 employees.

The average labour cost in the EU in 2021 amounted to about 28.5 EUR/h (EUROSTAT 2021a). This labour cost will be used for this evaluation.

Direct supervisory and clerical labour

These are costs of administrative, engineering and support personnel. Turton 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} .

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Maintenance and repairs

These are costs of labour and materials associated with maintenance. Turton et al. (2012) are proposing a factor of 0.02-0.10 linked to FCI. According to Cheuvel 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 et al. 2003). 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 equipment 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 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 et al. (2012), p. 204). For this cost item, Turton 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 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 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 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 et al. 2003) or 50-100% of labour costs (Sinnott (1999), p. 264).

Turton 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 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 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 et al. (2012), p. 205). Turton 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: 8.640 h/year (pilot plant); 29.400 h/year (commercial plant) Direct supervisory and clerical labour: $0.18*C_{OL}$ Maintenance and repairs: 0.02*FCIOperating supplies: 0.003*FCILaboratory 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 * OPEXResearch and development: 0.05 * OPEX



Summing up all of the above and solving for OPEX leads to the following equation:

 $\mathsf{OPEX} = 0.184*\mathsf{FCI} + 2.735*\mathsf{C}_{\mathsf{OL}} + 1.235*(\mathsf{C}_{\mathsf{UT}} + \mathsf{C}_{\mathsf{RM}})$

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

This chapter describes the goal and scope together with the methodological framework of the TEE study. More precisely, it comprises the objectives and intended application of the study, a general description of the product function and product system, the system boundaries together with the system function and functional unit as well as the methodological framework.

4.1 Goal

The goal of the study is to assess the economic performance of the AFTERLIFE process. In particular, the evaluation focuses on identifying cost hotspots to guide process optimisation. In addition to analysing pilot-scale data, assumptions for a potential commercial scale were made and evaluated, based on literature and expert consultation (especially from BBEPP). Further, results were compared with others TEE results for PHA production from different studies.

4.2 Scope

The scope of the TEE was defined in analogy to the scope description of the LCA (D7.2 'Final report Life-cycle assessment'). A definition follows in the coming chapters.

4.2.1 Targeted audience

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

4.2.2 Geographical and time representativeness

At the current status of the project the goal of the study is to reflect the European situation. Hence, the corresponding background data was selected, i.e. all materials and utilities are considered from datasets of production in Europe (RER) whenever available. Otherwise, global (GLO) production data are considered. Data reflects the current status of development on December 2021.

4.2.3 Function and functional unit

The functional unit in this assessment is defined as one kg of PHA polymer (namely poly(3-hydroxybutyrate) (P3HB)) with a purity of 99 %.

4.2.4 System boundaries

The assessment includes all production steps from <u>cradle-to-gate</u>, meaning that all production phases from Jake WW acquisition in the hypothetical AFTERLIFE factory to the final products are considered. As shown in Figure 2, the main production phases consist of: (1) VFA production, (2) PHA fermentation



(mixed or pure culture systems), (3) PHA purification downstream processing, (4) water purification and (5) biogas production.

In this assessment, the Jake WW input is considered as a waste product of candy and sweet manufacture, so that the wastewater entering the process does not bear any costs. However, costs may be incurred further down the AFTERLIFE process. Moreover, it was considered that the hypothetical AFTERLIFE production facilities would be located close to the Jake factory, thus neglecting possible costs of WW transportation. Clean water generated in step 4 is used in the PHA fermentation and purification phases. A detailed system description is provided in the inventory chapter. The assessment also assumed that the biogas and the digestate produced would be sold at a profit and not returned to the process.

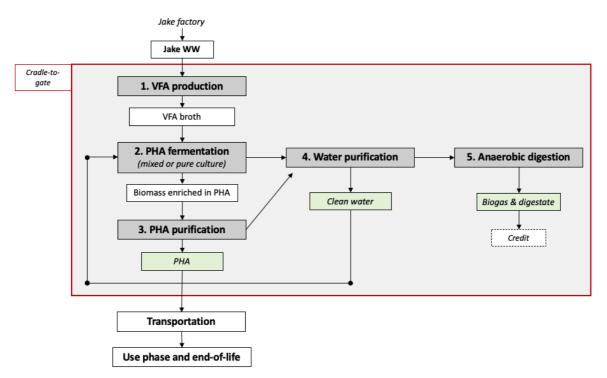


Figure 2 Jake WW system boundaries and main production phases. System boundaries are marked in red.

5 Life Cycle Inventory analysis

The Life Cycle Inventory (LCI) consists of detailed tracking of all flows into and out of the product system, including raw resources or materials, energy by type, water, and emissions to air, water and land by specific substance as well as wastes occurring in each process step. The in- and outputs of all necessary processes were collected during the data collection phase from project partners and literature.

5.1 Sources of Life Cycle Inventory data

The LCI data was obtained by several data exchange rounds along the project development with several consortium partners. Among all, the main partners involved in data gathering were: BBEPP for pilot plant mass balance, IDENER for pilot plant energy balance data, NID and CSIC for mixed and pure culture fermentation media components and INNOVEN for anaerobic fermentation information. **Foreground data** for wastewater to PHA processes were provided by the responsible project partners throughout bilateral email, conference calls. Further data of each process step were gathered through an excel data collection sheet, which was sent to the involved project partners. For **background processes** (e.g. feedstocks, materials, utilities and waste treatment), data were used from the Ecoinvent inventory database. This database is internationally recognized, both from a qualitative (completeness of data, quality of validation process) as well as from a quantitative perspective (scope of included processes). Background production data from Ecoinvent were kept as local (Europe, RER) as possible. When no local processes (RER) were available global data (GLO) were used as a reasonable alternative.

5.2 System description and inventory data

5.2.1 AFTERLIFE process

The process starts with converting Jake WW into VFA (volatile fatty acids). As mentioned, no transportation from the WW production point to the AFTERLIFE process facility is considered. In a first step WW is equalized with Calcium carbonate (CaCO₃) and mixed for further processing. The equalized medium is fermented to produce VFA by using anaerobic cultures. The fermentation liquid is further purified via ceramic microfiltration 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.

Two different fermentation techniques were tested in the pilot plant and therefore also analysed separately in this study: mixed and pure culture system. The differences between these systems, shown in Table 2 are in the fermentation medium components and pH control agents used and also in the respective amounts, the amount of VFA used per fermentation cycle and the system outputs. In both fermentations the water input, necessary for the dilution of the nutrients, comes from the clean water generated at the end of the water purification phase in step 4.2. In this way both systems do not need to acquire additional water sources but can merely reuse the water they produce themselves. A threshold of 1% on a mass basis was chosen, below which fermentation components

were considered as no relevant. All fermentation nutrient amounts reported in Table 2 are on a dry matter basis. The mixed broth enriched in PHA produced undergoes the PHA purification phase, while the supernatant broth is sent to the water purification step.

In the PHA purification phase, first the fermentation broth is transferred into a decanter in which two different fractions are obtained, the supernatant and the sediment. The first one is sent to the water purification phase, while the sediment continues the purification cascade. The next PHA recovery step consists of digestion with sodium dodecyl sulphate, dilution and homogenization, obtaining the homogenate. The homogenate is now processed via ceramic microfiltration; the retentate obtained continues the recovery phase while the filtrate is sent to the water purification step. The retentate from microfiltration is sent to digestion with H₂SO₄ at the end of which, similar to the previous process, the resulting retentate continues the recovery phase while the filtrate is sent to the water purification step. The next step is the last PHA recovery step to obtain 99% pure PHA, by means of ethanol wash and drying. It was assumed that 99% of the ethanol used in the process can be recycled via distillation, however the distillation burden was not included in the model due to data gaps. It is important to note that the PHA obtained from the mixed culture fermentation broth is less than that obtained from the pure culture system, in the former case 3 kg while in the latter 4.1 kg is obtained.

In the next phase all waste water streams generated along the processing cascade are sent to the water purification phase, in order to obtain pure water out of the AFTERLIFE system. As mentioned, this water is looped back into the system.

The last process phase is the biogas generation step, in which all solid streams from previous steps are turned into valuable energy and digestate. It is important to appreciate that the energy obtained from the mixed culture fermentation line is less than that obtained from the pure culture system, in the former case 177 MJ while in the latter 198 MJ is obtained as reported by the partners. The anaerobic digestion is also generating digestate as a side product, a valuable nutrient-rich substance that can be used as a compost fertiliser and soil enricher.

Table 2: Jake mixed and pure culture systems LCI.

1. VFA production						
1.1 Anaerobic Fermentation to VFA						
Material/energy	IN/OUT	Dimensional unit	Amount	Comments		
Jake WW (cycles)	IN	kg	1045,00	No costs considered		
Jake WW (startup)	IN	kg	200,00	No costs considered		
Agrodigestate		kg	22	neglected		
CaCO3	IN	kg	40			
Electricity	IN	kWh	0,04	Mixing		
Electricity	IN	kWh	1,77	Pumping		
Fermented VFA broth	OUT	kg	1045	next step		
WW to municipal treatment	OUT	kg	262,00	Own calculation for mass balance purposes		
		1.	2 Ceramic microfiltration (
Material/energy	IN/OUT	Dimensional unit	Amount	Comments		
Fermented VFA broth	IN	kg	1045			
Electricity	IN	kWh	0,26			
Retentate VFA	OUT	kg	200	to biogas production step		
Filtrate VFA	OUT	kg	800	next step		

AFTERLIFE

WW to municipal treatment	OUT	kg 45,00		Own calculation for mass balance purposes					
	2. PHA fermentation - <u>Mixed and Pure Culture</u>								
Material/energy	IN/OUT	Dimensional unit	Amount (Mixed Culture)	Amount (Pure Culture)	Comments				
Filtrate VFA	IN	kg	800	1244,3					
Water for dilution		kg	4956	897	This water input is supplied with the RO water generated at the end of the AFTERLIFE process				
NH4CI	IN	kg	66,50952	0,89					
K2PO4	IN	kg	26,96064	1,34					
(NH4)2SO4	IN	kg	//	8,07300000					
MgSO4.7H2O	IN	kg	5,9472	//	_				
HCI	IN	kg	90,447	//					
NaOH	IN	kg	99,12	17,94					
Electricity	IN	kWh	0,01	0,01	Mixing				
Electricity	IN	kWh	1,77	1,77	Pumping				
Electricity	IN	kWh	1,35	1,35	Aeration				
Mixed broth enriched in PHA	OUT	kg	1475	2500					

AFTERL!FE

Broth supernatant (to filtration cascade)	OUT	kg	4425	//	to water purification ste
		3.	PHA purification and pro	cessing	
Material/energy	IN/OUT	Dimensional unit	Amount	Comments	
Mixed broth enriched in PHA	IN	kg	1475		
Supernatant	OUT	kg	1393	to water purification step	
Sediment	OUT	kg	82	next step	
		3.2 Digestio	on with SDS, dilution and h	nomogenization	
Material/energy	IN/OUT	Dimensional unit	Amount	Comments	
Sediment	IN	kg	82		
Sodium dodecyl sulphate (SDS)	IN	kg	1		
decarbonised Water		kg	82	This water input is supplied with the RO water generated at the end of the AFTERLIFE process	
Electricity	IN	kWh	0,034	mixing	
Homogenate	OUT	kg	164	next step	
		3.3 Ceram	ic microfiltration (0.45) wi	ith diafiltration	

т



Material/energy	IN/OUT	Dimensional unit	Amount	Comments
Homogenate	IN	kg	164	
RO water		kg	327	This water input is supplied with the RO water generated at the end of the AFTERLIFE process
Electricity	IN	kWh	0,26	(in pure culture system it is 0,31)
Filtrate + diafiltrate (to step 4.9)	OUT	kg	232	to water purification step
Retentate	OUT	kg	259	next step
		3.4 Dig	estion with H2SO4 and r	nicrofiltration
Material/energy	IN/OUT	Dimensional unit	Amount	Comments
Feed	IN	kg	259	
H2SO4 (96%)	IN	kg	38	
RO water for dilution		kg	676	This water input is supplied with the RO water generated at the end of the AFTERLIFE process
NaOH (30%)	IN	kg	0,3	
RO water for diafiltration		kg	402	This water input is supplied with the RO water generated at the end of the AFTERLIFE process
Electricity	IN	kWh	0,034	
Heat	IN	MJ	7,49	
Filtrate + diafiltrate	OUT	kg	1173	to water purification step
Retentate	OUT	kg	201	next step

AFTERLIFE

WW to municipal treatment	OUT	kg	1,30	Own calculation assuming for mass balance purposes			
3.5 Ethanol wash and drying							
		Dimensional	Amount (Mixed		• · ·		
Material/energy	IN/OUT	unit	Culture)	Amount (Pure Culture)	Comments		
Feed	IN	kg	201	same as mixed			
EtOH	IN	kg	40,22	same as mixed	Assuming 99% of ethanol is recycled.		
RO water for EtOH washout		kg	302	same as mixed	This water input is supplied with the RO water generated at the end of the AFTERLIFE process		
Electricity	IN	kWh	0,26	same as mixed	pumping		
Steam	IN	MJ	20,12	same as mixed	Drying phase		
Wash water	OUT	kg	400	same as mixed	to water purification step		
РНА	OUT	kg	3,00	4,10	DM 100%		
			4. W	ater Purification			
			4.1 Ceramic	c microfiltration 0.2 μm			
Material/energy	IN/OUT	Dimensional	Amount (Mixed	Amount (Pure Culture)	Comments		
waterial/energy	114/001	unit	Culture)	Amount (Fure Culture)	comments		
All water							
streams from	IN	kg	7623	3198			
previous steps							
Electricity	IN	kWh	0,26	0,31			

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filtrate	OUT	kg	6861	2878	next step			
retentate	OUT	kg	762	320	to biogas production step			
4.2 RO filtration								
Material/energy	IN/OUT	Dimensional unit	Amount (Mixed Culture)	Amount (Pure Culture)	Comments			
Filtrate 4.9	IN	kg	6861	2878				
Electricity	IN	kWh	0,31	0,37				
filtrate (Final clean RO water)	OUT	kg	6175	2590	Looped in PHA fermentation and purification			
retentate	OUT	kg	686	288	to biogas production step			
			5. Bi	ogas production				
Material/energy	IN/OUT	Dimensional unit	Amount (Mixed Culture)	Amount (Pure Culture)	Comments			
All biogas streams from previous steps	IN	kg	1648	808				
Electricity	IN	kWh	1,95	2,08				
Heat	IN	MJ	125,82	140,59				
Energy produced by Biogas burning	OUT	MJ	177	198	Energy credit			
Digestate	OUT	kg	1318,70	646,10	Compost credit			

5.2.2 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 $4,000 \notin/t$ to $5,000 \notin/t$. In this study the target price is considered $4,900\notin/t$, which is an estimate by nova regarding the future trends of market needs for biodegradable polymers.

In/Outputs	Price per unit €/t	Source
Utilities		
Electricity	0.13 (€/kWh)	EUROSTAT (2021b)
Gas (for production of steam)	0.07 (€/kWh)	EUROSTAT (2021c)
Operating labour		
Average hourly wage in EU	28.50	EUROSTAT (2021a)
Used materials		
SDS Sodium dodecyl sulfate (NaC12H25SO4)	250.00	Zauba.com
Calcium carbonate (CaCO3)	140.00	Zauba.com
Sulfuric acid (H2SO4)	85.00	Zauba.com
Ethanol (C2H5OH)	650.00	Zauba.com
Sodium hydroxide (NaOH)	600.00	Zauba.com
Output		
PHA granulate	4,900.00	nova-Institut estimation
	(target price)	
Biogas	0.07 (€/kWh)	dena (2019)
Digestate	10.00	Jurgutis et al. (2021)
Wastewater for disposal in municipal	0.20	Mulder (2015)
wastewater treatment plant		

Table 3 Market price of inputs and outputs that have been used in this TEE

5.2.3 Assumptions

Below, the main assumptions taken in this TEE study are shown:

- In the calculation of the TEE, no costs have been allocated to the Jake wastewater 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 **PHA** production facility. No transportation costs for the wastewater transport have been considered.
- When Jake WW enters the VFA fermentation phase it already has the required processing temperature (37 Celsius), therefore it does not need to be further heated or cooled.

- 99% EtOH recovery was not included in the TEE assessment, but evaluated separately as a scenario.
- The infrastructure, for example reactor, facility or other equipment, needed for the foreground AFTERLIFE process was neglected.
- Electricity is supplied by medium voltage grid based on the average transformation technology and the average electricity loss during transmission in EU.
- Produced biogas and digestate are sold at a profit to increase turnover and reduce costs
- Annual operating hours are considered the same as for the previous hotspot analysis (4.200 h/year).
- All waste water streams generated along the processing cascade are sent to the water purification phase, in order to obtain pure water out of the AFTERLIFE system. This water is looped back into the system so that no costs for water input (demineralised water) is considered.

5.2.4 Data quality assessment and limitations

In the context of the life cycle assessment (LCA), the quality and limitations of the data have been examined. These results were adopted for the TEE.

Since LCA 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. A qualitative analysis of the uncertainty of the inventory data was carried out. 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 in Table 4 according to Weidema and Wesnæs (1996). The indicators are explained in Appendix 1

Overall uncertainty is present at inventory level, technical complications were encountered in the design of pilot plant operation by BBEPP. Moreover, the data gathered are not entirely experimental but also estimates, especially with regards to the energy balance which comes from the mathematical model developed by IDENER. Based on that, the AFTERLIFE LCI scores relatively bad in completeness, which is a measure of the representativeness of the data. All in all, the quality of the inventory is in line with the low TRL of the production process examined.

Table 4 Data quality assessment of AFTERLIFE and reference processes.Data Source: 1 primary (from experiments), 2 secondary (LCI databases), 3 tertiary (literature/estimates).Indicator score: 1-2 very good to good, 3- fair, 4-5, poor to very poor.

Source	Reliability	Completeness	Temporal correlation	Geographical correlation	Further technological correlation		
AFTERLIFE process							
1,3	2	4	1	1	2		

5.2.5 Upscaling approach towards commercial level operation

The evaluation of the Jake process is based on the data from the pilot plant. These are scaled up for economic analysis with regard to a commercial/industrial plant. For this purpose, a scenario is considered that assumes an increased capacity of the Jake wastewater input to produce commercial quantities of PHA annually. In the pilot plant, the production yield is 3.00 g PHA/L WW for the mixed culture and 4.10 g PHA/L WW for the process-only route. With an estimated annual wastewater input of about 22.5 m³ into the pilot plant and a PHA accumulation rate of 80 %, about 54 kg PHA is produced for the mixed and 74 kg PHA for the pure route.

After consultation with BBEPP, an effluent input of 1,500,000 m³ per year is required to produce commercial quantities of PHA, as assumed in Lauder (2021) TEE analysis. With the experimental design otherwise unchanged, this would result in annual PHA production values of 3,600 tonnes (mixed) and 4,920 tonnes (pure). The associated material costs were assumed to increase linearly with the production capacity. For the energy and labour costs, either results of the model from the hotspot analysis (D7.1 "Hotspot LCA analysis for further optimisation") or data from the BBEPP were used (Table 5).

	Pi	lot	Comm	nercial
Annual WW stream (m ³)	22.5		1,500,000	
Process Route	Mixed	Pure	Mixed	Pure
PHA annual yield (t/year)	0.054	0.074	3,600	4,920

Table 5 Annual yield of PHA (mixed and pure process route) at pilot and commercial scale

6 Results and discussion

For the implementation of the TEE, based on the material and energy flows, CAPEX and OPEX were calculated as described in chapter 3. Results of the pilot plant were transferred to an industrial level as outlined in section 5.2.6. In the following, these results of the TEE for the AFTERLIFE project are presented and discussed in detail. In the calculation of the TEE, no costs were applied for Jake wastewater as feedstock, as the PHA production plant will be constructed in the industrial park where the companies operate. Therefore, the water will be directed to the PHA production plant. The transport costs for wastewater transport were not taken into account.

6.1 Overview

Figure 3 shows an overview of the financial indicators of the mixed and the pure variant of the AFTERLIFE process for Jake. The results show that both process systems are to be considered unprofitable. However, it can be seen that the pure variant generates higher profit due to higher production assets. In addition, the mixed culture system has high costs due to the use of fermentation media and pH control agents. The high turnover from the sale of by-products from biogas production such as fermentation residues cannot compensate for this.

Figure 4 shows the financial indicators for one tonne of PHA. As in the hotspot analysis, the target price of 4,900 \in was set. However, it is important to note that the average price for PHA is between 4,500 \notin /t and 5,000 \notin /t. In both process routes, production is not profitable. Although it can be stated that, due to the higher production volumes, the pure system achieves a higher profit from PHA than the mixed alternative.

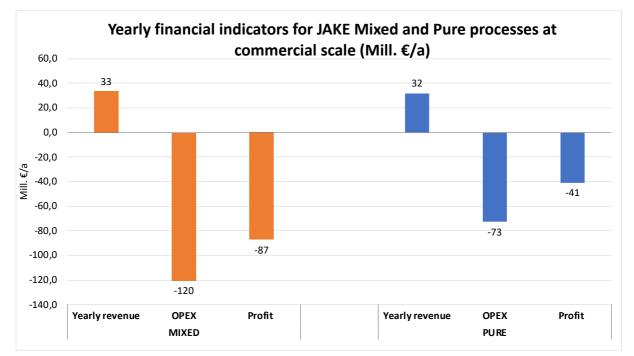
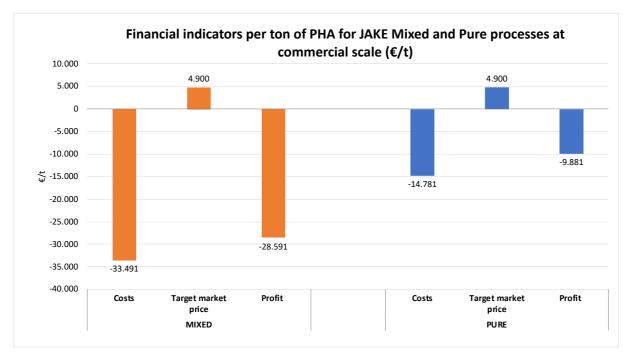


Figure 3 Yearly financial indicators for the JAKE mixed and pure process route



AFTERLIFE

Figure 4 Financial indicators per ton of PHA production for JAKE mixed and pure process route

6.2 TEE for Jake wastewater



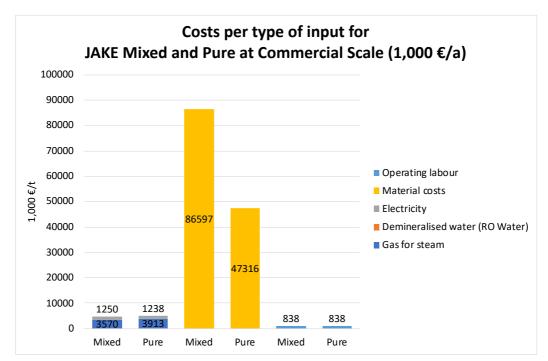


Figure 5 Costs per type of input for Jake mixed and pure process route

For the analysis, the annual capacity of Jake wastewater was set at 1,500,000 m³ to produce commercial quantities annually for both process routes (mixed: 3,600 t/year; pure: 4,920 t/year). The required energy, material and personnel input was adjusted accordingly for this capacity. In this scenario, as in the hotspot analysis, 4,200 h/year of operating time were taken into account. According to BBEPP, 7 full-time equivalents (FTEs) are planned for the operation/maintenance of the plant during the planned operating time.

Figure 5 illustrates the costs by type of input. It is obvious that material costs are much higher than energy costs and labour input costs. This not surprising considering that the figures are from linear scale up values from the pilot plant results. As Table 2 shows that the production of pilot quantities of 3 kg (mixed) and 4.1 kg (pure) PHA already requires 40 kg Calcium carbonate (CaCO₃) and 40 kg Ethanol (EtOH). When extrapolated, this results in high costs. The use of ethanol is one of the main contributors to the costs of material inputs for both process routes (Figure 6).

6.2.1.1 Material costs

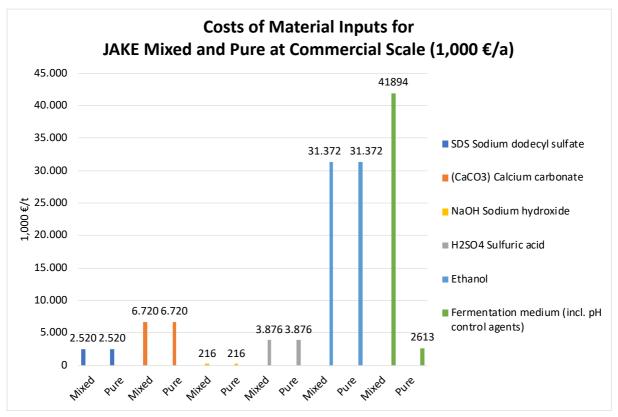


Figure 6 Costs associated with material inputs for Jake mixed and pure process route

Ethanol is used in the PHA recovery step to obtain 99% pure PHA, by means of ethanol wash and drying. It was assumed that 99% of the ethanol used in the process can be recycled via distillation, however the distillation was not included in the model due to data gaps. In 6.2.6 however, an attempt is made to show a scenario with 99% EtOH recovery.

However, it must be emphasised that the use of the fermentation medium and the pH control agents in the mixed culture system is the biggest cost hotspot in contrast to pure culture.

6.2.1.2 Utility costs

The energy demand of the facility is the cumulative energy demand of the mixed and pure process route (Figure 7).

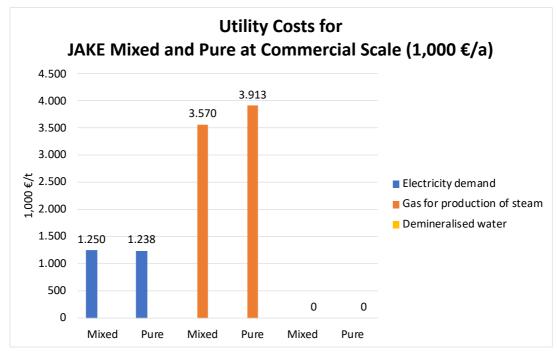


Figure 7 Utility costs for Jake mixed and pure process route

The contributors of electricity costs are mainly for the PHA processing and recovery phase. Costs of demineralised water has not been included in this calculation, as we assume that all water demand for PHA fermentation and purification can be met by recycled clean water (RO water) generated during the water purification step.

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 Ecovert v.3.4: 1 kg stem needs 0.09 m³ gas is necessary to produce 1 kg steam. 1 m³ gas converts into energy that is equal to 10.5 kWh electricity.

This evaluation also shows that gas for heat is the largest cost factor in both processes. During the PHA recovery phase, heat is needed mainly for drying the PHA. The greatest gas demand, however, is for biogas production, where the pure system has a greater demand than the mixed.

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, as it was in D7.1 "Hotspot LCA analysis for further optimisation". In this scenario it is considered that 7 employees will be necessary for the operation of the downstream processing at commercial scale. Thus, the costs associated with operating labour will equal to 29,400 working hours according to European average salary rate of 28.5 €/hour (EUROSTAT 2021a).

Operating labour		
Total hours worked per year (7 FTE each working 4,200	Hours	29,400.0
h/year		
Hourly wage	€/hour	28.5
Total costs for operating labour	€/year	837,900.0

Table 6 Operating labour for Jake

6.2.2 Outputs

PHA granulate is the main product of the AFTERLIFE process. The pure culture system has a higher production rate per 1 litre of wastewater and produces more PHA than the mixed process on an industrial scale (pure: 4,920 t/a; mixed: 3,600 t/a). In addition, biomass waste is produced during the manufacturing process, which feeds into the biogas production. In this assessment, it is assumed that the biogas produced and the resulting digestate are resold at a profit. It is also considered that the wastewater produced during the production process is discharged into the municipal wastewater system.



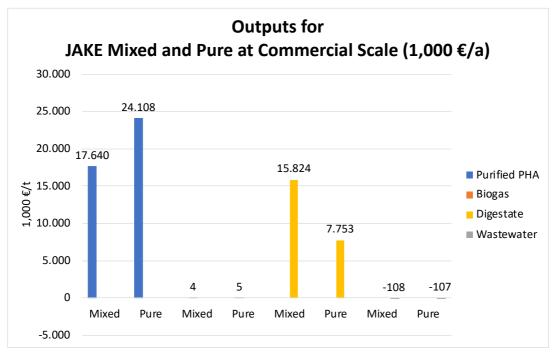


Figure 8 Outputs of the Jake mixed and pure process route

6.2.3 Capital expenditures (CAPEX)

production, resulting in a higher CAPEX estimation.

Calculations for CAPEX have been carried out as described in paragraph 3.1. Table 7Table 8**jError! No se encuentra el origen de la referencia.** show the results of CAPEX for Jake WW process. In addition, a heat integration of 40 % and an average additional power of 10 % were included in the calculation. As already described, the pure system has a higher energy demand, especially for biogas

Mixed:

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 = 43.37. Mill. Euro**

Table 7 Capital ex	penditures for Jo	ake WW process	(Mixed)
--------------------	-------------------	----------------	---------

Capital expenditures (CAPEX):	Value (Mill. €)
Fixed capital investment (FCI), ISBL	28.9
Engineering costs (C _{ENG})	5.78
Contingency charges (C _{cc})	5.78
Total FCI (TFCI)	40.48
Working capital investment (WCI; 10 % of FCI)	2.89
Total Capital Investment TCI = TFCI + WCI	43.37

Pure:

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 = 45.36. Mill. Euro**

Table 8 Capital expenditures for Jake WW process (Pure)

Capital expenditures (CAPEX):	Value (Mill. €)
Fixed capital investment (FCI), ISBL	30.24
Engineering costs (C _{ENG})	6.05
Contingency charges (C _{cc})	6.05
Total FCI (TFCI)	42.34
Working capital investment (WCI; 10 % of FCI)	3.02
Total Capital Investment TCI = TFCI + WCI	45.36

6.2.5 Operating expenditures (OPEX)

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 mixed and pure Jake wastewater systems are shown in Figure 9Figure 10.

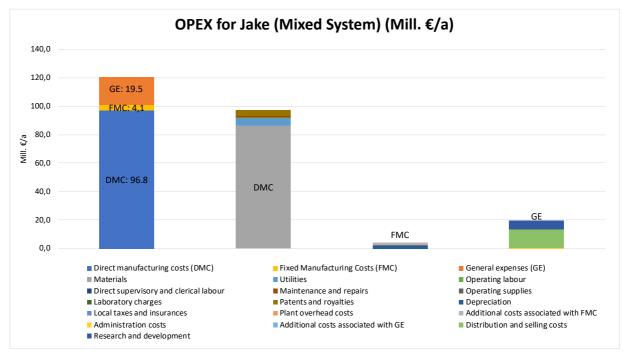
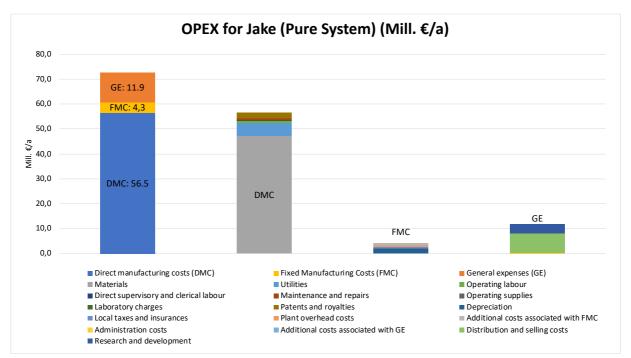


Figure 9 Overall picture of OPEX for Jake WW process (Mixed)



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Figure 10 Overall picture of OPEX for JAKE WW process (Pure)

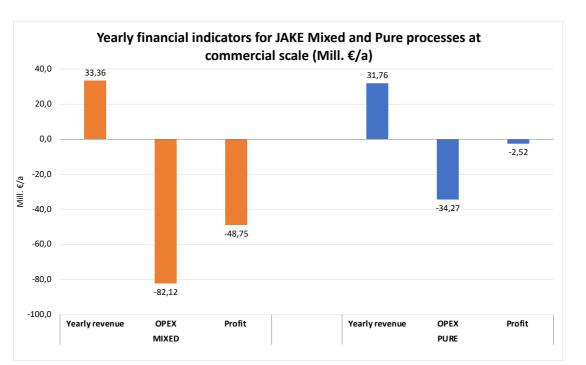
As already noted in section 6.2.1.1, material costs, especially for ethanol, are the largest cost factor in both systems, resulting in very high direct manufacturing costs. Ethanol accounts for about 26% of OPEX in the mixed system and around 43% of OPEX in the pure process route. In addition, the use of a large amount of fermentation medium in the mixed system leads to an excessively high cost of the operating system.

6.2.6 Scenario: 99% EtOH recycling

The integration of an ethanol recycling step via distillation shows significant cost reductions for both process systems (Figure 11). The results show that OPEX can be reduced from 120 million Euros to about 82 million Euros (mixed system), or from 73 million Euros to about 34 million Euros (pure system). Furthermore, the results show that for the pure production process, it can be assumed that production is almost profitable. This is due not only to the reduction in ethanol use, but above all to the revenue that can be generated from the sale of by-products like digestate from biogas production. The production of PHA systems alone is not yet economical, although it is just below the zero-cost limit (Figure 12).

In the mixed system, costs could be reduced, but the costs for the fermentation medium and the associated pH control agents remain high.

It should be noted that for this scenario, no potential energy costs for an additional distillation step were considered.



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Figure 11 Yearly financial indicators for the JAKE mixed and pure process route (99% EtOH recycling)

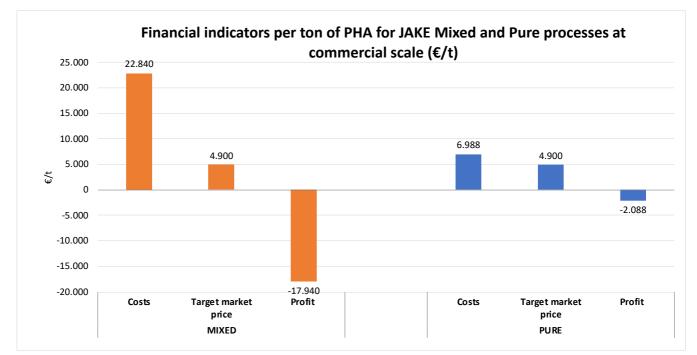


Figure 12 Financial indicators per ton of PHA production for JAKE mixed and pure process route (99% EtOH recycling)

6.2.7 Scenario: Increasing the rate of PHA yield

In addition to reducing material costs, there is also the possibility of evaluating the prospect of increasing the production rate of PHA outputs produced in the process. In this scenario, all the assumptions and considerations made in the baseline scenario are retained, except for the consideration of higher yields of PHA. Figure 13 shows that even a quadrupling would lead to economic results in the pure system. For the mixed cultures system, an eightfold increase in PHA yield would be required to make the process profitable. In this scenario, however, it must be considered whether such yield increases are at all possible in the future.

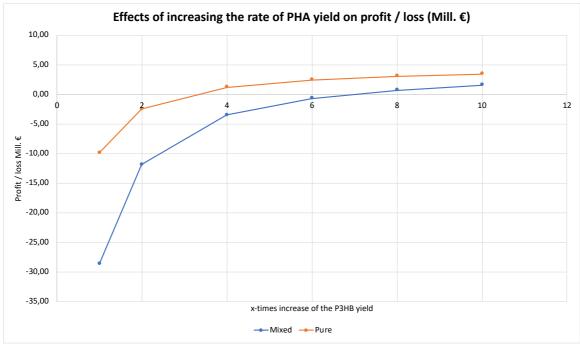


Figure 13 Effects of increasing the rate of outputs on profit / loss

6.4 Benchmark comparison

Study by	Annual production rate (tonnes/year)	Carbon source used	CAPEX (\$)	CAPEX (€, 2021)	OPEX (\$)	OPEX (€, 2021)	Final cost of production of PHA (\$/kg)	Final cost of production of PHA (€/kg) estimated for the year 2021
Choi and Lee (1997)	2850	Glucose	27,000,000	42,000,000	18,000,000	27,500,000	5.58 – 9.16	8.56 – 14.05
Mudilar et al. (2007)	46	Activated sludge	500,000	590,000	34,000	40,000	11.80	14.02
Rumjeet (2015)	2929	Glucose	59,600,000	62,000,000	24,000,000	25,100,000	8.40	8.73
Leong et al. (2017)	9000	Glycerol	160,000,000	161,000,000	58,000,000	58,000,000	5.77	5.80
	·		without	99% EtOH recy	cling			
AFTERLIFE (Mixed)	3600	Wastewater		43,000,000		120,460,000		33.49
AFTERLIFE (Pure)	4900	Wastewater		45,000,000		72,620,000		14.78
	with 99% EtOH recycling							
AFTERLIFE (Mixed)	3600	Wastewater		43,000,000		82,000,000		22.84
AFTERLIFE (Pure)	4900	Wastewater		45,000,000		34,000,000		6.99

Table 9 Comparison of selected studies on large scale PHA production

The comparison shows that the results of the TEE study are only comparable with the selected studies to a limited extent. In particular, the relatively high costs of the mixed culture system already exclude it from comparison with the other studies, regardless of the integration of an ethanol recovery. In the pure system, especially the assumption with 99% EtOH recovery shows promising competitive potential compared to the other processes, so that we focus exclusively on this variant in this comparison (Table 9).

Thus, it can be seen that the AFTERLIFE technology appears to be more economical and less costintensive compared to the processes considered. The comparison with Choi and Lee (1997), with the values transferred to the year 2021, shows that the CAPEX values of both studies are almost identical (42 million to 45 million Euros). Only the OPEX is slightly higher for the AFTERLIFE variant (34 million to 27.5 million Euros), although the annual production rate is higher (4950 tonnes to 2850 tonnes). This is also reflected in lower production costs (6.99 \notin /kg) compared to Choi and Lee (1997) study (8.56-14.05 \notin /kg). Furthermore, the economic analysis of Rumjeet (2015), which dealt with PHA production from glucose as carbon source, also shows similar production costs (8.73 \notin /kg) with a similarly large annual production volume. (2929 tonnes). Again, compared to this process, AFTERLIFE is more cost-effective. In contrast, the study by Leong et al. (2017) conducted an economic evaluation for very large commercial production volumes. 9000 tonnes of PHA were produced using glycerol as a carbon source. This is about double the amount compared to the present study. This resulted in CAPEX of 161 million Euros and OPEX of 58 million Euros. The cost of producing 1 kg of PHA was about \notin 5.8, which would be cheaper than AFTERLIFE's pure system (\notin 6.99/kg). However, it should be noted that the data for the study by Leong et al. (2017) came via modelling software. These can help to better close weaknesses such as data gaps or to better implement assumptions, for example on upscaling, than in the present study.

When looking at the market in addition to the scientific work, the hotspot analysis has shown that the market price for PHA granulate is between 4000 \notin /t and 5000 \notin /t. In other sources, this range is even slightly wider (4000 \notin /t to 6000 \notin /t) (Fantinel 2020).

At the moment, the pure AFTERLIFE process (with EtOH recycling) would not be competitive on the market. Thus, the process would have to set a price of about 7000 \notin /t as a target price to generate revenue from the sale of PHA in order to become viable in the market.

For this reason, it is crucial that the AFTERLIFE process routes close the most important cost points and make further optimisations to make it even more profitable. Besides increasing the production potential, the integration of an EtOH recovery seems to be one of the most important factors to reduce costs in the AFTERLIFE system.

Conclusions

The economic feasibility of the process developed in the AFTERLIFE project to recover and valorise relevant fractions from Jake wastewater was evaluated using TEE. Several cost factors were investigated, resulting in a comprehensive picture of the most important economic factors influencing the production system with mixed and pure cultures. The identification of hotspots can also lead to the identification of approaches to reduce costs.

The foreground AFTERLIFE processes are based on mainly pilot scale data from the project partners, which were scaled up to an industrial scale process by using calculation models, assumptions and estimates from the literature and partners.

It is shown that both the mixed and the pure culture production systems generate high costs and are currently not economical.

The following conclusions can be drawn about the TEE:

- Neither the mixed nor the pure process route prove to be economical in the current process scheme. However, it can be seen that the pure route generates more profit. This is because the pure system produces more PHA per litre of wastewater.
- The main cost items are the material expenditures. Ethanol is one of the main contributors in both systems. In the mixed system, however, there are also high costs due to the use of fermentation medium and pH control agents which makes it less economical than the pure process route.
- The mixed variant produces more digestate from biogas production. The resulting potentially higher turnover that the mixed variant could achieve through the sale of the by-product digestate compared to the pure system cannot currently lead to profitable results.
- The high input quantity and price of ethanol drive up the costs. More than 40 kg of EtOH are needed to produce 3 kg (mixed) or 4.1 kg (pure) PHA at pilot level. On a commercial production scale, this would lead to massive cost points. The TEE shows in a scenario that a 99% ethanol recovery via distillation could lead to significant cost savings.
- The results of the TEE show that, because of the low production rate of PHA per litre wastewater (mixed: 3.0 g/L WW; pure: 4.1 g/L WW), commercial production rates could currently only be achieved by using high volumes of Jake wastewater (at least 1,000,000 m³). Thus, increasing production efficiency should be a main objective in further research, as it could lead to significant cost reductions.
- Utility costs were significantly reduced compared to the hotspot analysis by using recycled water (RO water) from the water purification step. Future economic analyses could look at assumptions about what would change if the water did not go back into the process but was sold for profit.
- In both processes, the revenue and energy reduction potential of the biogas produced is low.
 Upcoming evaluations of the system need to examine whether biogas production would be the most economically viable option, or whether there would be another end uses for the accumulated retentate.
- In addition, it must be taken into account that in this TEE it was assumed that there are no costs for wastewater from Jake as feedstock, as the PHA production plant will be built on the

Jake Industrial Park (no transport costs). Further research needs to investigate how realistic this assumption is and how the economic performance would change if costs for wastewater were incurred.

In conclusion, despite its current limitations, the AFTERLIFE technology is promising and should be further developed. In particular, the pure system shows promising potential, which can be made more economical, for example, by increasing the production rate or integrating EtOH recycling. Further optimisation options need to be explored that could lead to increased production efficiency (lower material costs, lower material requirements per unit, lower energy demands).

The TEEs conducted in this study take place in the experimental and modelling phase of development. As there is some uncertainty at the level of the dataset, the potential economic outcomes are to be considered informative and are likely to decrease as knowledge increases and uncertainty decreases along the development pathway.

7 Appendix

Appendix 1 Indicator of Inventory data quality assessment adapted from	n Weidema and Wesnæs (1996)
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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 periods 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 businesses	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

9. References

Bureau of Labour Statistics 2019: CPI Inflation Calculator. (Ed.), Download at <u>https://data.bls.gov/cgi-bin/cpicalc.pl</u>

Cheuvel, A., and, G. F. and Raimbault, C. 2003: Manual of Process Economic Evaluation. Institut Français du pétrole publications (Ed.), Download at

Choi, J.-i. and Lee, a. S. Y. 1997: Process analysis and economic evaluation for Poly(3-hydroxybutyrate) production by fermentation. (Ed.), Download at

dena 2019: dena-Analyse Branchenbarometer Biomethan 2019. Deutsche Energie-Agentur GmbH (dena) (Ed.), Berlin, Download at <u>https://www.dena.de/fileadmin/dena/Publikationen/PDFs/2019/dena-Analyse_Branchenbarometer_Biomethan_2019.pdf</u>

EUROSTAT 2021a: Wages and labour costs. (Ed.), Download at <u>https://ec.europa.eu/eurostat/statistics-explained/index.php/Wages_and_labour_costs</u>

EUROSTAT 2021b: Electricity prices (including taxes) for household consumers, first half 2021. (Ed.), Download at <u>https://ec.europa.eu/eurostat/statistics</u> explained/index.php/Electricity price statistics#Electricity prices for non-household consumers

EUROSTAT 2021c: Natural gas price statistics. (Ed.), Download at <u>https://ec.europa.eu/eurostat/statistics-explained/index.php/Natural_gas_price_statistics</u>

Fantinel, F. 2020: Deliverable 5.3 - RES URBIS (Ed.), Download at https://www.google.com/url?sa=t&rct=j&q=&esrc=s&source=web&cd=&ved=2ahUKEwiM-JPMqPf0AhVYi_0HHfP5B20QFnoECAwQAQ&url=https%3A%2F%2Fec.europa.eu%2Fresearch%2 Fparticipants%2Fdocuments%2FdownloadPublic%3FdocumentIds%3D080166e5cffe89f0%26appId% 3DPPGMS&usg=AOvVaw3Km3LvzmLPpJ-paKr5ZY0s

Fernando D. Ramos, C. A. D., Marcelo A. Villar, M. Soledad Diaz (Bioresource Technology. Klöpffer, W. a. B. G.) 2019: Design and optimization of poly(hydroxyalkanoate)s production plants using alternative substrates. (Ed.), Download at

Jurgutis, L., A. Šlepetiene, J. Šlepetys and Ceseviciene, J. 2021: Towards a Full Circular Economy in Biogas Plants: Sustainable Management of Digestate for Growing Biomass Feedstocks and Use as Biofertilizer. Lithuanian Research Centre for Agriculture and Forestry, Institute of Agriculture (Ed.), Download at

Lange 2013: Personal Communication

Lange, J.-P. 2001: Fuels and chemicals manufacturing; guidelines for understanding and minimizing the production costs. (Ed.), Download at

Lauder, A. 2021: Personal Communication. BBEPP,

Leong, Y. K., P. Show, J. Lan, H. Loh, H. L. Lam and Ling, T. 2017: Economic and environmental analysis of PHAs production process. (Ed.), September 2017. Download at

Mudilar, S. N., Vaidya, A. N., Suresh Kumar, M., Dahikar, S. and Chakrabarti, T. 2007: Technoeconomic evaluatuon of PHB production from activated sludge. (Ed.), Download at

Mulder, M. 2015: Costs of removal of micropollutants from effluents of municipal wastewater treatment plants (Ed.), Download at

OFX 2021: View twenty years of exchange rate data for over 55 currencies. (Ed.), Download at <u>https://www.ofx.com/en-au/forex-news/historical-exchange-rates/monthly-average-rates/</u>

Peters, M. S. and Timmerhaus, K. D. 1991: Plant design and economics for chemical engineers. (Ed.), McGraw-Hill New York, Download at

Piotrowski, S., M. Carus, Cibilla, F. and Raschka, a. A. 2014: New nova Methodology for Techno-Economic Evaluations of Innovative Industrial Processes (nTEE). (Ed.), Download at

Rumjeet, S. 2015: Systematic investigation of potential factors that affect the production costs of the bio-based and bio-degradable plastic polyhydroxyalkanoates (PHAs) by a costing analysis based on early process simulation. University of Cape Town (Ed.), Faculty of Engineering and the Built Environment, 20 November 2015. Download at https://open.uct.ac.za/bitstream/item/23346/thesis ebe 2016 rumjeet shilpa.pdf?sequence=1

Sinnott, R.-K. (Heinemann, B.) 1999: Coulson & Richardson's Chemical Engineering. (Ed.), Oxford, UK Download at

Towler, G. and Sinnott, a. R. (Elsevier) 2013: Chemical engineering design: principles, practice and economics of plant and process design. (Ed.), Download at

Turton, R., R. C. Bailie, Whiting, W. B. and Shaeiwitz, a. J. A. 2012: Analysis, synthesis and design of chemical processes. (Ed.), Pearson Education, Download at

Weidema, B. P. and Wesnæs, a. M. S. 1996: Data quality management for life cycle inventories—an example of using data quality indicators. (Ed.), Download at