Lessons from combining techno-economic and life cycle assessment – a case study of polyphenol extraction from waste resources

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Abstract

Purpose: To analyze the environmental and economic performance of polyphenol extraction methods being developed within the NoAW project to valorize agricultural residues. And to utilize life cycle and techno-economic assessment as tools for this purpose.

Methods: LCA is applied at an early design stage to obtain a preliminary carbon footprint of the polyphenol extraction methods. The extraction methods tested are solvent extraction and pressurized liquid extraction (PLE). Subsequently, TEA-LCA is applied in simulated industrial conditions, optimized with guidance from literature and the preliminary LCA.

Results: The lab scale results highlight the need to reduce solvent use and maximize yields. The best option selected through the TEA-LCA is PLE, using CO2:EtOH:H2O as solvent with a solvent to dry weight ratio of 5, and 2 extraction steps (PLE-EtOH-5). This is in part due to higher yields for the TEA, and the use of ethanol for the LCA, which is a less environmentally burdensome solvent than acetone.

Conclusions: If the same yields as in lab scale can be attained at the designed industrial scale, then the PLE-EtOH-5 option leads to the highest environmental and economic benefits, despite higher capital expenditure. The LCA at lab scale was useful in pointing out potential environmental hotspots, which served to guide the TEA in order to design a better performing process from both an environmental and economic perspective.

1. Introduction

Biomass demand for the production of bioenergy, biomaterials and biochemicals is estimated to increase by 70-110 % by 2050 compared to 2005 levels [1]. A paradigm shift to renewable sources of production has long been discussed, in the context of circular economy and valorization of biomass waste resources produced through the agricultural value chain. The bioeconomy today is estimated to have a 2.4 € billion annual turnover, which is only expected to increase in the future [2]. Yet, the prefix bio does not guarantee sustainability. For example, growing biomass for biofuels has long been debated, prompting the Renewable Energy Directive [3] at a European level to ensure validity of greenhouse gas reductions claims. In this regard, integration of quantitative sustainability assessment such as life cycle assessment (LCA) and techno-economic (TEA) assessment have been regarded as valuable. Combined TEA-LCA has been applied in many occasions to assess the environmental and economic ramifications of implementing new technologies. Amongst the many of the studies utilizing this method are: the novel use of lignocellulosic material for production of biodiesel from palm oil residues [4], production of biofuels and bioresins [5], and bioblend stocks for the light and heavy-duty transport [6]. More interestingly, TEA-LCA has been used for quantifying and monetize externalities in the form of Disability Adjusted Life Years (DALY) to provide a more complete picture of the financial burdens arising from environmental problems [7], [8]. Recently, combining TEA and LCA has been used to optimize new production routes from an early design phase, such as the integration of wastewater into microalgae production for biodiesel production [9], or the integration of power-to-gas technology of methane and photovoltaics [10]. Combined TEA and LCA lends itself well to finding production hot spots and opportunities for optimization. This is even more relevant when applied to renewable resources such as biomass, which have to be managed sustainably.

Agricultural residues are an increasingly important biomass resource, which continues to be studied to increase maturity level of 2G and 3G production. In this context, the H2020 No Agricultural Waste (NoAW) project is working toward the development of sustainable value added products from agricultural residues, such as biocomposites, biodegradable bioplastics, and others [11]. Among these agricultural residues, wine pomace is a residue rich in polyphenols, which are compounds with high antioxidant value [12]. Polyphenol extraction methods at the laboratory scale can be analyzed using TEA-LCA in order to identify hotspots and potentially environmentally problematic production steps. Therefore, in this study LCA is applied at an early design stage to obtain a preliminary carbon footprint of the polyphenol extraction methods. Subsequently, TEA-LCA is applied in simulated industrial conditions, optimized with guidance from literature and the preliminary LCA. The goal is to obtain a holistic picture of the economic feasibility and possible environmental impacts of each polyphenol extraction method.

2. Methodology

Results of laboratory scale experiments of different methods for the extraction of polyphenols from red grape pomace were evaluated using a combination of LCA and TEA. Based on the preliminary LCA of the laboratory scale experiments, industrial scale processes were designed. The industrial scale processes were thereafter analyzed with both LCA and TEA.

2.1. Polyphenol extraction methods and laboratory experiments

Various polyphenol extraction methods developed within the NoAW project were assessed. The extraction methods include both solvent extraction and pressurized liquid extraction (PLE).

2.1.1. Extraction with acetone – S-AcN

Batch extraction was performed in the laboratory with 75% acetone, 25% water as solvent, with a solvent to dry weight (DW) ratio of 11. Extraction was performed in an air tight vessel at 50°C at atmospheric pressure. The solvent and pomace were kept in contact for 2 hours. After this time the polyphenols were dissolved in the liquid phase from which they could be isolated and obtained as a powder. The polyphenol content was then analyzed. This set up was also tested for 1 and 4 hours.

2.1.2. Extraction with ethanol – S-EtOH

The same procedure as in 2.1.1 was tested with ethanol as solvent. Equal parts ethanol:H_2O were used for the extraction. Extraction times of 1, 2 and 4 hours were tested to observe their influence on yield. The S-EtOH was only examined at industrial scale (section 2.3 and 2.4).

2.1.3. Pressurized liquid extraction with ethanol – PLE-EtOH

Three different options for PLE were studied in the lab. PLE-EtOH-75 with 75% co-solvent composed of equal parts ethanol and water and 25% liquid CO_2. PLE-EtOH-100 is performed without liquid CO_2 and instead there is 100% co-solvent composed of equal parts ethanol and water. The extraction is performed at 80°C and 100 bar. While the third PLE option, PLE-EtOH-oil, is divided into two extraction steps. One with 100% supercritical CO_2 at 350 bar and 80°C for one hour, with a flow of CO_2 of 30g per minute, leading to the production an oily phenolic extract. A second extraction step with the same EtOH:H_2O:CO_2 ratio as applied for PLE-EtOH-75 is performed to obtain polyphenols as dry extract. The solvent flow for the second step was 8g per minute. As this is a continuous set up, both of these steps lead to an extremely high solvent to DW ratio. All extraction operational parameters are presented in Table 1.

All extraction processes listed leave behind the pomace residue, which can be further valorized using different methods not assessed in this study [11].

Table 1 Operational parameters of laboratory experiments.

Scenario Name	**S-AcN**	**PLE-EtOH-75**	**PLE-EtOH-100**	**PLE-EtOH-oil**
Yield (g polyphenol/kg DW)	47	48	44	49
Solvents				
- Water	25%	37.5%	50%	37.5%**
- Ethanol		37.5%	50%	37.5%**
- Acetone	75%			
- CO2		25%		100%*, 25%**
Solvent to DW ratio	11	101	101	583
Stages (no.)	1	1	1	2
Total extraction time (min)	120	30	30	90
Temperature (°C)	50	80	80	80
Pressure (bar)	1	100	100	350*, 100**

*first stage
** second stage

2.2. LCA of laboratory scale experiments

A preliminary LCA was performed on the extraction methods described above, using only the Global Warming potential (GWP) impact category as the environmental indicator. The ReCiPe 2016 Midpoint Hierarchist method [13], which has a 100 year time horizon from point of emission, was used as impact assessment method, supplied by the Ecoinvent 3.4 Database [14]. The functional unit for the LCA is 1 kg of polyphenols assuming equal functionality. The process design software, Superpro designer [15], was used to simulate the polyphenol extraction methods with industrial scale equipment. However, all operating parameters such as temperature, solvent to DW ratio, polyphenol yield, pressure, and extraction times among others, were kept equal to laboratory conditions (Table 1). Simplified flow diagrams with the industrial equipment used are shown in Figure 1 and Figure 2. The polyphenol producing plant is assumed to be placed in Italy and thereby, background processes for Italy from the Ecoinvent database were used as much as possible, e.g. the electricity grid.

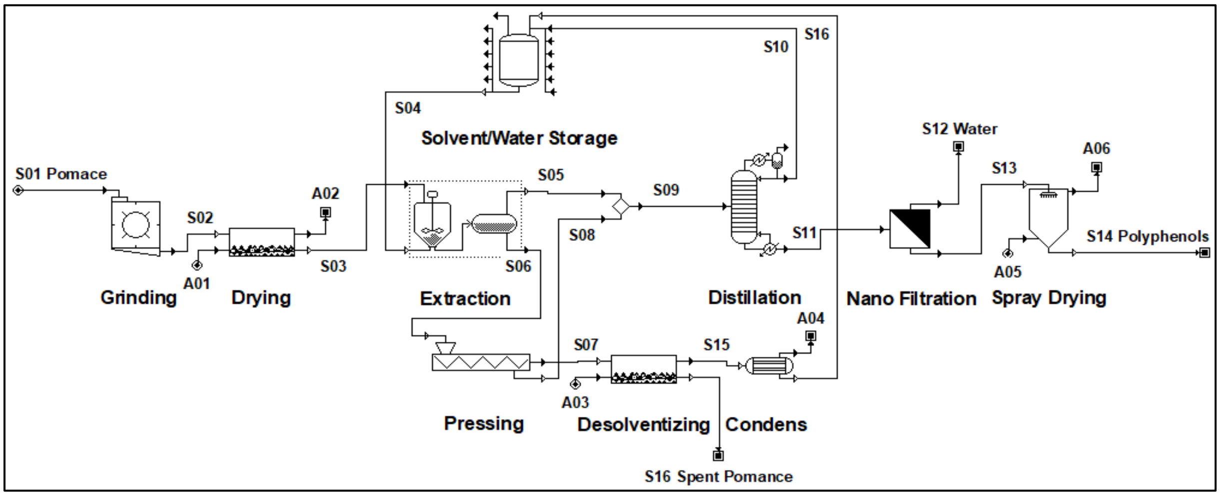

Figure 1 Solvent extraction with either acetone or ethanol at atmospheric pressure. The pomace dryer is optional.

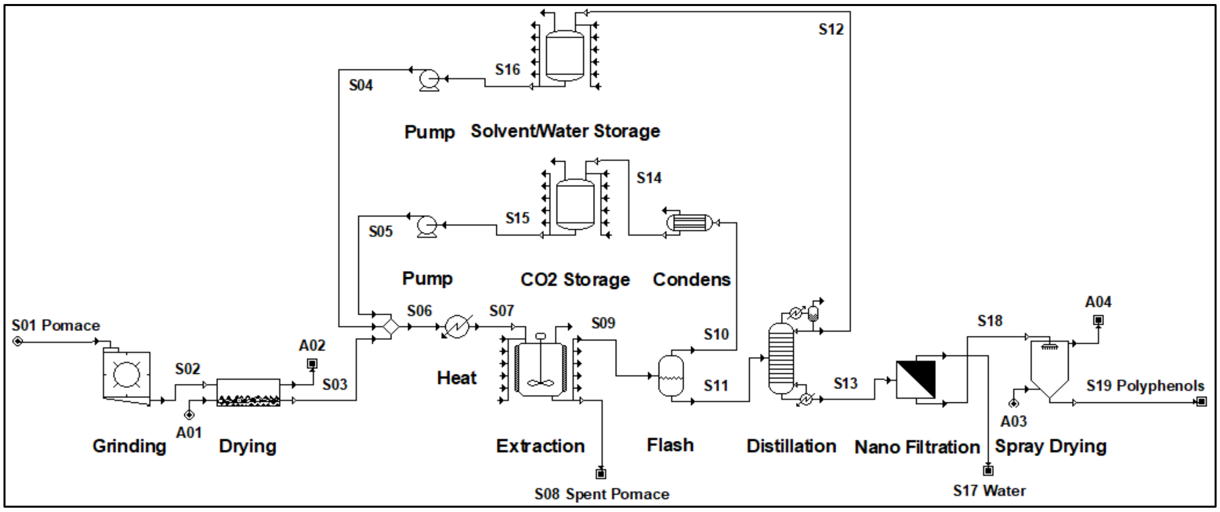

Figure 2 Pressurized liquid extraction with ethanol, water, and supercritical CO_2. The pomace dryer is optional.

2.3. TEA of industrial scale processes

Based on the results of the laboratory scale experiments, the preliminary LCA, and literature [16]–[20], industrial scale processes for solvent extraction and PLE were designed. TEA of the industrial scale processes designed was carried out in order to investigate the economic repercussions of installing a polyphenol extracting plant. The TEA includes Capital Expenditure (CapEx) and Operating Expenditure (OpEx). Assumptions and simplifications were made in order to fill data gaps. Assumptions of economic parameters and estimates of fixed capital costs were based on [15], [21]–[24]. The most important assumptions are reported in Table 2.

Table 2 Parameters for the techno-economic assessment.

Production	8000	h/y
Red pomace	20	kton wet/y
	2500	kg wet/h
	36.2%	DW
Labour related costs	891	k€/y
Plant related costs	10%	of fixed capital/y
Financing costs	10%	of fixed capital/y
Electricity	10%	€/kWh
Steam	25	€/ton
Solvent price		
- Water	0.00	€/kg
- Ethanol	0.80	€/kg
- Acetone	1.20	€/kg
- CO_2	0.50	€/kg
Solvent ΔH evaporation		
- Water	2260	kJ/kg
- Ethanol	841	kJ/kg
- Acetone	539	kJ/kg
- CO_2	380	kJ/kg
Solvent loss	2%	of recycle
Energy solvent recycle	2	x ΔH_{vap}

The labour related costs were assumed to be the same for all processes and are based on: 2 shift positions, an operator salary of k€ 30/y including supervision, direct salary overhead, and general plant overhead. The plant related costs include maintenance, tax, insurance, rent, overhead, environmental charges, and royalties. The financing costs are based on an amortization of the fixed capital costs over 10 years with no interest.

For all processes, a solvent loss of 2% of the solvent in the recycle is assumed. The energy which is required to recycle the solvent is estimated as two times the heat of evaporation. For the recycle of water, acetone, and ethanol, thermal energy is required, while for the recycle of CO_2, electricity is required.

2.4. LCA of industrial scale processes

Following the TEA, a complete accounting LCA was performed on the same systems analyzed for the TEA. The system boundary for the accounting LCA includes all actions carried out in order to obtain 1 kg of polyphenols from when the grape pomace enters the production system to the product leaving the production facility, e.g. all processing steps, such as grinding, drying, adding solvents, filtering, distillation and more (Figure 1 and Figure 2). On the other hand, the “gate-to-gate” LCA does not include end of life of the polyphenols or any transport throughout the life cycle. Furthermore, no allocation is performed on the impacts of polyphenol production, i.e. the entire burden of production is assigned to the main product, the polyphenols. Likewise, no credits are assigned for the production of polyphenols potentially replacing similar products in the market.

The LCA includes all 18 impact categories in ReCiPe 2016 Midpoint (H) methodology. As for the LCA at lab scale, the geographical location of the polyphenol plant is assumed again to be Italy.

To ease interpretation of results, a simple multi-criteria decision assessment (MCDA), was performed. First, results for the 18 impact categories were normalized within each impact category to the worst performing scenario and ranked. Second, normalized results for all impact categories were averaged for each extraction method respectively to obtain a single score per scenario, which was then used to single out the best performing scenario. The average results were compared with normalized Global Warming results in order to assess the possibility of burden shifting between GWP and other environmental impacts (categories).

3. Results

3.1. LCA of laboratory scale experiments

The carbon footprint analysis clearly shows that if laboratory conditions are maintained when implementing a polyphenol extraction plant, then the acetone based solvent extraction method outperforms all other scenarios by a large margin, in terms of global warming potential (GWP). This is largely due to the amounts of solvent used in each scenario, which are lowest for the S-AcN scenario. The large amount of solvent used in the continuous set up for all PLE scenarios results in a very high electricity and heating demand in, for example, electricity for compressing of the system, heating during polyphenol extraction, and heating during distillation to recover the solvents.

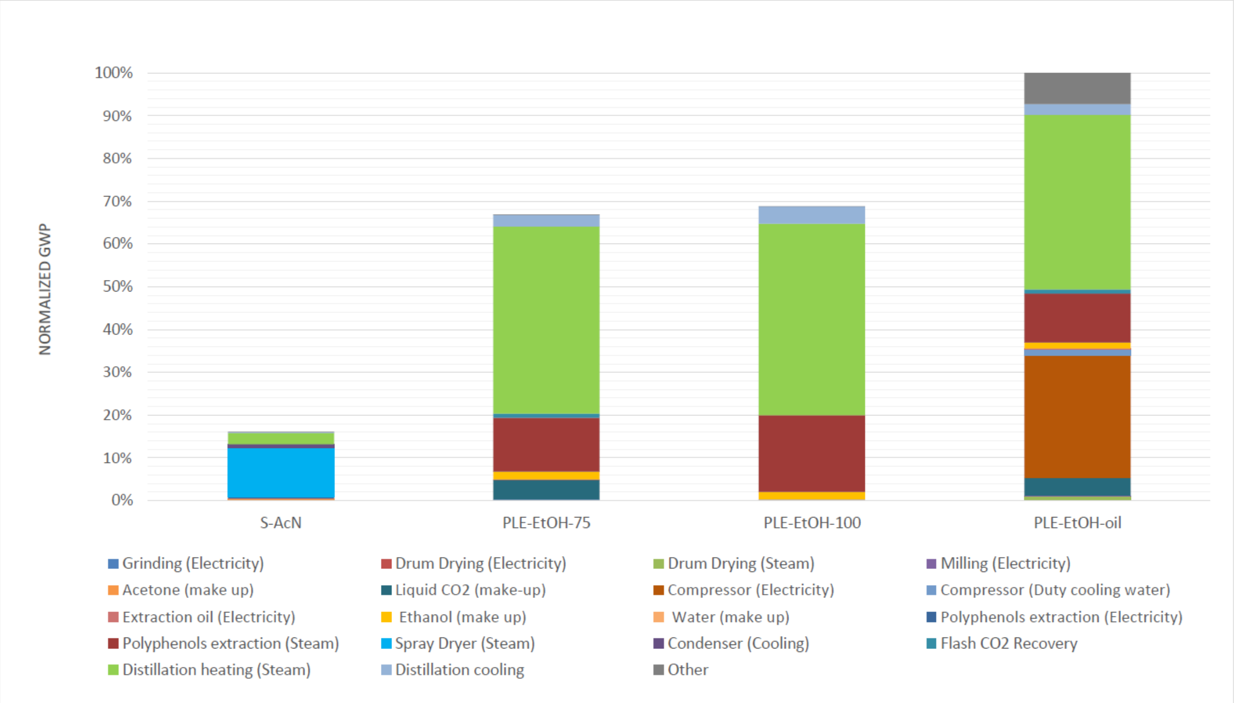

Figure 3 Normalized global warming potential results of polyphenol extraction scenarios at lab scale. Functional unit is 1 kg of polyphenols. Normalization to worst performing scenario PLE-EtOH-oil.

From the preliminary LCA, the importance of keeping the solvent ratio as low as possible is evident. This has a trickle down effect on the energy demand of the whole system. It was also proposed that the contact between solvent and pomace could be increased by changing the set up of the system. Systems with multiple extraction stages and lower solvent to pomace DW ratios were considered in the TEA.

3.2. TEA of industrial scale processes

The TEA focused on optimizing the operational parameters so that it would be economically feasible to implement a polyphenol extraction at industrial scale. Based on laboratory scale experiments and literature

[16]–[20], extraction steps were increased and as a result the solvent to pomace DW ratios decreased. Because water is already present in the pomace, it is necessary to dry the pomace prior to the extraction to maintain a solvent to DW ratio of 2 (S-AcN-2 and S-EtOH-2). Total extraction time was assumed to be 60 minutes for all processes. Equipment was scaled based on the flow sizes and subsequently the purchased equipment costs and fixed capital costs were estimated. The operational parameters and assumed extraction yields are given in Table 3.

Table 3 Operational parameters of designed industrial scale processes.

Scenario Name	**S-AcN-5**	**S-AcN-2**	**S-EtOH-5**	**S-EtOH-2**	**PLE-EtOH-10**	**PLE-EtOH-5**
Yield (g polyphenol/kg DW)	47	47	40	40	79	79
Solvents						
- Water	33%	33%	50%	50%	37.5%	37.5%
- Ethanol			50%	50%	37.5%	37.5%
- Acetone	67%	67%				
- CO2					25%	25%
Solvent to DW ratio	5	2	5	2	10	5
Stages (no.)	2	5	2	5	2	2
Total extraction time (min)	60	60	60	60	60	60
Temperature (°C)	50	50	50	50	80	80
Pressure (bar)	1	1	100	100	100	100
Fixed capital (M€)	4.6	4.1	4.7	4.0	9.4	6.5

The best performing scenario, in economic terms, is PLE-EtOH-5, which also has the highest polyphenol extraction yield. Despite lager fixed capital costs, the costs expressed per kg polyphenol are lower compared to the solvent extraction processes (Figure 4). The second best scenario is S-AcN-2, which has the advantage of a low solvent to DW ratio of 2 and similar cost range for plant related and financing cost. However, the heat demand for S-AcN-2 is larger, because drying of the pomace is required.

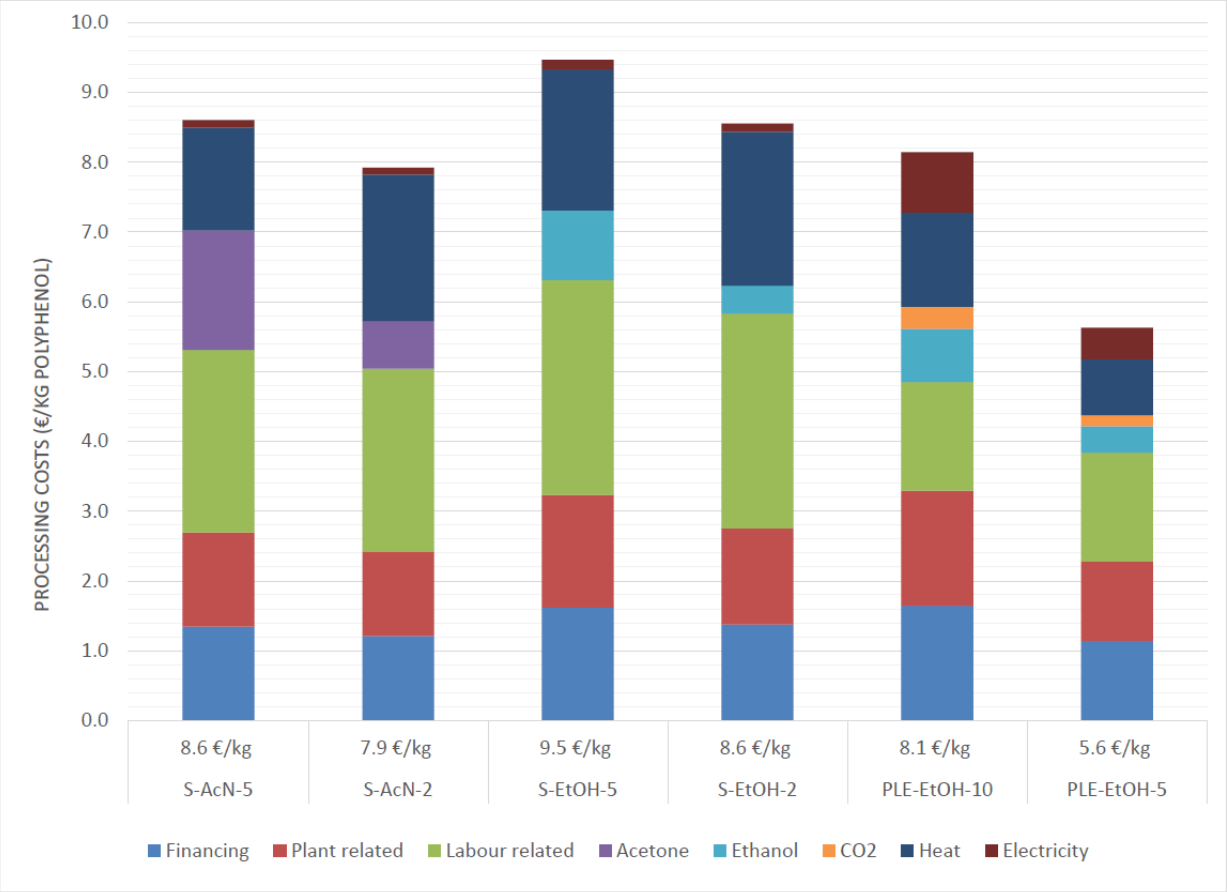

Figure 4 Techno-economic assessment results of optimized polyphenol extraction at industrial scale.

3.3. LCA of optimized industrial scale design

The LCA of optimized operational conditions showed that if seeking to alleviate environmental problems it would be preferable to choose PLE-EthOH-5, that is to say, a pressurized extraction that uses ethanol, water and supercritical CO_2 as solvent, with a solvent ratio of 5 and 2 extraction steps (blue bars, Figure 5). It is noteworthy to say that a solvent extraction using acetone with a solvent ratio of 2 (S-AcN-2) is potentially within the same range of impact when all impact categories for the LCA are equally weighted i.e. all environmental problems encompassed in the LCA are equally valued. If instead, the goal is to reduce global warming at the potential cost of other environmental problems, then the best choice is PLE-EtOH-5. PLE-EtOH-5 is the best performing scenario in terms of GWP. The upper error bar for this scenario represents the worse possible outcome for the scenario, when uncertainty is taken into consideration, which is here called the “GW acceptable value”. As such, scenarios above the dashed line will most likely lead to higher GWP impacts than PLE-EtOH-5. As can be seen in Figure 5, scenario S-AcN-2 just barely falls below the GW acceptable line, and only when taking into consideration a -10% uncertainty.

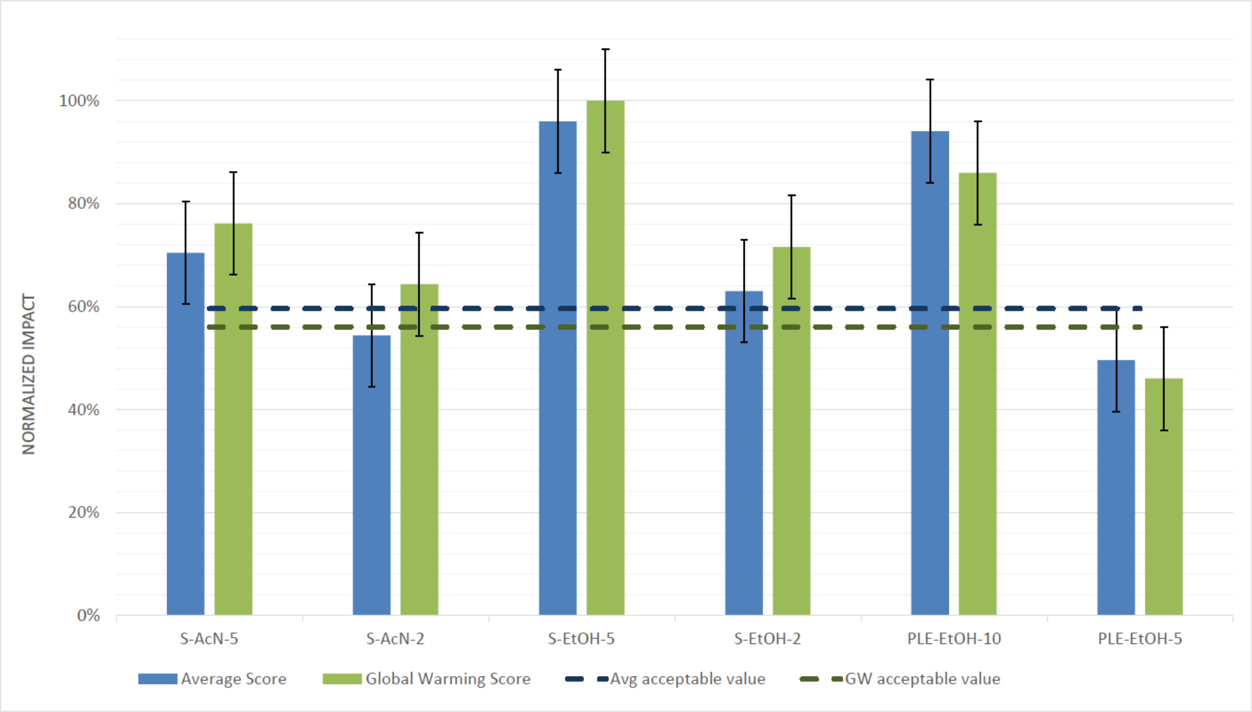

Figure 5 Single score impact results from the full LCA. Single scores are derived by internally normalizing results to the worst performing scenario and averaging all impact categories into a single score (blue bar). While for GWP, internally normalized results for each scenario are shown (green bar). An arbitrary uncertainty value of ±10% is depicted for each single score by the dashed lines, to show distance to the best solution. Error bars also show ±10% uncertainty level.

Results from the TEA align well with the LCA, which points out that, at least in this case, the same parameters that are "expensive" for the environment, are also costly for the investment.

4. Discussion

The preliminary LCA assessment performed on the lab scale emerging technologies can be used in the early design phase, in order to avoid excessive environmental burden later on. By identifying hot spots early on, it is possible to envision adjustments to the production set up, so that the identified hot spots are addressed. In this case, the environmental hot spots coincide well with economic costs, as is shown by the successive TEA-LCA. For both of these assessments, one of the most important parameters was solvent to wine pomace dry weight ratio. High use of solvent leads to high operational costs and increased demand for electricity and heat, which affect the results of both TEA and LCA. On the other hand, higher yields allow more leeway for higher energy consumption. This is observed in the results for PLE-EtOH-5, which has a very high electricity demand, due to the compressed system, but at the same time produces one of the highest yields out of the assessed scenarios. The high yield translates into reductions in the energy demand when looking at the results on a per kilo of product basis.

Results for the TEA showed that increasing the number of extraction steps has consequences for vessel volumes, which can be kept smaller if there is a higher number of extraction steps. In turn, this results in lower fixed capital costs for the extraction. On the other hand, to keep solvent ratios low, it is necessary to add a drying step before mixing the wine pomace, which contains water in itself. The extra drying incurs extra costs for heating, while at the same time saving some costs for material expenditure. These results are mirrored in the LCA, where results benefit from lower solvent use, while impacts are increased due to the extra heating needed. In this regard though, it was clear in the LCA that solvent use, especially if the solvent is acetone, comes with higher impacts than electricity or heat use. This is easily illustrated when looking at the GWP impacts of 1 kg of acetone compared to 1 kg of ethanol or 1 kWh of electricity, as shown in Figure 6, but also when looking at other impact categories (not shown here). From the figure it is possible to visualize that, in terms of the overall LCA assessment, added acetone or ethanol weigh more than added heat or electricity, with acetone being two times more burdensome than ethanol.

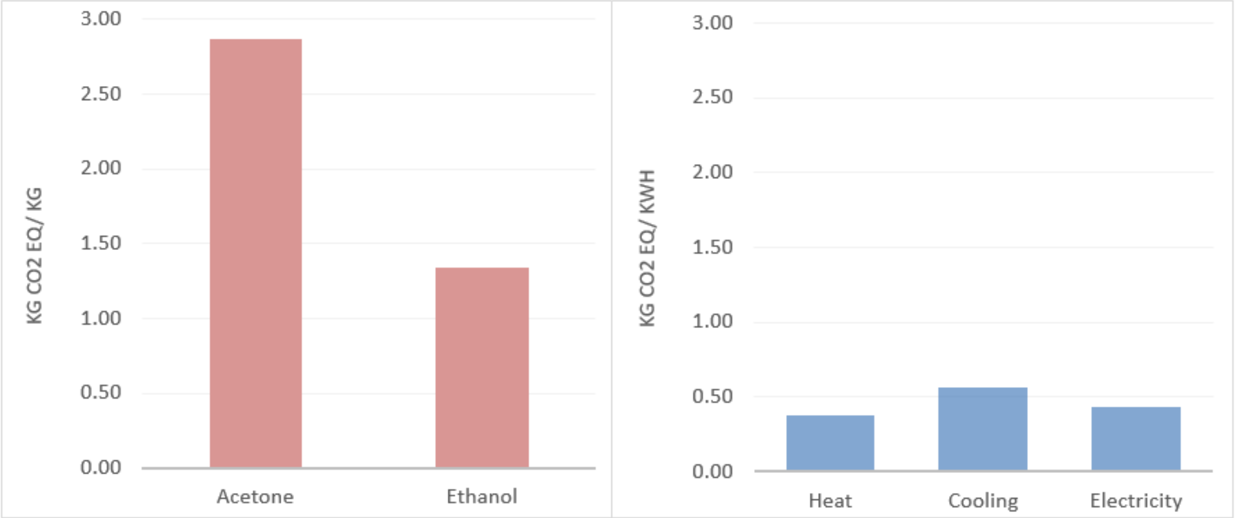

Figure 6 Global warming potential of 1 kg of acetone or ethanol. GWP of 1kWh of cooling, Italian electricity or heating. For illustrative purposes.

In this regard, it is also worth mentioning that the ethanol used for this assessment is of petrochemical origin. However, since the waste being treated is wine pomace, it is quite possible that a biorefinery treating this waste would also produce bioethanol. This is true for distilleries placed in Italy and France, which currently treat wine pomace in order to produce ethanol, bioenergy and food additives, among others.

Furthermore, the TEA in this study considers the processing costs including the financing costs. The market price of the product, the extracted polyphenols, and the market volume are yet to be explored. Once a market price or price range is known, then fixed capital costs and processing costs can be compared to the benefits, and profitability indicators, such as net present value (NPV) and internal rate of return (IRR), can be taken into consideration. A larger investment for more complex technology (PLE instead of solvent extraction) might be justified if the benefits are significantly lager.

Besides the economic (TEA) and environmental (LCA) aspects investigated, it is also useful to consider the technology readiness level (TRL) of the evaluated processes in the future. Solvent extraction, with both acetone and ethanol, is a mature process technology, which is currently implemented at large scale. PLE is a less mature technology for which extra measures might be required for large scale implementation.

5. Conclusion

Polyphenol extraction methods developed in the NoAW H2020 project were assessed using LCA at different maturity levels and with TEA-LCA at industrial scale. The lab scale results highlight the need to reduce solvent use and maximize yields. The best option selected through the TEA-LCA is pressurized liquid extraction, using CO2:EtOH:H2O as solvent with a solvent to DW ratio of 5, and 2 extraction steps (PLE-EtOH-5). If the same yields as in lab scale can be attained at industrial scale, then this option leads to the highest environmental and economic benefits, despite higher CAPEX. The most important parameter for optimization indicated by the LCA results is reducing solvent amounts. The most important parameters indicated by the TEA are the polyphenol extraction yield and the solvent to DW ratio. The LCA at lab scale was useful in pointing out potential environmental hotspots, which served to guide the TEA in order to design a better performing process from both an environmental and economic perspective.

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