Technoeconomic and environmental assessment of alternative biorefineries for bioenergy and polyphenolic production from pomace biomass

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Abstract

Pomace is generated during fruit processing and is regarded as a highly polluting waste stream due to its high moisture content, biological instability and acidic properties. To facilitate pomace management, this study has applied the biorefinery concept to develop systems that facilitate value extraction. To this regard, alternative scenarios for the production of polyphenolic compounds and bioenergy from apple pomace were investigated using ASPEN Plus for process modelling, simulation and analysis. Systems facilitating the production of polyphenols via the use of the green solvents (i.e. subcritical water in scenario (a) and ethanol-water in scenario (b)), while also co-producing bioenergy, were compared to a system that produced only bioenergy (i.e. scenario (c)). Comparisons of profitabilities and environmental performances were achieved via considerations of the net present values (NPVs) and potential environmental impacts (PEIs) of all scenarios. The study was able to show that scenario (a) constituted the only economically viable strategy, with a NPV of US$19.86 million, while scenarios (b) and (c) were determined to have NPVs of US$-88.12 million and US$-4.05 million respectively. Scenario (b) was also determined to have the poorest environmental performance with a PEI of 148 kPEI/h. Notably, although scenario (c) (PEI of 0.21 kPEI/h) was determined to present a better environmental performance than scenario (a) (PEI of 47 kPEI/h), its economic infeasibility indicated that it will be impractical to consider it as a viable pomace valorization strategy in a scaled-up system. This study therefore proposed that scenario (a) may constitute a preferred pomace valorization strategy provided technological innovations, i.e. use of alternative energy sources and gas filters, are explored to reduce its major existing challenge of global warming potential due to greenhouse gas emissions. This study therefore provides critica information regarding the sustainability implication of executing different biorefinery scenarios for pomace management in the fruit processing industry.

Keywords: waste valorization; apple pomace; anaerobic digestion; subcritical water extraction; solvent extraction.

1 Introduction

The fruit processing industry is responsible for the generation of pomace (i.e. waste) that must be managed in an environmentally sustainable and cost-effective manner [1]. This pomace, which is the residual ‘press cake’ that is generated after fruit juicing operations are undertaken, is characterized by its high moisture content, biological instability and low pH that ranges from ∼3 to 5 [2,3]. These properties hinder pomace’s functionality as an animal feed [2], and reduces the scope of viable management strategies that can be employed. To this regard, previous studies explored the potential of employing apple pomace as a resource for bioenergy and organic fertilizer production [4,5]. Notably, although biomass is largely employed in the production of carbon neutral fuels, biomass such as pomace may also be employed as a sustainable source of value-added products such as polyphenolic compounds [5,6]. Indeed, the potential of employing green extraction techniques for the recovery of high value bioactive compounds such as p-coumaric, chlorogenic etc. from apple pomace waste in accordance of the circular economy, was previously explored in the literature [4]. Similarly, other studies in the literatures have investigated the potential of recovering functional ingredients such as carbohydrates, pentacyclic triterpenes etc. from pomace[5,7]. For instance, in the study undertaken by Hobbi et al. [7], fruit apple pomace (AP) was investigated as a source of polyphenolic compounds (PPCs) with the authors suggesting that the abundance (i.e.~ 4 million tons generated/y globally [4]) of AP may facilitate sustainable production of PPCs in scaled-up systems. In the study by Hobbi et al. [7], the production of PPCs from apple pomace via of green extraction (i.e. using water and ethanol solvents) strategies was investigated. These strategies were hypothesized to facilitate the management of AP, without compromising favorable economic and environmental outcomes, in scaled-up systems. It is now crucial to assess the validity of the hypothesis via the evaluation of the technical, economic and environmental performances of PPC production from apple pomace in large-scale biorefineries. Furthermore, although the use of green solvents of ethanol/water and subcritical water extraction (SWE) led to vastly different PPC yields of 9.19 mg/ g of dry pomace ash [7] and 39.09 mg/ g of dry pomace [8] respectively, concerns were raised regarding the risk of an increased energetic penalty arising from the application of the energy intensive SWE process. This concern is worthy of further investigation and will therefore be explored. Additionally, the circular economy paradigm will be facilitated by ensuring that all non-PPC components in the AP are utilized as sources of bioenergy via the integration of the anaerobic digestion (AD) technology and co-generation systems. This is because of the reported potential of employing AD to produce biomethane m^3/kg-volatile solids) from AP [9,10]. The biomethane could be employed as a cheap fuel for electricity production [9,10].

This study therefore aimed to undertake comparative evaluations of three alternative AP valorisation scenarios; (a) a phase II biorefinery that employs the AP in the production of PPC using subcritical water extraction technology and bioenergy; (b) a phase II biorefinery that employs AP in the production of PPC using ethanol-water mixture as the green solvent and bioenergy, and (c) a phase I biorefinery that employs the AP in sole production of bioenergy. In all scenarios, the biofuel from the integrated AD process was used in electricity production using simple conceptual co-generation systems. Thus, electricity constituted a product in all scenarios. Technical assessments were undertaken using ASPEN plus as the preferred process simulation tool, with economic performance and environmental performance assessed using the net present value (NPV) and the potential environmental impact (PEI) metrics, respectively. It is important to recognize that some studies in the area have previously been undertaken. For instance, in the study by Todd, Baroutian [11], PPC extractions from grape pomace using subcritical water, ethanol-solvent and supercritical CO_2 technologies were investigated. The study showed the supercritical CO_2 extraction and ethanol-solvent strategies constituted the worse performing and the best performing technologies, respectively. Similarly, Uyttebroek et al. [12] investigated the economics of PPC recovery from AP using the ethanol-water mixture and determined that the process was not economically viable. Best et al. [13] also assessed the perfomances of ethanol-water and supercritical CO_2 enabled extractions of PPCs from *Mauritia flexuosa*. In the study, Best et al. [13] was able to show that the use of the PPC extraction technologies presented the best economic performance when both highlighted technologies were combined. Crucially, a further review of the literature shows that no study has explored the technoeconomic and environmental performance of apple pomace valorisation using the scenarios highlighted in this study. For emphasis the originality of the present investistigation is elaborated in Table 1. This study also acknowlegdes that the use of technoeconomic, energy, and environmental analyses as a basis for the assessments of alternative pomace valorisation strategies, although being powerful tools, do not constitute perfect solutions to sustainability concerns [14]. Indeed, the functionality of the approaches employed will depend on process complexity, the level of precision and study objectives [14]. Crucially, given the objectives of the study, system complexity and precison requirements, the integrated use of the metrics of NPV and PEI are considered sufficient for this preliminary comparative study.

Table 1: The novelty of the present study compared to other major studies in the literature

PPC production	Apple pomace	Bioenergy production	SWE technology	Ethanol-solvent technology	Economic performance	Environmental performance	References
✓	✗	✗	✓	✓	✓	✓	[11]
✓	✓	✗	✗	✓	✓	✗	[12]
✓	✗	✗	✗	✓	✓	✗	[13]
✓	✗	✗	✓	✗	✓	✓	[15]
✓	**✓**	**✓**	**✓**	**✓**	**✓**	**✓**	**This study**

✓: Included, ✗: Not Included, PPC: polyphenolic compounds, SWE: subcritical water extraction

2 Materials and methods

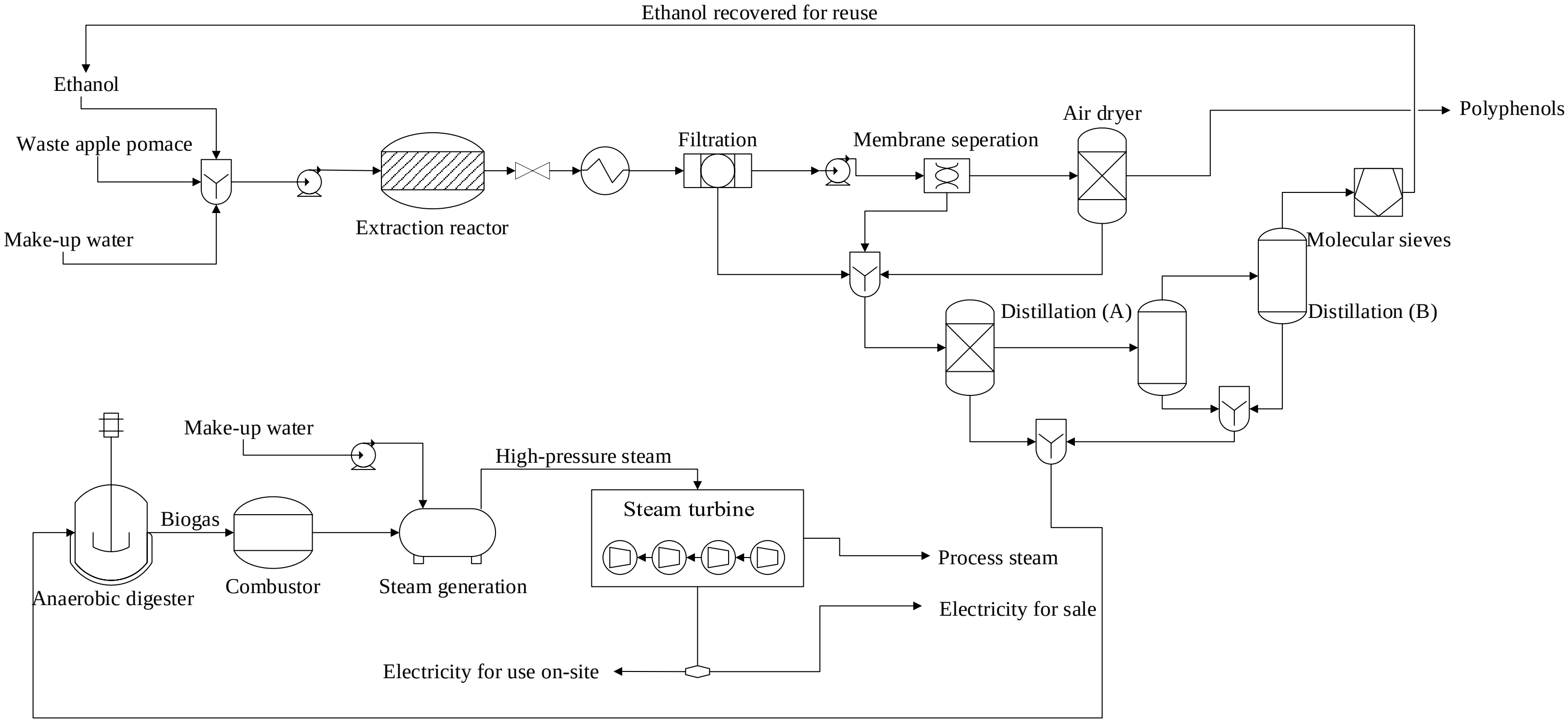
The alternative scenarios were modelled using ASPEN Plus® v 11 software for the three specified configurations (Figure 1); (a) The production of PPCs and electricity from AP using subcritical water used as the green solvent; (b) The production of PPCs and electricity from AP using ethanol-water mixture as the green extracting solvent, and (c) The production of only electricity from AP. The AP was modelled based on its composition in the literature. The AP was modelled as being composed of 71.9 wt.% carbohydrates, 5.94 wt.% protein, 1.3 wt.% lipid, 1.3 wt.% ash [7], 3.9 wt.% polyphenols [8] with the residual fraction assumed to be lignin, on the dry basis. The AP was also modelled as containing 67.3 wt. % moisture[7]. The carbohydrate present in the AP was modelled as starch, since starch constitutes the main reserve of polysaccharides in fruits [16,17]. Protein was modelled as L-phenylalanine, since it is an essential amino acid present in food materials and constitutes a vital component of proteins in living organisms [16,18]. Lipid was modelled as triolein. Polyphenolic compounds were modelled as gallic acid since it constitutes a major polyphenol compound present in apples [19]. Furthermore, gallic acid is widely used as a reference standard when the total polyphenolic content of biomass is quantified [7]. The components of lignin and ash were modelled using properties in the literature [20] and the Non-Random Two Liquid (NRTL) was specified as the preferred thermodynamic property model for phase equilibria calculations. The NRTL model was employed due to its sufficiency in undertaking calculations in complex multi-component systems, containing multiple polar and nonpolar components [21]. In addition to ASPEN Plus, other software systems employed in this study include Microsoft Excel®, Visio®, and the EPA Waste Reduction (WAR) Algorithm.

2.1 Process description and model development.

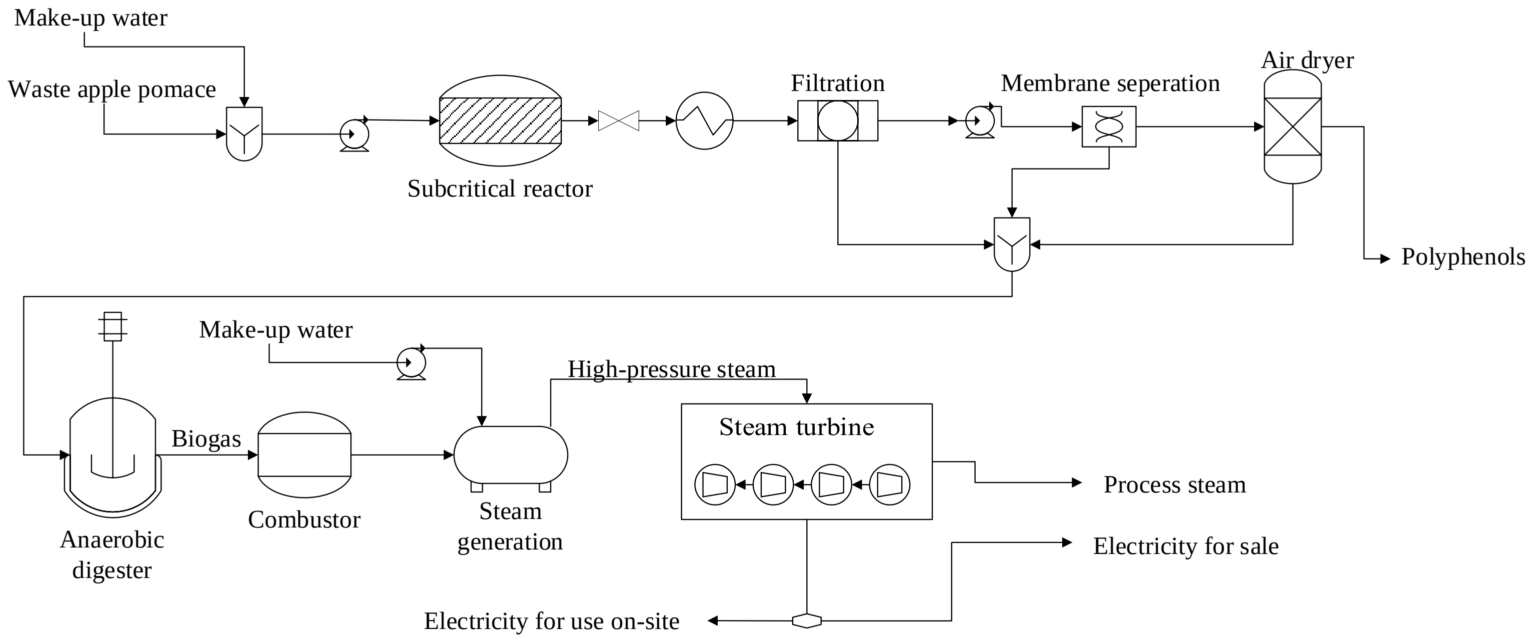
Figure 1 highlights the three competing scenarios investigated. Figure 1 (a) shows that PPC and electricity is produced via the integration of subcritical water extraction (SWE), an AD process and a simplified combined heat and power (CHP) system. In Figure 1 (a), the AP is initially homogenized at a pressure and a temperature condition of 1 atm and 25 °C, respectively, with make-up water introduced to achieve a solid-solvent ratio of 1 g/100 mL as specified in our work [8]. An electricity input of 1.5 kWh per ton for homogenizing the AP slurry was introduced in the model and executed using calculator blocks containing relevant FORTRAN commands. In Figure 1 (a), the well-mixed AP slurry is then transferred to the SWE reactor, which is modelled as an RSTOIC reactor operating at 203.7 ^{o}C [8]. The pressure was specified as being autogenously generated and assumed to reach 16.55 atm in accordance with Antoine equation [22]. It is assumed that in addition to PPC extraction, hydrolysis reactions involving starch, (97 % conversion), and lipid (% fatty acid yield of 72%) to produce glucose, and fatty acids respectively, also occur [17,23]. The proteins are assumed to exist as monomers of L-Phenylalanine, for simplicity.

At the conclusion of the SWE of PPCs from the AP, the exit stream is de-pressurized to 1 atm, using a valve and subsequently cooled to 25 ^{o}C using a cooler. The cooled stream from the subcritical reactor is then subjected to a filtration operation to facilitate the removal of insoluble solids after which the filtrate is fed to a nanofiltration (DURACID membrane) unit to facilitate the separation of the PPCs [24]. The recovered PPCs are then subjected to air dying at 30 ^{o}C with the dried polyphenols recovered. Figure 1 (a) also shows that non-PPC components in the AP (i.e. hydrolysates of carbohydrates, lipids, etc.) are recovered and mixed prior to being transferred to a reactor for anaerobic digestion at 1 atm and the mesophilic temperature of 37 °C. The anaerobic digester is modelled using an RSTOIC reactor with the degradation reaction assumed to occur in accordance with Boyle's equation [25] as shown in Table S1 in the supplementary file. Figure 1 (a) shows that the resulting biogas is employed as a combustion fuel for heat generation in the boiler to facilitate steam generation in the CHP system.

To facilitate high-pressure steam generation, water at 25 ^{o}C and 1 atm is initially pressurised to 20 atm, then heated using heat generated from the combustion of biogas. Additional heat recovered from the cooling of the subcritical reactor exit stream (i.e. from 203.7 ^{o}C to 25 ^{o}C) is also introduced to further enhance the heating utility available to generate the high pressure steam (HPS). The produced HPS at 20 atm and 213 ^{o}C is then used in electricity generation via its expansion to 1 atm in an isentropic turbine. The mass of water required to achieve the target temperature of the HPS was calculated based on fundamental knowledge of energy balance and incorporates latent (phase change) heat and specific heat components. Generated energy balance equations were introduced in the model using FORTRAN codes in calculator blocks. Similarly, in Figure 1 (b), the AP is initially homogenized as discussed above with ethanol introduced such that the ethanol-water v/v ratio of 50-50 and the solid-solvent ratio of 1 g/80 mL, are maintained [26].

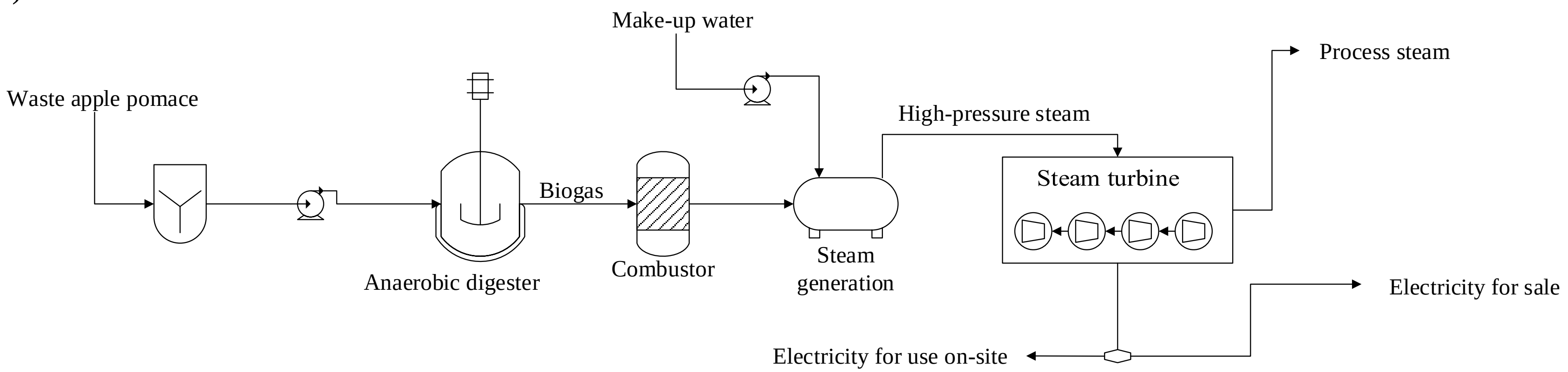

Ethanol recovered for reuse
Ethanol
Waste apple pomace
Make-up water
Extraction reactor
Filtration
Membrane seperation
Air dryer
Polyphenols
Molecular sieves
Distillation (A)
Distillation (B)
Make-up water
High-pressure steam
Steam turbine
Biogas
Anaerobic digester
Combustor
Steam generation
Process steam
Electricity for sale
Electricity for use on-site

(a)



Make-up water
Waste apple pomace
Subcritical reactor
Filtration
Membrane seperation
Air dryer
Polyphenols
Make-up water
High-pressure steam
Steam turbine
Biogas
Anaerobic digester
Combustor
Steam generation
Process steam
Electricity for sale
Electricity for use on-site

(b)



Make-up water
Process steam
Waste apple pomace
High-pressure steam
Steam turbine
Biogas
Anaerobic digester
Combustor
Steam generation
Electricity for sale
Electricity for use on-site

(c)

Figure 1 : Alternative waste apple pomace valorisation pathways. Scenario (a): biorefinery that employs the AP in the production of PPC and biofuel with subcritical water used as the green solvent; Scenario (b): biorefinery that employs AP in the production of PPC and biofuel, with an ethanol-water mixture used as the green solvent ; Scenario (c): biorefinery that employs the AP in production of biofuel only. PPC denotes polyphenolic compounds

The well-mixed AP slurry is then transferred to a reactor modelled as an RSTOIC reactor operating at 60 ^{o}C and 1 atm to facilitate PPC extraction. It is assumed that the hydrolysis of starch, lipids and proteins, to produce their associated monomers, do not occur since the reaction conditions are considered too mild to facilitate hydrolysis transformations [27,28]. The exit stream from the reactor is then cooled to 25 ^{o}C using a heat exchanger model and the PPC stream subsequently recovered via stepwise filtration, nanofiltration and air drying operations as discussed earlier above.

The stream composed of the aqueous (ethanol-water) and solid fractions is filtered to facilitate the recovery of the filtrate with the solids subsequently transferred to AD reactor for biogas production. The filtrate is then transferred to a distillation column to strip the ethanol from the ethanol-water mixture. The study initially employed the Fenske–Underwood–Gilliland (FUG) method in ASPEN Plus to provide initial estimates of the design variables for all the columns (i.e. theoretical number of stages, reflux ratio, etc) prior to undertaking rigorous distillation simulation calculations. A further separation operation, to increase ethanol concentration is facilitated using a rectification column, to produce a distillate stream containing mainly (>90 wt. %) ethanol. To enable the production of anhydrous ethanol, further water removal is achieved using molecular sieves. The bottom streams from both columns, are transferred to the anaerobic digester for biogas production with the biogas subsequently employed as a cheap biofuel for electricity generation as discussed earlier above.

Figure 1 (c) shows that AP is employed solely for electricity production. As described earlier above, the AP is initially homogenized prior to being fed to the AD reactor for biogas production. The biogas produced is then employed as a fuel for electricity generation using a CHP system. In all scenarios, the heating and the cooling utilities were further assessed using the ASPEN Energy Analyzer, with heat integration via pinch analysis undertaken such that an assumed minimum allowable temperature difference of 10 °C, between the 'hot' and 'cold' streams at 'pinch point', was imposed [29]. The heating requirements were assumed to be satisfied using HPS at 230 ^{o}C and 20 bar and cooling requirements were satisfied using cooling water with a coefficient of performance of 12 [29].

2.2 Economic performance assessment and sensitivity analysis

The net present value (NPV) metric was selected as the preferred economic metric such that a project is considered profitable when the NPV is greater than zero. The NPVs, in MUS$ (i.e. M denotes million), for the different scenarios were determined using discounted cash flow tables that were developed in accordance to Equations (1) and (2) [30];

$$\mathrm{NPV} = \sum_{1}^{n} DF \times A - \mathrm{TCI} \tag{1}$$

$$DF = \frac{1}{(1+i)^n} \tag{2}$$

where the net cash flows arising from polyphenol and electricity sale, total capital investment and life span of the project are denoted by *A* in MUS$, TCI in MUS$ and *n* in y, respectively. *DF* denotes the discount factor.

The total capital investment (TCI), was determined using established costing correlations and assumptions in Tables S2 and S3 in the supplementary file and is based on equipment purchase costs determined. These correlations are well-known an employed in other studies [21,30]. The purchase costs of common equipment (i.e. pumps, columns, separators etc) were obtained using the ASPEN economic analyzer V11. Notably, these costs were based on 2016 data, highlighting the need to introduce correction methodologies to account for time-dependent, inflationary effects on money. The Chemical Engineering Plant Cost Index (CEPCI) was therefore employed as shown in Equation (3);

$$p_{\mathrm{i},_{2021}} = p_{\mathrm{i},_{\mathrm{ref}}} \left(\frac{\mathrm{CEPCI}_{2021}}{\mathrm{CEPCI}_{\mathrm{ref}}} \right) \tag{3}$$

where the *i*th equipment purchase costs in the year 2021 and the reference year are denoted by $p_{i,2021}$ and $p_{i,ref}$. The CEPCI_{2021} was specified as 776.9 (https://www.chemengonline.com), with $\mathrm{CEPCI}_{\mathrm{ref}}$ specified for the reference year (https://www.chemengonline.com). The CEPCI for 2021 was employed since at the time of drafting this manuscript the CEPCI for 2022 was not yet available.

The equipment cost of the specialized stainless steel subcritical reactor was obtained as a quote from the manufacturer as US$1445 for a 250 mL reactor (IEUZON,China, quoted price). Due to differences in processing capacity, the purchase cost of the scaled-up subcritical reactor was adjusted using Equation (4) as follows;

$$p_{i,Q} = p_{i,Q_{ref}} \left(\frac{Q}{Q_{ref}} \right)^f \tag{4}$$

where $p_{i,Q}$ is the purchase cost of the subcritical reactor in US$ for the desired capacity (or characteristic factor) and $p_{i,Qref}$ denotes the purchase cost of the subcritical reactor in US$ for the reference capacity. Q_{ref}, Q and f denote the reference capacity and the desired capacity respectively with the scaling factor specified as 0.65 [31,32]

Total operating cost (TOC) is determined based on the total variable costs and total fixed costs [33]. The total variable cost refers to costs that are directly dependent on plant capacity such as the cost of consumables, while the total fixed cost refers to costs that are not directly dependent on processing capacity such as labor cost [33]. The economic data input employed in calculating the TOC are summarized in Tables S4 and S5 of the supplementary file. The correlations used are well-known an employed in other studies [21,30]. Recognizing that the economic calculations discussed above incorporate several underlying assumptions, it is crucial to assess the impact of variations in the underlying assumptions on the profitabilities (i.e. NPVs) of the competing scenarios using sensitivity analysis. The sensitivity of the generated NPVs to -50% to +50% variations in the important parameters of TCI, TOP, electricity cost, discount rate, plant life span, processing capacity and cost of polyphenol (i.e. gallic acid) was therefore assessed for the different scenarios. The sensitivity analysis was undertaken by assessing the impact of each parameter, independently, while keeping the other parameters constant. Tornado plots were subsequently constructed relative to the baseline scenarios.

2.3 Environmental performance

The environmental performances of the alternative scenarios were investigated using the waste reduction (WAR) algorithm [34]. This algorithm employs conceptual potential environmental impact (PEI) balances and is based on mass and energy balance data generated from the simulation study. The mass and energy balance results are combined with conventional toxicity data associated with the inlet and exit streams of chemical processes [34]. The WAR algorithm is established to be functional and sufficient in assessing processes at the conceptual, design and/or retrofitting stages [34]. Furthermore, the WAR algorithm is reported as being sufficient when comparing different chemical processing facilities and is characterized by its vast implementation opportunities [35]. In the simplest terms, the WAR seeks to determine the PEI balance by considering the PEI of the inlet (mass and energy) streams and outlet (mass and energy) streams, defined using Equations (5) and (6) respectively as follows [34];

$$\dot{I}_v^{cp} = \sum_i^{cp} \dot{I}_i^{v} = \sum_i^{cp} \dot{M}_i^{v} \sum_k x_i \phi_k \quad (5)$$

$$\dot{I}_v^{ep} = \sum_i^{ep-g} \dot{M}_i^{v} \sum_k x_{ki} \phi_k \quad (6)$$

where $\dot{I}_v^{cp}$, $\dot{I}_v^{ep}$, $\dot{M}_i^v$ and x_{ki} denote the rates of PEI out or in from chemical transformations, PEI out or in from energy production, mass flow (kg/h) from or into the *i*th process and mass fraction of component *k* in the exit or inlet stream *i* . The potential environmental impact due to component *k* in streams is denoted by $ø_k$ such that the PEI generated within the chemical process is determined as the difference between the PEI out and PEI in of the system. An extensive discussion of the WAR algorithm is beyond the scope of this study and is available in the literature [34,36]. To determine the value of $ø_k$, the summation of the separate PEIs from the disposal of component *k* responsible for the impacts of *l* is undertaken with the categories of impacts *l* summarized in Table 3.

Table 2: Category of impact [36]

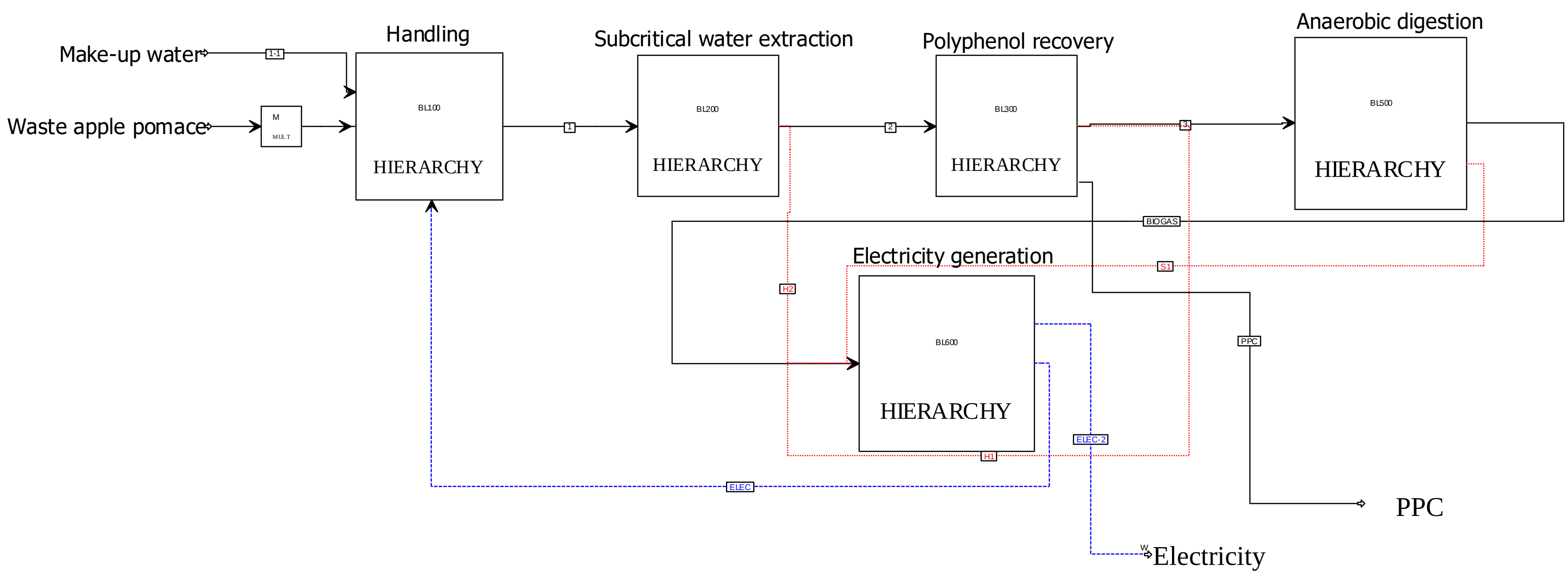
Category of impact	Measure of Impact Category
Ingestion (HTPI)	LD50
Inhalation/dermal (HTPE)	OSHA PEL
Aquatic toxicity (ATP)	Fathead Minnow LC50
Terrestrial toxicity (TTP)	LD50
Global warming potential (GWP)	GWP
Ozone depletion potential (ODP)	ODP
Acidification Potential (AP)	AP
Photochemical oxidation potential (PCOP)	PCOP

For simplicity, in all scenarios, the current study has assumed that the AP is freely available, with supply chain concerns and environmental impacts associated with AP collection not considered. Such supply chain assessments/considerations may constitute the basis of future work and will focus on only the preferred AP valorization strategy.

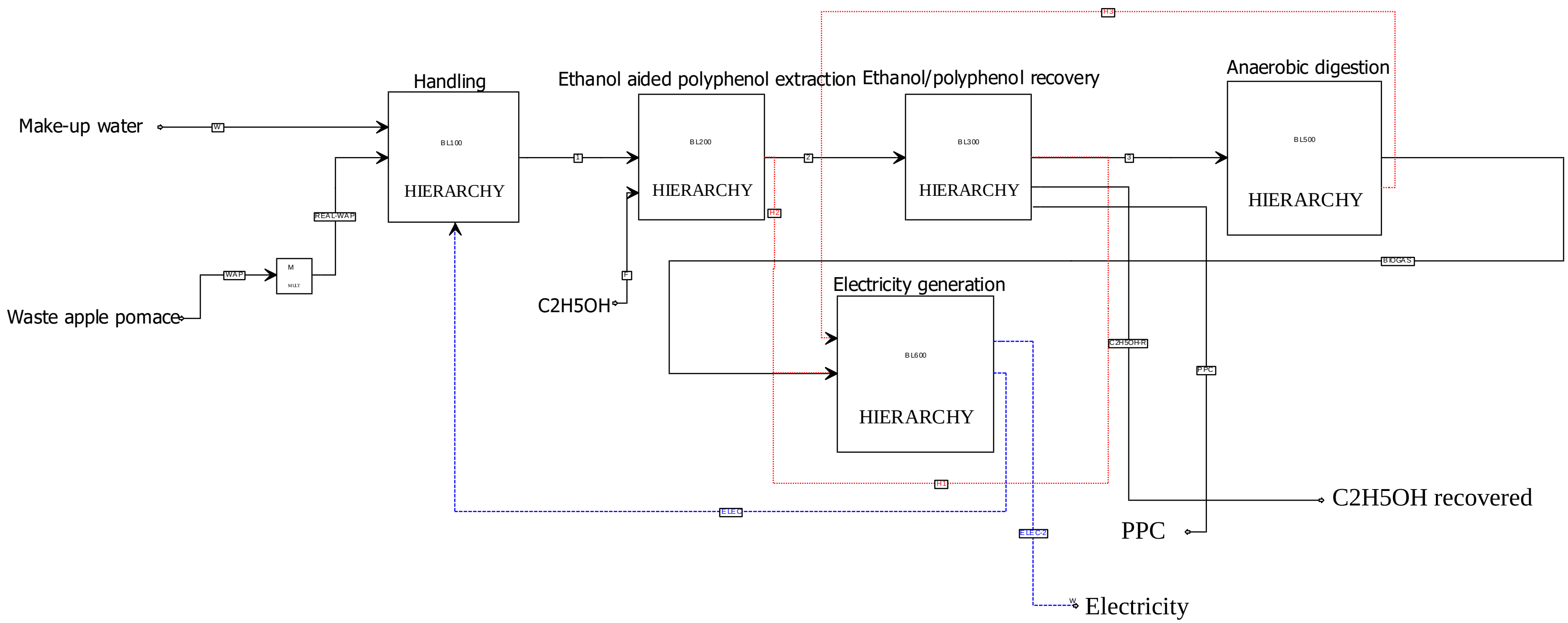
3 Results and discussion

3.1 Process simulation results

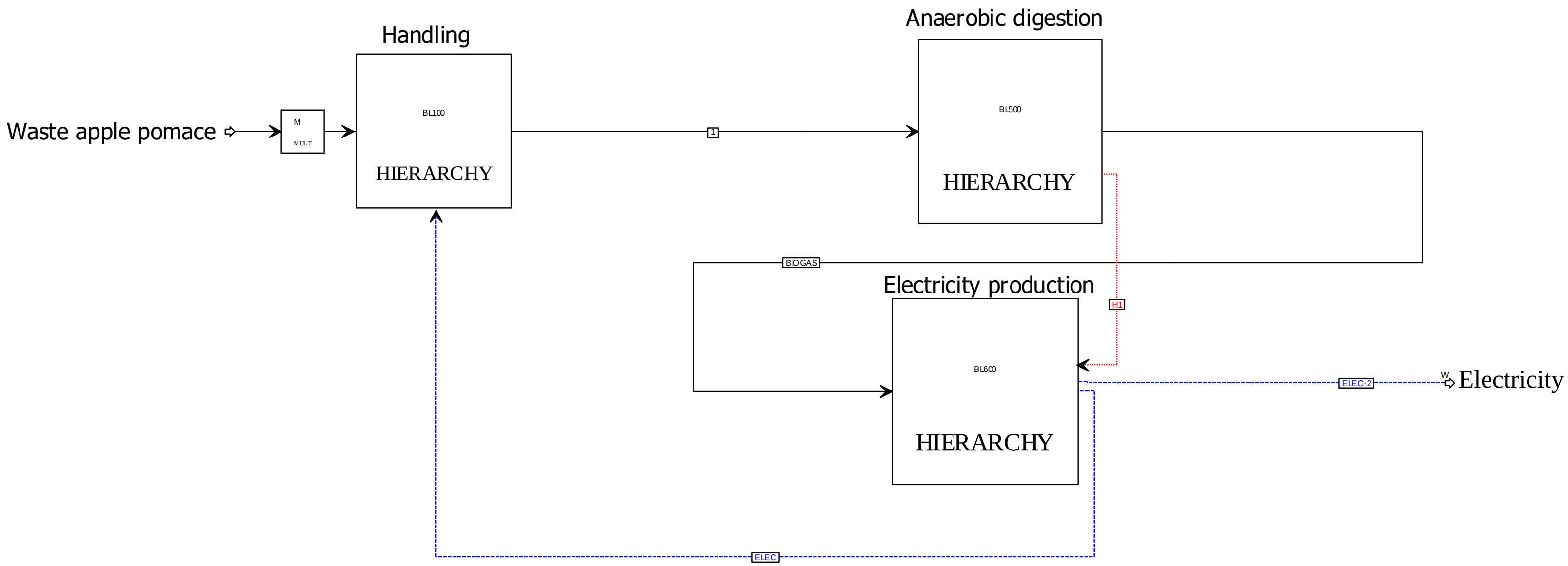
In the study, 5000 kg/h of AP (wet basis) has been assumed in all scenarios with the simplified ASPEN simulation output presented in Figure 2. Figure 2 highlights that in scenarios (a) and (b), PPCs and electricity constitute the major products, with scenario (b) showing that ethanol employed in PPC extraction is also recovered. In scenario (c) however, only electricity is produced. The major assessment results are summarized in Table 3. Table 3 shows that the PPC yields for scenario (a) and scenario (b) of 38.20 g/kg dry AP and 8.27 g/kg dry AP are comparable to the experimentally determined yields of 39.09 g/kg dry AP and 9.19 g/kg dry AP respectively. Furthermore the biomethane yields were observed to range from 0.257- 0.271 m^3/kg dry AP, with the yields varying as follows; scenario (c) > scenario (b) > scenario (a). In addition to the biomethane yield being within the range reported in the literature (i.e. 0.22- 0.89 m^3/kg-volatile solids) [10,37], the trend of the biomethane yields is also expected. This is because of the reduction in the mass of biodegradable macromolecules (i.e. scenario (a) <scenario (b) < scenario (c)) as more of the inherent PPCs are progressively recovered. These combined observations support the sufficiency of the modelling approach applied.


Make-up water
1-1
Waste apple pomace
M
MULT
Handling
BL100
HIERARCHY
1
Subcritical water extraction
BL200
HIERARCHY
2
Polyphenol recovery
BL300
HIERARCHY
3
Anaerobic digestion
BL500
HIERARCHY
BIOGAS
Electricity generation
S1
H2
BL600
HIERARCHY
PPC
ELEC-2
H1
ELEC
PPC
Electricity

(a)


Make-up water
Waste apple pomace
Handling
HIERARCHY
Ethanol aided polyphenol extraction
HIERARCHY
C2H5OH
Ethanol/polyphenol recovery
HIERARCHY
Anaerobic digestion
HIERARCHY
Electricity generation
HIERARCHY
C2H5OH recovered
PPC
Electricity

(b)



(c)

Figure 2 : ASPEN plus simulation output for the alternative waste apple pomace valorisation pathways. Scenario (a): biorefinery that employs the AP in the production of PPC and biofuel with subcritical water used as the green solvent; Scenario (b): biorefinery that employs AP in the production of PPC and biofuel, with an ethanol-water mixture used as the green solvent ; Scenario (c): biorefinery that employs the AP in production of biofuel only. Red, blue and black lines indicate heat, electricity and mass flows. PPC denotes the polyphenolic compounds

Table 3: Simulation results highlighting the major product and inlet streams for the scenarios considered

Stream name	Scenario (a)	Scenario (b)	Scenario (c)
Apple pomace (AP), dry basis (kg/h)	1635	1635	1635
Simulated solid (AP) to solvent ratio (kg/L)	0.010	0.0126	-
Experimental solid (AP) to solvent ratio (kg/L)	0.010	0.0125	-
Polyphenol yield simulated (kg/kg dry AP)	0.0382	0.008	-
Polyphenol yield experiment (kg/kg dry AP)	0.0391	0.009	-
Biomethane yield simulated (m^3/kg dry AP)	0.257	0.269	0.271
Electricity produced (MW)	3.38	2.18	0.85
Externally sourced heating requirement (MW)	49.62	155.52	0.09

Scenario (a): biorefinery that employs the AP in the production of PPC and electricity with subcritical water used as the green solvent; Scenario (b): biorefinery that employs AP in the production of PPC and electricity, with an ethanol-water mixture used as the green solvent, and ; Scenario (c): biorefinery that employs the AP in production of electricity only.

Table 3 also shows that the external heating requirement based on the ASPEN energy analyzer varies as follows; scenario (b) > scenario (a) > scenario (c). This observation is due to the inlet energy required to supply heat to the reboilers of the two distillation columns employed in ethanol recovery plus the heating duty of the extraction reactor, with their combined energy input, in scenario (b), estimated to exceed the net energy input requirement of the one-step SWE process in scenario (a). As expected, the low temperature mesophilic AD process was determined to require the lowest energy input when the three scenarios were considered. It is also observed that the net electricity generated ranged from 0.15 MW to 3.38 MW and varied as follows, scenario (a) > scenario (b) > scenario (c). This observation is anticipated since the electricity generated is also dependent on the heating utility available for the production of the HPS, after heat integration. Thus, scenarios characterized by a higher number of exit hot streams, when integrated, will be produce higher masses of HPS, for enhanced electricity generation. Additionally, since the yields of biomethane in the scenarios are not substantially different (i.e difference maximum ~5 %), similar heating duties were calculated from the combustion of the biomethane for HPS generation.

3.2 Economic performance

Employing the methods discussed in section 2.2. above, the costing components for the three scenarios are presented in Table 4 and the economic performance summarized in Figure 3.

Table 4: The major cost components for the three scenarios considered

Cost components	Scenario (a)	Scenario (b)	Scenario (c)
Total equipment purchase cost (MUS$)	8.054	13.106	0.129
Total equipment installation cost (MUS$)	13.787	29.662	0.239

Warehouse cost (MUS$)	0.551	1.186	0.010
Home office and construction fee (MUS$)	3.240	6.971	0.056
Project contingency (MUS$)	1.620	3.485	0.028
Other costs (start-up, permits) (MUS$)	1.620	3.485	0.028
Fixed capital investment (MUS$)	25.920	55.765	0.449
Determined Lang factor	**3.22**	**4.26**	**3.47**
Working Capital	1.296	2.788	0.022
Total capital investment (MUS$)	**27.216**	**58.553**	**0.471**
Labor cost (MUS$)	1.062	1.062	0.708
Labor burden (MUS$)	0.956	0.956	0.637
Maintenance cost (MUS$)	0.242	0.393	0.004
Property insurance (MUS$)	0.181	0.390	0.031
Total variable cost (MUS$)	1.410	5.923	0.060
Fixed operating cost (MUS$)	2.441	2.801	1.380
Total operating cost (MUS$)	**3.850**	**8.724**	**1.440**

M denotes million

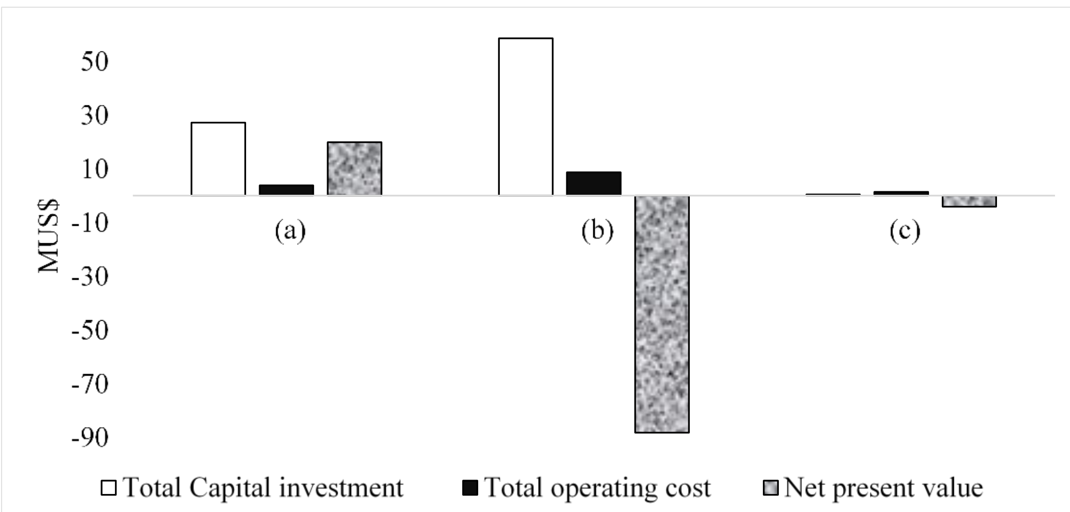


Figure 3 : Economic performance determinants for scenarios (a), (b) and (c). M denotes million

Table 4 and Figure 3 show that scenario (a) , scenario (b) and scenario (c) have TCIs of US$ 27.2 million, US$ 58.55 million and US$ 0.47 million respectively. This observation is consistent with previous studies since higher capital costs were determined for processes composed of more unit operations and higher complexities [30,38]. Table 4 also shows that the Lang factors based on the costing estimates ranged from 3.22 to 4.26. This range is consistent with literature predictions since the Lang factors of chemical processes typically ranges from 3 to 6 [39,40]. Furthermore, Figure 3 shows that scenario (a) constitutes the only profitable project with an NPV of US$19.86 million. This observation is due to the higher yield of polyphenols (i.e 0.0382 kg/kg dry AP) and additional electricity (i.e. 3.38 MW) generated in scenario (a) relative to other scenarios. Crucially, the economic performances (i.e. NPVs) of scenarios (b) and (c) calculated to be US$-88.12 million and US$-4.05 million, respectively, show that the biorefinery that employs ethanol for polyphenol recovery constitutes the least economically viable valorization strategy. Indeed, the study determined that it would be preferable to simply valorize the AP via a one-step AD process for bioenergy production rather than the execution of a polyphenol recovery process using ethanol.

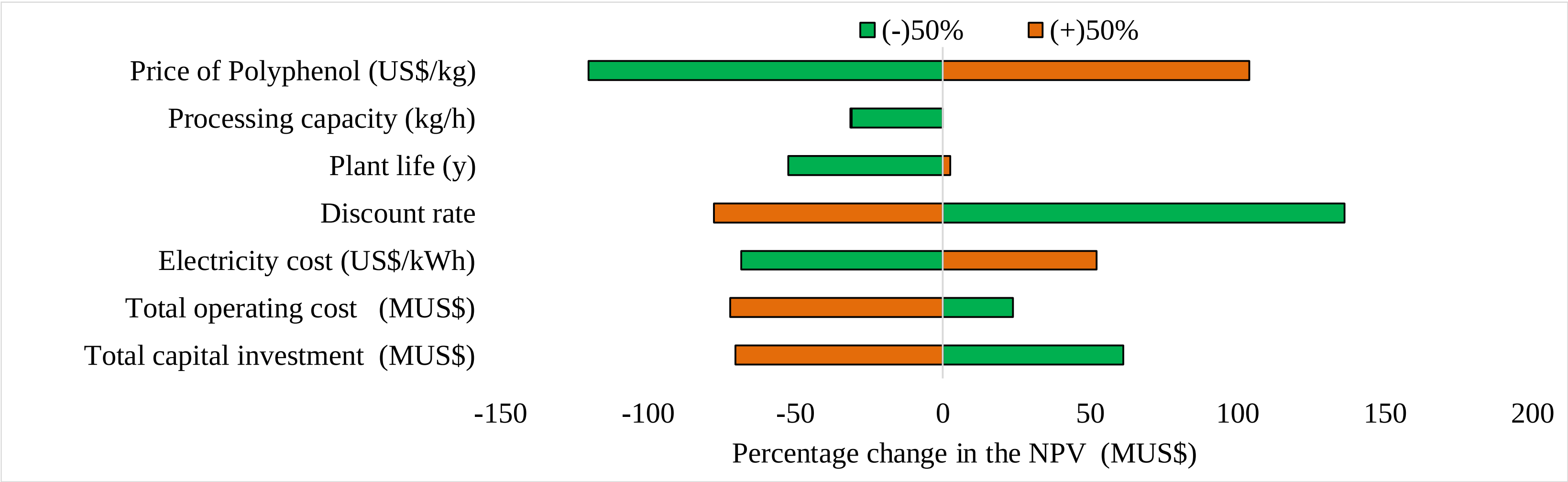
It is acknowledged that no studies in literature have comparatively explored the use of AP as a resource for PPC production using the comprehensive approaches presented in the study. However, to aid discussions, the economic performace results of other studies, exploring the production of valuable products such as PPCs, bioenergy etc are presented in Table 5. In considering the results presented in Table 5, it must be recognized that the economic performance results are largely dependent on the underlying assumptions, the feedstock type and the process design developed. Table 5 shows the studies by Todd, Baroutian [11] and Manhongo et al. [41], using the SWE for PPC production from grape and mango pomaces, respectively. In both cases, the SWE process was determined to be economically feasible with NPV values of US$ 6.76 million and US$ 311 million. These outcomes were similar to the result presented in this study since a positive NPV was also calculated. The higher NPV value from the study of SWE of PPCs from mango pomace [41] is due to the co-production of pectin as a high value co-product that was sold as a revenue source. On the other hand the lower NPV value from the study of SWE of PPCs from grape pomace [11] may be due to the absence of on-site electricity generation, which could have been sold as an additional revenue source. Similarly, the studies presented by Best et al. [13] and Uyttebroek et al. [12], reported that the ethanol (solvent) enabled PPC extraction did not present viable scale-up opportunities. These conclusions were consistent with the result presented in this study. A contrary result was however presented in the study by Todd, Baroutian [11]. In the study, the ethanol solvent enabled PPC extraction was determined to be economically feasible.

Table 5: Economic performance outcomes of the valorisation of different feedstocks for PPC and bioenergy production

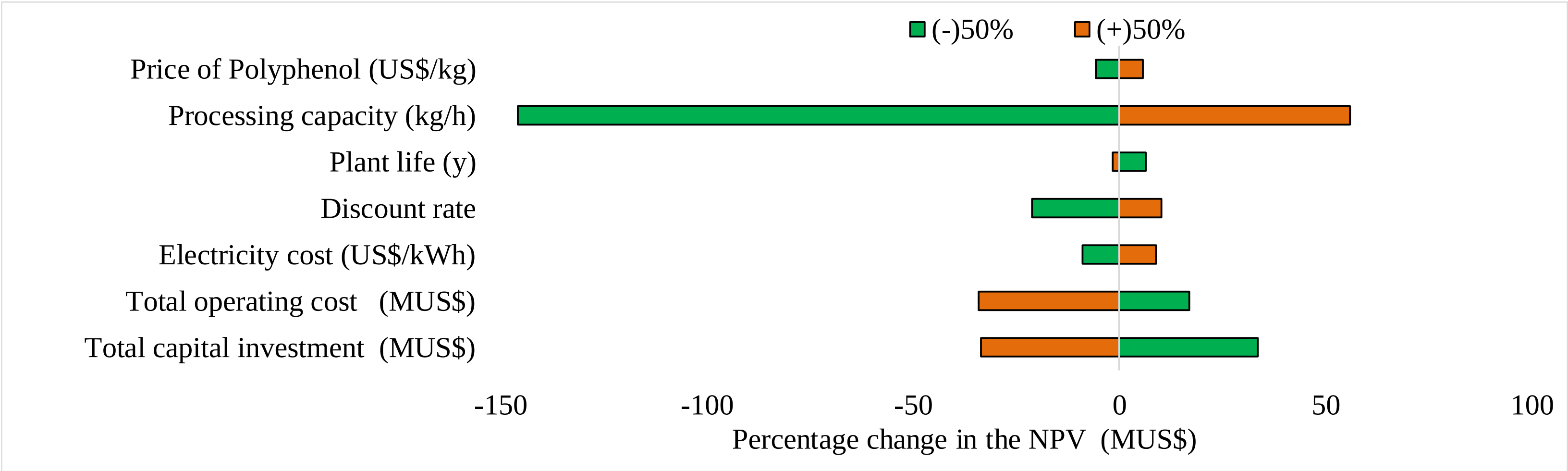
Valorisation technology	The present study using apple pomace as feedstock	The study using *Mauritia flexuosa* as feedstock	The study using grape pomace as feedstock	The study using apple pomace as feedstock	The study using mango pomace as feedstock
Ethanol solvent extraction	NPV is negative and project is infeasible (-US$ 88.12 million)[a]	NPV is negative and project is infeasible (not reported) [13]	NPV positive and technology feasible (US$ 16.60 million) [11]	NPV is negative and project is infeasible (-US$ 5.810 million) [12]	N/A
Subcritical-water extraction technology	NPV positive project feasible (US$ 19.86 million)[a]	N/A	NPV positive and technology feasible (US$ 6.76 million) [11]	N/A	NPV positive project feasible (US$ 311 million)[c][41]
Anaerobic digestion for bioenergy production	NPV is negative and project is infeasible (-4.05 M)[b]	N/A	N/A	N/A	N/A

[a]PPC and bioenergy produced, [b]bioenergy produced only, [c]pectic produced and sold, N/A: not available

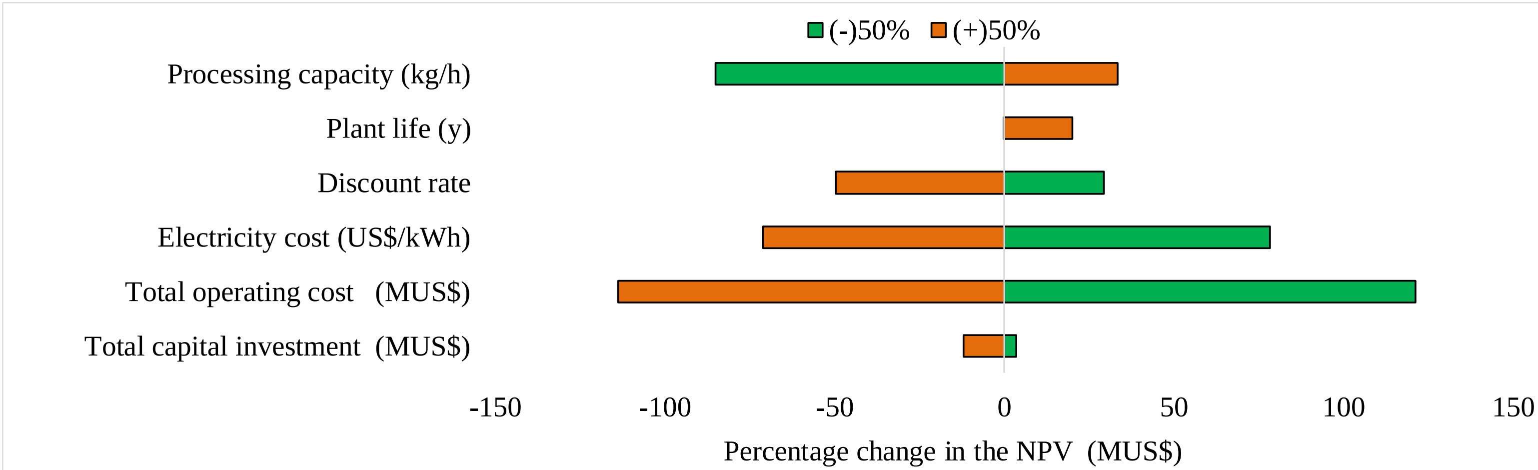
In the study by Todd, Baroutian [11], it was assumed that the ethanol and the SWE technologies had similar similar PPC extraction potentials. This assumption is however incorrect since the SWE technology typically facilitates improved PPC production compared to the ethanol solvent technology [42]. Furthermore, recognizing that plant costing was determined based on the inclusion of several underlying assumptions, it was determined that the assessment of the effects of major cost items on the plant's economic performance must be undertaken to assess the dependence of the plant profitability on variations in these major cost items. To this regard, sensitivity analysis was undertaken according to methods discussed earlier in section 2.2 above with results presented in Figure 4. Figure 4 shows that the scenario (a) constitutes a viable investment in most cases, except when the polyphenol price is reduced by 50 %. Figure 4 shows that a 50% reduction in the price of polyphenols (i.e. reduction from US$ 15 per kg to US$7 per kg) will lead to a 120.13 % reduction in the NPV of scenario (a) to an unfavorable value of -US$4 million. Indeed, the reduction in the price of polyphenols constitutes the most impactful costing parameter that negatively influences the economic feasibility of scenario (a). It must however be stated that such an unfavorable outcome is highly unlikely, since US$ 15 per kg constitutes the lower limit of the typical polyphenol prices [43]. It is also observed that while a 50 % reduction in the production capacity led to a 30.8% reduction (i.e. US$ 13.74 million) in the NPV of scenario (a), negligible changes in the NPV were observed when the production capacity was increased by 50%. This observation suggests that economic changes associated with increments in production capacity were not significant in scenario (a).


(-)50%
(+)50%
Price of Polyphenol (US$/kg)
Processing capacity (kg/h)
Plant life (y)
Discount rate
Electricity cost (US$/kWh)
Total operating cost (MUS$)
Total capital investment (MUS$)
-150
-100
-50
0
50
100
150
200
Percentage change in the NPV (MUS$)

(a)


(-)50%
(+)50%
Price of Polyphenol (US$/kg)
Processing capacity (kg/h)
Plant life (y)
Discount rate
Electricity cost (US$/kWh)
Total operating cost (MUS$)
Total capital investment (MUS$)
-150
-100
-50
0
50
100
Percentage change in the NPV (MUS$)

(b)



(c)

Figure 4 : Sensitivity of the net present value (NPV) to -50% to +50 % variations in major performance parameters in scenario (a), scenario (b) and scenario (c).

The positive effects of economies of scale as illustrated by the increase in NPVs were however demonstrated in Figure 4 (b) and Figure 4 (c) for scenarios (b) and (c) respectively. This is because in scenarios (a) and (b), a 50 % increase in production capacity led to a 55.91% (NPV of -US$38.85 million) and a 33.47 % (NPV of -2.69 million) increase in NPVs, while a 50 % reduction in the production capacity led to a 145.78 % (NPV of -216.66 million) and 85.05 % (NPV of -7.74 million) reduction in the NPVs respectively. The effect of changes in the TOCs on NPVs was shown to be most impactful on the economic performance of scenario (c), with a 50 % increase in TOC translating to a 113.75% (NPV of -8.65 million) decrease in NPV. Similarly, a 50 % decrease in TOC led to a 121.3 % (NPV of 0.86 million) increase in the NPV. As expected, in all scenarios, the 50% increase and a 50 % decrease in TOCs led to unfavorable and favorable effects on profitabilities (i.e. NPVs) respectively, with similar trends observed when the TCIs of the scenarios were considered. These observations reinforce the crucial role of production costs on the profitability of large-scale production processes. Figure 4 also shows that a 50 % increase in plant lifespan leads to positive effects of +20.36% and +20.11% on NPVs of scenario (a) and scenario (c) respectively. A similar increase in plant lifespan however presented a minor negative effect of -1.55 % on NPV in scenario (b). These observations suggest that in scenarios (a) and (c), increments in project lifespan cost will facilitate sustained production of polyphenols and electricity products, with the associated revenue having the capacity to offset the capital/cost expenditure. However, such a trend is not expected in scenario (b). This observation is due to the substantially higher TCI of scenario (b) (US$ 58.55 million) compared to scenario (a) (NPV of US$ 27.22 million) and scenario (c) (NPV of US$ 0.47 million). Additionally, scenarios (a), (c) and (b) also show that the 50 % increase in discount rate leads to a 77.56 % (-US$ 4.45 million) decrease, 49.56 %(-US$ 6.05 million) decrease and a 10.18 % (-US$ 79.15 million) increase in NPVs. On the otherhand, a 50 % decrease in discount rate leads to a 136.38% (-US$ 46.94 million) increase, 29.44 %(- US$2.85 million) increase and a 21.16 % (-US$ 106.77 million) decrease in NPVs respectively. These observations presented in scenarios (a) and (c) are expected, since smaller discount rates will lead to higher discount factors such that if the cash flow (*A*) is positive, the NPV becomes larger, or vise versa. If the cash flows are however negative, such smaller discount rates will lead to more negative NPV values as observed in scenario (b).

3.3 Environmental performance

Employing the method discussed in section 2.3 above, the environmental performances of the three scenarios were compared based on the PEI performance metric with the results presented in Figure 5.

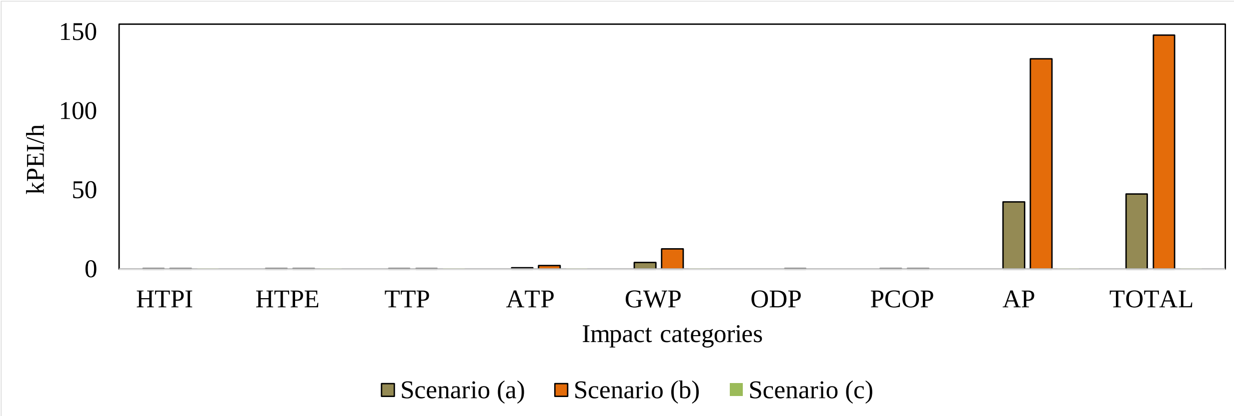


Figure 5 : The potential environmental impacts of apple pomace valorization strategies of scenario (a), scenario (b) and scenario (c).

Figure 5 shows that the environmental performances were as follows scenario (c) > scenario (a) >scenario (b), with scenario (b) presenting the poorest environmental performance with a PEI of 148 kPEI/h. Scenario (c) and scenario (a) were determined to have environmental performances of 0.21 kPEI/h and 47 kPEI/h respectively. Figure 5 also shows that acidification potential (AP) and global warming potential (GWP) constitute the major impact categories responsible for the relatively poorer environmental performances in scenarios (a) and (b). The AP index impact category in scenarios (a) and (b) of 42.40 kPEI/h and 133 kPEI/h respectively is due to the significant consumption of fossil fuels for energy generation to satisfy the heating requirements for the high-temperature SWE process and the sequential distillation processes for ethanol recovery, respectively. The use of these fossil fuels will result in the release of unwanted gases such as CO_2, which in the presence of atmospheric moisture, leads to the formation of weak acids (i.e. H_2CO_3). Such weak acids are recognized as responsible for the production of the so-called acid rain [53], which increases the AP of the processes. Crucially, the higher GWPs determined in scenarios (a) and (b) of 4.09 kPEI/h and 12.80 kPEI/h respectively are also a consequence of the use of externally sourced fossil fuels to satisfy the heating requirements of the processes, since the associated production of greenhouse gases (i.e. CO_2) will increase the GWPs of the processes. Crucially, although scenario (c) is presented as the most favorable process when environmental performances are considered, its selection is not encouraged for further development due to its determined economic infeasibility. It is suggested that introducing approaches to enhance the environmental performance of scenario (a) may constitute a more prudent strategy to ensure that favourable economic and environmental performance goals are achieved. To this regard, this study proposes the utilization of alternative energy sources i.e. solar power to fully/partly satisfy the heat energy needs of scenario (a). Additionally, the possibility of utilizing low-cost 'filters' to clean gaseous emissions may be explored when fossil energy is employed as the energy source.

The authors acknowledge that the results of the simulation study may be limited by significant variations in the composition of the apple pomace. This is because, the composition of the apple pomace may vary with location, collection method, pretreatment processing strategy, etc. This implies that APs from different sources may contain different concentrations of TPCs leading to variations in revenue generation and thus, economic performance outcomes. Furthermore, in simulating the anaerobic digestion process, possible risks of digestion failure due to low pH values, poor mixing, ineffective microbial population etc, were not considered. This suggests that the performances of the AD processes, with respect to the biogas yields in all scenarios, may be optimistic, since the theoretical biomethane potential employed in the study assumes complete degradation of the macromolecules present in the AP. Limitations associated with economic performance estimations are also acknowledged. Specifically, sensitivity analysis determined that variations in the cost of inputs and market prices of product streams (i.e. bioenergy, polyphenols etc.) serve as major sources of uncertainty in predicting economic viabilities. Additionally, since the NPV metric is based on an assumed discount rate and future cash flows, its use in economic assessment is limited. This is because, the discount rate and the future cash flows can not be predicted with a 100 % certainty. In comparing the environmental performances of the alternative valorization strategies, it must be acknowledged that WAR algorithm considered only the anticipated environmental impacts associated each facility. Thus, possible environmental impacts associated with the transfer of the AP to the processing facility were not considered. While this (WAR) approach was sufficient for comparing scenarios in this study, comparing the results in the study with any results in the literature may be futile due to differences in system boundaries. It must be noted that, although most of these limitations highlighted were addressed in the sensitivity study, it is proposed that the results presented in this study are employed as a 'first-level' and a preliminary screening tool for the benefit of policy makers.

3.4 Technological challenges, future directions and practical implications

Due to the limitations of the approaches employed in the study, it is anticipated that future studies may incorporate integrated exergy-based approaches such as exergoeconomic, exergoenvironmental, and exergoeconoenvironmental investigations [14,44]. This is because, such exergy-based analyses facilitate the identification of breakthrough points for additional environmental improvements, thus can outperform other sustainability assessment tools and serve as more informative indicators, in this regard [14,45]. Additionally, although not considered in this study, it is possible that the higher TPC of the SWE technology may be due to the depolymerization of lignin bonds, for phenolic acid production, when high temperatures are imposed. This production of phenolic acids contributes to the TPC yield [46]. The possible depolymerization of lignin therefore limits its use an important biopolymer or as a solid fuel in the CHP plant. Crucially, it was also reported in the literature that the high temperature imposed during SWE may lead to the oxidation of PPCs. This enhanced risk of oxidation may be exacerbated during the post PPCs recovery stage which involves a (time-consuming) drying operation for water vaporization/removal. This oxidation may translate to loss of the antioxidant activity of the TPCs [47], and thus limit its functionality in some biomedical applications. Additionally, the imposition of high temperatures in the SWE technology may also translate to an increased need for caution to ensure safe operation [48]. It is also suggested that the SWE technology may be hindered by the requirement for frequent plumbing, since blockage may occur during dynamic processes, thus leading to higher maintenance costs [48]. Inspite of the aforementioned challenges of the SWE technology for PPC extraction, the overall favourable performances reported in this study provide a compelling basis to explore its scale-up. It is therefore proposed that future research focuses on pilot-scale operations of SWE of PPCs in continuous mode, with the actual (pilot-scale) equipment cost employed as a basis for calculating the industrial-scale capital cost for higher costing accuracy. The possibility of employing a freeze-drying operation for TPC recovery from the water extract, to reduce PPC degradation/oxidation, as well as its associated cost implications must be investigated in future works. It is also recommended that future research futher explores practical (beyond theory) heat integration opportunities during SWE and explore conditions that reduce or eliminate TPC degradation. The findings herein have therefore broadened the application of AP as a sustainable source of high value PPC and bioenergy, which have applications in the biomedical, food and energy industries.

4 Conclusion

This study comparatively investigated alternative AP valorization schemes that focused on the production of polyphenols, using green solvents of subcritical water and ethanol, and bioenergy. The study determined that the SWE of PPC from AP constituted the most profitable strategy compared to alternative biorefinery pathways of using ethanol solvent for PPC extraction from AP and using the anaerobic digestion technology for only bioenergy production from AP. Recognising the need to further improve the environmental performance of the SWE of PPC from AP, the study proposed several technologies and the future use of exergy-based approaches to aid in the identification of specific sections of the SWE system that must be improved.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability statement

The authors confirm that the data supporting the findings of this study are available within the article.

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Author Contribution

Conceptualization: O.V.O, Methodology: O.V.O, L.N., Formal analysis and investigation: O.V.O, A.S., Writing - original draft preparation: O.V.O, D.P., Writing - review and editing: O.V.O, L.N., D.P., A.S., Supervision: A.S..

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Data Availability

All data generated or analysed during this study are included in this published article [and its supplementary information files.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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