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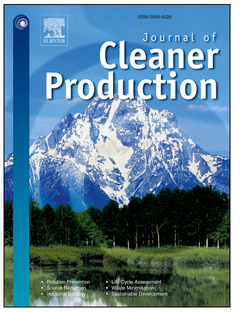

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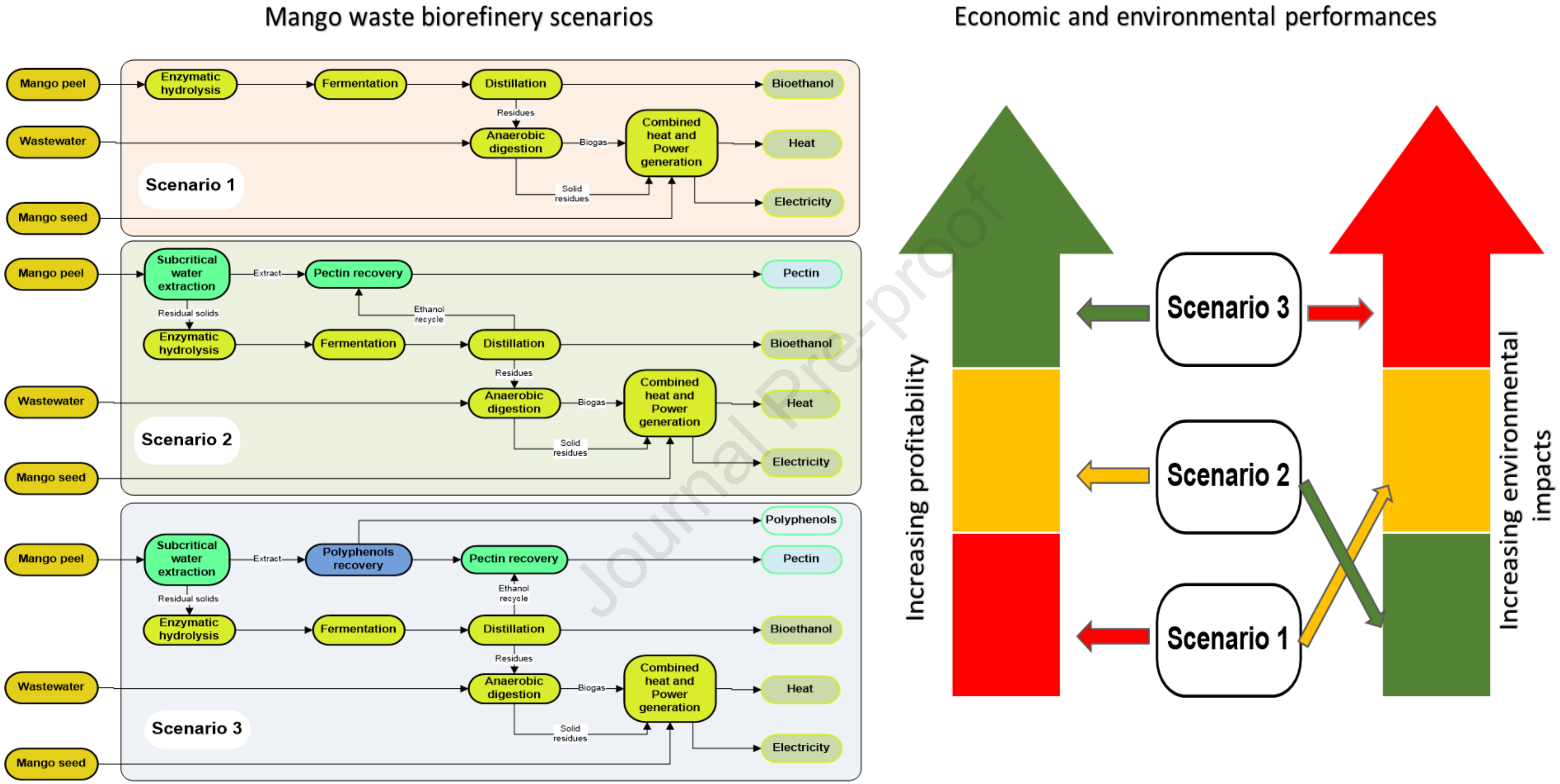
Annie Chimphango: Conceptualization, Funding acquisition, Resources, Supervision, Writing - review & editing.

Patricia Thornley: Formal, analysis, Funding acquisition, Resources, Supervision

Mirjam Order: Formal analysis, Writing - Review & Editing

Graphical abstract



Techno-economic and environmental evaluation of integrated mango waste biorefineries.

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Abstract

An analysis of process feasibility, economic and environmental performances of mango processing waste biorefineries is presented. Three biorefinery scenarios were modelled in Aspen Plus to integrate the recovery of high-value bioactive compounds, bioethanol, and bioenergy. Fermentation of mango peel to produce bioethanol was evaluated in Scenario 1. Scenario 2 considered the recovery of pectin from mango peel prior to ethanol fermentation while Scenario 3 assessed the sequential recovery of pectin and polyphenols from mango peel before ethanol fermentation. In all three scenarios, anaerobic digestion of wastewater and stillage produced biogas which was co-combusted with mango seed to generate heat and electricity. Co-producing pectin and polyphenols with bioethanol and bioenergy (Scenarios 2 and 3) promotes product diversification and improves profitability. Although Scenario 1 is the least capital intensive, with a total capital investment of 77.1 million USD (compared to 85.2 and 87.5 million USD for Scenarios 2 and 3, respectively), it is not economically attractive with a negative Net Present Value (-142 million USD). Scenario 3 is the most attractive in terms of profitability, with a Net Present Value of 311 million USD compared to 238 million USD for Scenario 2. However, Scenario 2 has the least environmental impacts, with Global Warming Potential at 16.6 kg CO_2 equivalent per tonne of mango waste and Fossil Resources Consumption at 5.55 kg oil equivalent per tonne of mango waste compared to Scenarios 1 and 3 with Global Warming Potential values of 21.9 and 32.7 kg CO_2 equivalent per tonne of mango waste and Fossil Resources Consumption values of 6.68 and 10.3 kg oil equivalent per tonne of mango waste, respectively. Accordingly, the economic and environmental results suggest that trade-offs between profitability and environmental impacts for the biorefineries should be established in implementation decisions.

Keywords

Integrated biorefineries; mango processing waste; process modelling; economic viability; environmental life cycle analysis.

Abbreviations and nomenclature

AD	Anaerobic digestion	TPC	Total Production Costs
CHP	Combined Heat and Power	TS	Total Solids
COD	Chemical Oxygen Demand	USD	United states Dollars
CSL	Corn Steep Liquor	VOC	Variable Operating Costs
DAP	Diammonium Phosphate	WC	Working Capital
EH	Enzymatic hydrolysis	WCo	Water consumption
FCC	Fixed Capital Costs	WWT	Wastewater Treatment
FRS	Fossil Resource Scarcity	**Nomenclature**	
FU	Functional Unit	CO_2	Carbon dioxide
GHG	Greenhouse gases	°C	Degree Celsius
GWP	Global Warming Potential	%	percent
IRR	Internal Rate of Return	g	gram
IPCC	Intergovernmental Panel on Climate Change	h	hour
LCA	Life Cycle Analysis	kg	kilogram
MWB	Mango Waste Biorefineries	kWh	kilowatt hour
MPF	Mango Processing Facility	L	Litre
MPSP	Minimum Product Selling Price	m^3	Cubic metre
MPW	Mango Processing Waste	mg	milligram
NPV	Net Present Value	MJ	Mega Joule
SWE	Sub-critical Water Extraction	MWh	Mega Watt hour

TEA	Techno-economic Analysis	v/v	Volume by volume
TCI	Total Capital Investments	w/w	Weight by weight
TDC	Total Direct Costs		

1. Introduction

With a global production exceeding 55 million tonnes in 2019 (FAOSTAT, 2019), the mango is the world's second most-produced tropical fruit (Jahurul et al., 2015). Owing to its high moisture content, the mango is highly perishable, leading to considerable post-harvest losses (Sehrawat et al., 2018). Mango processing, mainly into dried slices, juices, and powders, preserves the fruit and extends its shelf-life. In addition, mango processing enables all-year-round availability and reduces post-harvest losses. Despite lucrative benefits, the mango processing sector is perceived as a residual industry, processing ≈30% and 0.22% of South African (Directorate Statistics and Economic Analysis, 2018) and world mangoes (Link et al., 2018), respectively.

The processing of mango generates substantial quantities of residues (≈350 – 600 kg/tonne of fruit) in the form of peels and seeds (Banerjee et al., 2018). Landfilling of the residues comes at a cost and is often associated with undesired environmental concerns. If poorly managed, landfilling of highly biodegradable material such as mango residues contaminates water bodies and releases greenhouse gases (GHG). Incineration of the waste is also discouraging due to excessive moisture content and the associated release of gaseous emissions and particulates. On the other hand, South African thermal energy needs for mango processing are met by coal combustion, while electricity supply is erratic such that it is complemented by diesel or petrol generators (Dzigbor and Chimphango, 2019).

Global initiatives including the Intergovernmental Panel on Climate Change (IPCC) advocate for sustainable processing which reduces greenhouse gas releases (Tursi, 2019). The South African Department of Science and Technology (DST) launched the Bioeconomy Strategy in 2014 (DST, 2013) aimed at encouraging the transition towards a bioeconomy. Valorization of waste biomass forms is an alternative waste management strategy which supports the mentioned initiatives. Mango residues, like most biomass forms, are a potential renewable resource with attractive compositions for biorefining into multiple products including bioenergy and bioactive compounds that could reduce the reliance on fossil fuels and improve revenue flows. However, current biomass utilization is still low, with estimated contributions of 14% to global energy (Tursi, 2019).

Laboratory scale studies have successfully recovered valuable products from the mango peel (Banerjee et al., 2018; Berardini et al., 2005). Among the high-value compounds recoverable from the peel, pectin which constitutes 20 – 30% of the peel weight (Banerjee et al., 2016) and polyphenols (93.0 – 96.2 mg/g of dry peel) (Ajila et al., 2007), have the potential for economic extraction at a large scale (Mugwagwa and Chimphango, 2019). Pectin is a cell-wall polysaccharide widely used as a gelling, stabilizing, and emulsifying additive in the food and cosmetics industries. Selling at $15/kg, the pectin market has been expanding owing to its upcoming uses in pharmaceuticals, for drug delivery, and preparation of neutraceuticals (Ciriminna et al., 2015). Mango peel polyphenols exhibit antioxidant characteristics that have attracted their use as health-promoting agents in the food, health, and pharmaceutical sectors (Masibo and He, 2008). Starch, polyphenols, oil, and nanocellulose have also been obtained from the seed (Arora et al., 2018; Henrique et al., 2013).

Existing process feasibility studies on mango waste biorefineries are limited in terms of the number of products and generate waste streams that need further treatment and disposal. Moreover, the reported studies considered valorization of one form of the waste, either peel or seed. For example Mahadevaswamy and Venkataraman (1990) and Madhukara et al. (1993) reported on the anaerobic digestion of mango peel for biogas production. Jawad et al. (2013) and Reddy et al. (2011) assessed the feasibility of mango peel as a feedstock for lactic acid and bioethanol, respectively. Banerjee et al. (2018, 2016) and Berardini et al. (2005) evaluated the co-recovery of pectin and polyphenols from the mango peel. Mugwagwa and

Chimphango (2019) assessed the feasibility of sequential recovery of pectin, polyphenols, and anthocyanins from the peel.

The residues from the bioactives extraction, for example, have been characterized as having attractive composition for further conversion into biofuels, and bioenergy, potentially promoting cleaner production and full utilization of the biomass (Banerjee et al., 2018). Considering that the mango seed is a potential biofuel, with a calorific value of 17 – 18 MJ/kg (Perea-Moreno et al., 2018), mango processing residues can be utilized in integrated multi-product biorefineries for co-producing valuable products including pectin, polyphenols, biofuels, and bioenergy.

Despite the lucrative potential, commercialization decisions may be misguided without comprehensive economic viability and sustainability assessments (Aghbashlo et al., 2018). Preliminary estimates for revenue generation from the sale of pectin, phenolics, lipids, and starch recovered from mango peel and seed provided encouraging results for commercialization (Banerjee et al., 2017). Also, a cost-benefit analysis of mango waste biorefinery scenarios reported by Arora et al. (2018) demonstrated economically viable conversion of mango waste to co-produce pectin, polyphenols, seed oil, starch, and protein using three different biorefinery scenarios. However, the lucrative economic gains do not guarantee environmental sustainability (Vega et al., 2021) and should not be prioritized over environmental detriments. Thus, environmental sustainability assessment must accompany economic analysis in feasibility studies.

Engineering tools for process simulation, for example, Aspen Plus, have been employed in assessing the feasibility and limitations of combining unit processes to come up with integrated biorefineries for multi-product recoveries (Aghbashlo et al., 2018; Dávila et al., 2015; Humbird et al., 2011; Lohrasbi et al., 2010). Process simulation models generate mass and energy balances that are used in equipment sizing and estimation of equipment costs. When combined with economic modules such as Aspen Process Economic Analyzer, the approach is useful for cost-benefit analysis, informing research and investment on development, scale-up, and improvement of new technologies and their economic viability.

Process modelling can be combined with environmental impact assessments to identify related environmental bottlenecks and hotspots for technological improvement (Kwant et al., 2018). Life cycle analysis (LCA) is a commonly used standardized method for predicting the lifetime environmental impacts of products. Coupled with techno-economic analysis (TEA), LCA provides information that limits burden-shifting and aids the selection of products and processes that are both economically and environmentally favorable.

Many studies combining TEA and LCA for quantitative biorefinery sustainability analysis have been published. For example, Budzinski and Nitzsche (2016) analyzed the economic and environmental benefits of four beech wood-based biorefinery scenarios against reference systems. Combined economic and environmental studies have been used to compare the performances of biorefineries utilizing sugarcane bagasse and trash as possible annexes to existing sugar mills (Farzad et al., 2017; Mandegari et al., 2017, 2018). A comparison of the economic and environmental efficiencies of sugarcane molasses-derived vs agave juice-based bioethanol was reported by Parascanu et al. (2021). Calicioglu et al. (2021) combined TEA and LCA sustainability for wastewater-based duckweed biorefinery to inform decisions that support the circular bioeconomy. Croxatto Vega et al. (2021) used a combined TEA-LCA study to compare two technologies for recovering polyphenols from red wine pomace. However, studies on combined TEA and LCA of mango waste biorefineries co-producing bioenergy, bioethanol, and bioactive compounds have not been reported.

The present study evaluated the process feasibility, economic viability, and environmental life cycle impacts of mango waste biorefineries (MWB) co-producing bioethanol, bioenergy, pectin, and polyphenols. The economic analysis provided information on the capital and operating cost requirements, revenue flows, and profitability while environmental analysis provided information on the biorefineries' contribution to global warming, and consumption of fossil fuels and water. The study results are envisaged to inform investments decisions on the selection of economically viable and sustainable mango waste utilization options.

2. Methods

The study approach (summarized in Figure 1) is detailed in the subsequent sections.

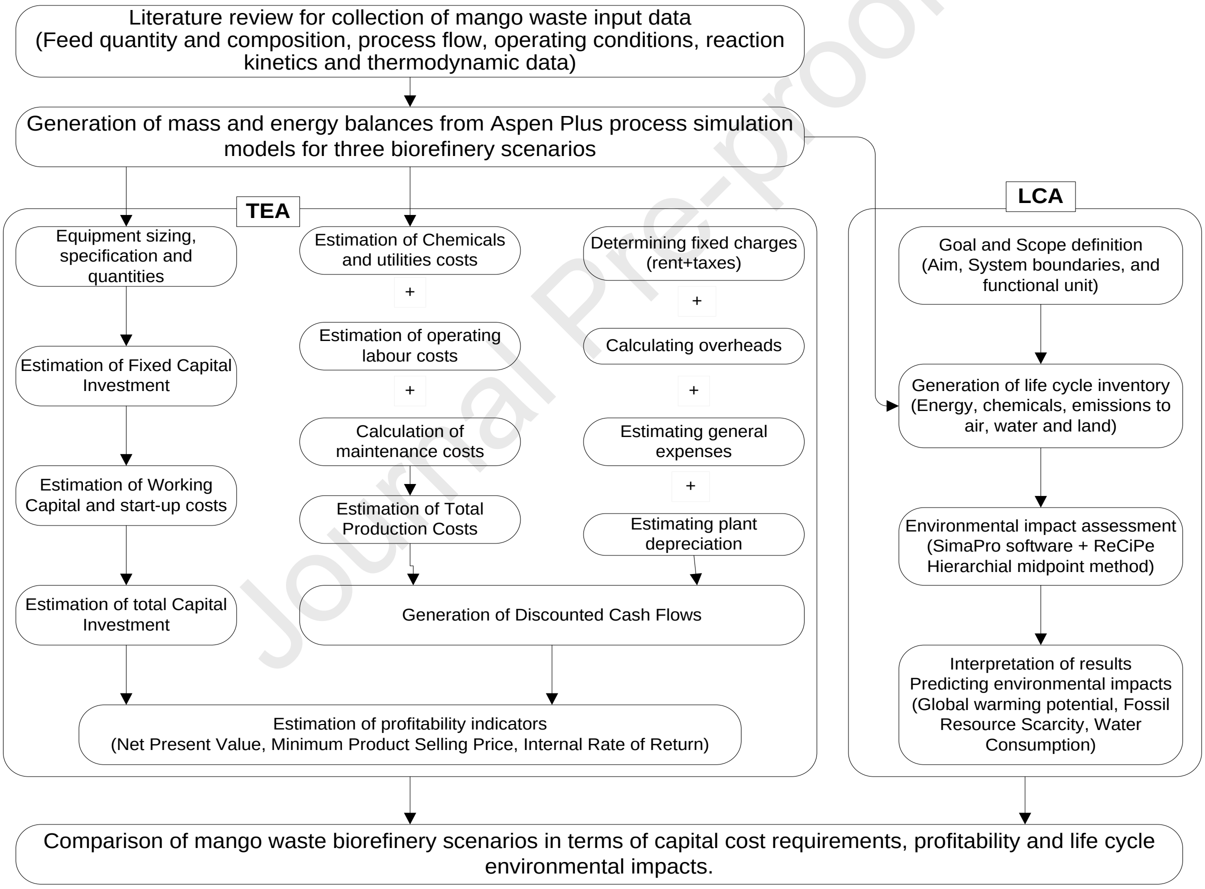

Figure 1: Study method followed for evaluating the techno-economic viability (TEA) and environmental life cycle impacts (LCA) of mango waste biorefineries.

2.1 Process design and Aspen process modelling

With the physical properties of non-conventional components (e.g., cellulose, hemicellulose, lignin) adopted from the National Renewable Energy Laboratory (NREL) database, the Electrolyte Non-Random Two liquid (ELECNRTL) was selected as the general thermodynamic model for the process simulation in Aspen Plus®. The process was developed following the NREL Aspen simulation models (Davis et al., 2018; Humbird et al., 2011) and valorization data from literature of mango peels and other pectin-rich feedstocks of comparable compositions (Banerjee et al., 2018; Grohmann et al., 1996a, 1996b; Jahid et al., 2018; Talekar et al., 2018) including citrus peel, apple pomace, and sugar beet pulp (Edwards and Doran-peterson, 2012). Electricity demands for the different sections were simulated basing mainly on the ethanol model developed by NREL (Humbird et al., 2011).

2.1.1 Plant capacity and waste composition

Plant capacity was estimated as 62.5 tonnes/h (50.0 tonnes process wastewater + 5.56 tonnes peel + 6.94 tonnes seed) for biorefineries annexed to a dried mango chips processing facility (MPF) (capacity ≈27.8 tonnes/h) (Arora et al., 2018) which generates 0.45 tonnes solid waste (44.4% peel + 55.6% seed) (Banerjee et al., 2016; Reddy et al., 2011) and 1.8 m^3 of wastewater (chemical oxygen demand (COD) ≈4 000 mg/L) (Khan et al., 2015) per tonne of mango processed. The annual plant operating time is 24 h/day for 330 days. The *Totapuri* cultivar composition was adopted for the peel (Arora et al., 2018; Reddy et al., 2011) while the seed waste was assumed to constitute 55% kernel and 45% seed coat with specified compositions from literature (Table A.1) (Arora et al., 2018; Henrique et al., 2013).

2.1.2 Description of scenarios

Major stages of the MWBs include feedstock preparation, subcritical water extraction (SWE), pectin and polyphenols recovery, ethanol production/recovery (enzymatic hydrolysis (EH), fermentation, and distillation), combined heat and power (CHP), and anaerobic digestion (AD) & wastewater treatment (WWT). These processes were combined into three scenarios, described in the next subsections. Feed preparation in all scenarios includes separate shredding and milling of the peel and seed, following which, the seed is conveyed to the CHP section while the peel is screw pressed. The resultant liquid together with process wastewater is pumped to the AD & WWT section while the solid is conditioned using rectifier bottoms and direct steam injection in preparation for EH in Scenario 1 or SWE in Scenarios 2&3.

Scenario 1: Production of ethanol, heat, and electricity.

Scenario 1 (Figure 2) assesses the production of bioethanol, heat (steam), and electricity. The bioethanol is upgraded to fuel-grade while heat is exported to the host facility, and electricity is consumed within the biorefinery.

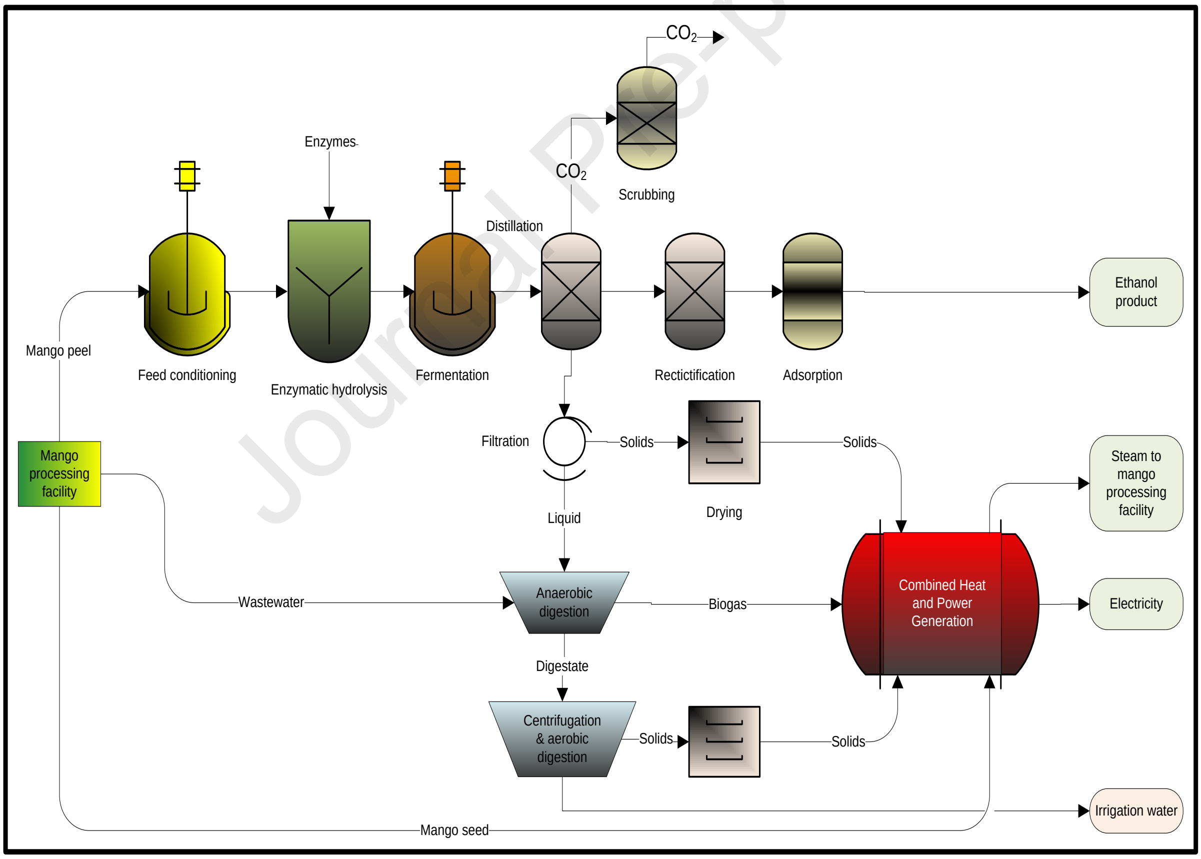

Figure 2: Process flow diagram depicting Scenario 1 for the mango waste biorefinery co-producing ethanol, steam, and electricity.

Enzymatic hydrolysis, fermentation, and ethanol recovery

Considering the high pectin content in the peels (≈20 – 35%) (Banerjee et al., 2016), which interacts with the cellulose, hemicellulose, and free monosaccharides (e.g. glucose), hydrolysis of the pectin, together with cellulose and hemicellulose ensures full utilization of the peel. The breaking down of pectin linkages not only produces pectin-derived fermentable sugars but also facilitates enzyme access to cellulose, thereby releasing more glucose. Process conditions utilizing enzyme cocktails that allow concurrent breakdown of pectin and cellulose were adopted from Grohmann et al. (1996a, 1994).

The hydrolysate, containing pentose and hexose sugars, as well as galacturonic acid is fermented at 35°C, with corn steep liquor (CSL) and diammonium phosphate (DAP) as nutrient supplements (Grohmann et al., 1996a, 1996b). For the fermentation microorganism, *Escherichia coli (E.coli KO11)* has been considered over yeasts (*Saccharomyces Cerevisiae)* due to its ability to co-ferment pentoses, galacturonic acid, and glucose, thus simultaneously fermenting the EH sugars with 25 – 35% higher yields (Grohmann et al., 1996a). The fermentation broth is concentrated to fuel-grade ethanol via distillation and adsorption processes suggested by the National Renewable Energy Laboratory (NREL) (Humbird et al., 2011). The distillation bottoms product is treated at the AD section.

Anaerobic digestion and wastewater treatment

Process wastewater, distillation bottoms, boiler blowdown, cooling tower blowdown, and mango process wastewater are anaerobically digested under conditions adopted from the NREL ethanol model (Humbird et al., 2011). The AD effluent is further treated in the WWT section constituting aerobic sludge lagoons for further reduction of the COD (Humbird et al., 2011). Dewatered sludge from AD and aerobic sludge lagoons is dried and co-combusted with mango seeds and biogas whereas the liquid effluent is discharged as irrigation water.

Urea is added to the anaerobic digestor as a nitrogen supplement whereas caustic is used in the aerobic sludge lagoons for pH control (Humbird et al., 2011).

Combined Heat and Power generation

A combustor capable of handling biogas and wet solids, a boiler, and an extraction-condensing turbo-generator (Humbird et al., 2011) make up the CHP section. Mango seed, residual solids, and biogas are combusted to produce high-pressure steam. Part of the steam drives a turbo-generator for electricity production, and part is extracted at different points from the multi-stage condensing turbine for use in peel conditioning, at the distillation section, and for drying mango chips.

Scenario 2: Recovery of pectin coupled with the production of ethanol, steam, and electricity from mango processing waste.

Scenario 2 (Figure 3a) adopted subcritical water conditions to recover pectin and assessed the feasibility of utilization of the residues in ethanol and biogas production. The solid residue is used in bioethanol production and the liquid stream is anaerobically digested for biogas production. Part of the bioethanol supplements the ethanol demand for pectin recovery and the balance is upgraded to fuel-grade. The biogas is co-combusted with solid residues and mango seeds for CHP generation.

Subcritical water extraction and pectin recovery

Process conditions for SWE were adopted from literature (Banerjee et al., 2018). The resultant slurry from SWE is pressure filtered, then the extract and solids streams are transferred to the pectin recovery and EH sections, respectively. The pectin recovery process includes vacuum evaporation to reduce the volume followed by pectin precipitation using an equal volume of 96% (w/w) ethanol (Pourbafrani et al., 2010), and drying of the pectin gel mass to 10% moisture. The ethanol is recovered in the ethanol recovery section.

Enzymatic hydrolysis, fermentation, and ethanol recovery

An enzymatic hydrolysis and fermentation process developed for pomegranate peel residues (Talekar et al., 2018) was adopted for mango peel residues. EH was assumed achievable with commercial cellulases and the hydrolysate is fermented at 37°C using the yeast *Saccharomyces cerevisiae* (Talekar et al., 2018) with CSL and DAP as nutrient supplements (Grohmann et al., 1996b). Assuming 90% conversion of sugars (Talekar et al., 2018), the fermentation broth is mixed with ethanol-rich streams from the pectin recovery section and purified via a distillation and adsorption process similar to the one in Scenario 1.

Scenario 3: Sequential recovery of pectin and polyphenols coupled with the production of steam and electricity from the mango processing waste.

Scenario 3 is an extension to Scenario 2, whereby, the SWE extract in Scenario 2 is first processed to recover polyphenols prior to pectin recovery. The extract flows through an Amberlite XAD 16 HP resin bed to recover polyphenols (Berardini et al., 2005; Schieber et al., 2003). Berardini et al. (2005) reported an 82% increase in recovered polyphenols through a process that recovers polyphenols before pectin precipitation compared to one recovering pectin before polyphenols. Thus, compared to the polyphenols recovery yield of ≈5 g/kg dry peel reported for the adopted method which recovers pectin before polyphenols (Banerjee et al., 2018), the polyphenol recovery yield at this scenario is assumed to be 82% higher.

The polyphenols are eluted with ethanol, followed by vacuum evaporation of the alcohol to ≈30% TS, then homogenization with 10% (w/w) maltodextrin, and spray drying to 6% moisture (Paini et al., 2015). The ethanol is recovered at the ethanol recovery section while the residual liquid from the polyphenol adsorption column is fed to the pectin recovery section described under Scenario 2. Similar to Scenarios 1 and 2, all residual liquid streams from the biorefinery are co-digested with the wastewater from the host facility to produce biogas for co-combustion with mango seed.

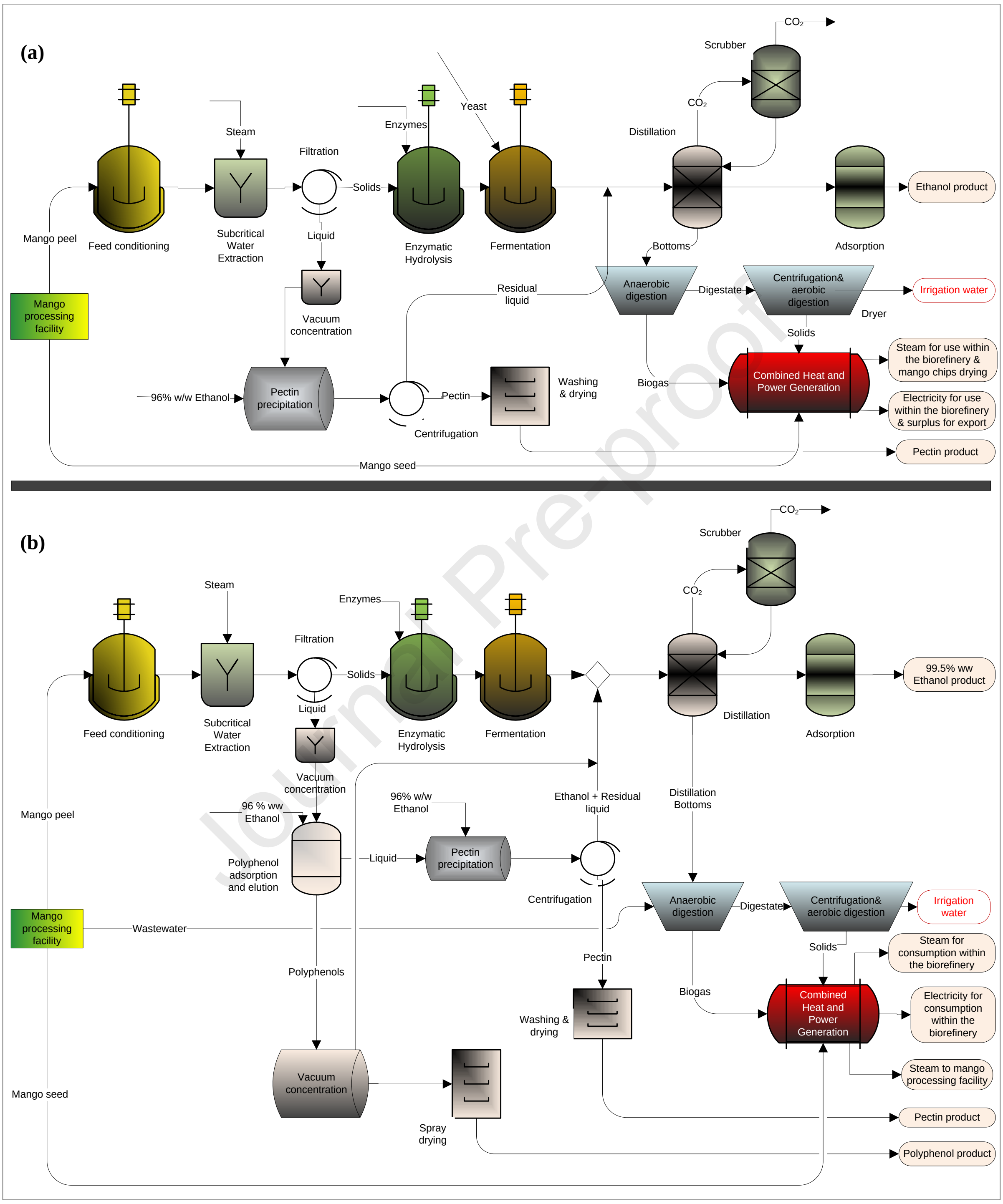

Figure 3: Mango waste biorefineries where (a) is Scenario 2: Recovery of pectin coupled with co-production of ethanol, steam, and electricity and (b) is Scenario 3: Sequential recovery of pectin and polyphenols coupled with co-production of bioethanol and bioenergy.

2.2 Economic analysis

Total Capital Investments (TCI) and Total Production Costs (TPC) were estimated using Aspen Plus Economic Analyser® (APEA) and Microsoft Excel. The TCI is the sum of Fixed Capital Costs (FCC) and Working Capital (WC), where the FCC constituted Total Direct Costs (TDC) and Total Indirect Costs (TIC). TDC include the cost of equipment purchase and installation, instrumentation, control, piping, and electrical elements (Peters and Timmerhaus, 1991). Relevant literature was consulted for purchased costs of equipment that could not be predicted using the Aspen Plus Economic Analyser® database. Literature values were adjusted for time and capacity using the Chemical Engineering Plant Cost Index (CEPCI) (Peters and Timmerhaus, 1991). TIC were estimated as 60% of TDC constituting the costs of freight to deliver the equipment to the plant site, contractor expenses, and contingencies (Seider et al., 2015) while the WC was estimated as 5% of the FCC.

Estimates for the TPC comprised direct production costs or variable operating costs (VOC), fixed charges (FC), and plant overheads (Peters and Timmerhaus, 1991). The VOC include directly associated costs of manufacturing such as procurement of the feedstock, utilities, labor, and disposal of waste while FC comprise depreciation, property insurance, taxes, and rent. Plant overheads were estimated as costs associated with plant maintenance, as well as warehouse and storage facilities. The analysis was performed in United States dollars (USD) for a 30-year plant life. Equipment depreciation was calculated using the straight-line method at zero salvage value and a recovery period of 20 years. Other assumptions include a 3-year period for land acquisition, equipment purchase, and construction; a 6-month initiation of biorefinery operations; a 40% equity and 60% loan finance scheme (loan term of 8% interest and a repayment period of 10 years). The net present value (NPV), minimum product selling price (MPSP), and internal rate of return (IRR) were calculated using discounted cash flow analysis assuming relevant South African economic parameters (Table 1).

Table 1: Assumed economic parameters for evaluating the economic viability of mango waste biorefineries

Parameter	Value
Base year	2019
Construction time	3 years (10%, 60%, and 30% capital allocation in year -2, year -1 and year 0, respectively)
Average annual tax rate	28% (Nieder-Heitmann et al., 2020)
Discount rate (real-time)	9.7% (Nieder-Heitmann et al., 2020)
Ethanol price	USD 1.08/kg (Nieder-Heitmann et al., 2020)
Pectin price	USD 15/kg (Ciriminna et al., 2016)
Polyphenols price	USD 82.5/kg (Arora et al., 2018)
Enzymes price	USD 4.24/kg protein (Magyar et al., 2016)
Diammonium phosphate price	USD 0.38/kg (Davis et al., 2018)
Corn steep liquor	USD 0.079/kg (Davis et al., 2018)
Cooling tower chemicals	USD 4.15/kg (Davis et al., 2018)
Boiler chemicals	USD 6.92/kg (Davis et al., 2018)
Caustic	USD 0.11/kg (Davis et al., 2018)

2.3 Life cycle analysis

The environmental burdens from the conceptualized MWB were evaluated using attributional LCA following the ISO 14040 guidelines. Using data generated from Aspen-based process models and economic analysis, the LCA was carried out to evaluate the environmental impacts of the three scenarios presented in section 2.1.2. The analysis demonstrates the impacts of product choice on the environmental burdens of MWBs. In addition, hotspot unit processes along the biorefinery process routes are identified. The LCA results are essential for decision-making and policy formulations concerning the valorization of MPW, particularly on the selection of environmentally sustainable product combinations and processing routes for investment.

The function of the biorefinery is to valorize MPW, thus, the study's functional unit (FU) was defined as 'per tonne of processed MPW, constituting 80% wastewater, 11.2% mango seed, and 8.8% mango peel by mass'. The study system boundaries (depicted in Figure 4), encompass energy/material inputs for the unit operations in the MWB boundaries described in Section 2.1.1, and the production of chemicals/utilities consumed within the MWB. Capital goods and construction of the MWB were assumed to have negligible environmental impacts. Inventories for the MWB processes (summarized in supplementary Table A.4) were derived from mass and energy balances generated by the Aspen process simulation models for a 62.5 metric tonne/hr plant capacity and were adjusted to suit the FU. Supporting data for the production of chemicals and materials used in the biorefineries including boiler and cooling tower chemicals, electricity, and make-up water was extracted from the Ecoinvent v3.5 database for cut-off unit production processes (Ecoinvent, 2018).

The inventory was translated to environmental burdens through the use of the ReCiPe Hierarchist (H) 2016 v1.1 methodology available in SimaPro v9.0 (PRé Sustainability) software. The ReCiPe 2016 method is the most recent upgrade of the ReCiPe 2008 method which was formed after the harmonization of the CML 2001 and Ecoindicator 99 methods, (Huijbregts et al., 2017). The method is non-region specific and translates life cycle inventory into 18 midpoint impact categories that can be holistically interpreted in terms of the environmental burdens that can be incurred. Global warming potential (GWP), fossil resource scarcity (FRS), and water consumption (WCo) were selected as relevant categories for discussion. The selection was made because first-generation biorefineries reportedly impact the energy-food-water nexus with effects mainly on land, water, and fossil energy resources (Martinez-Hernandez and Samsatli, 2017).

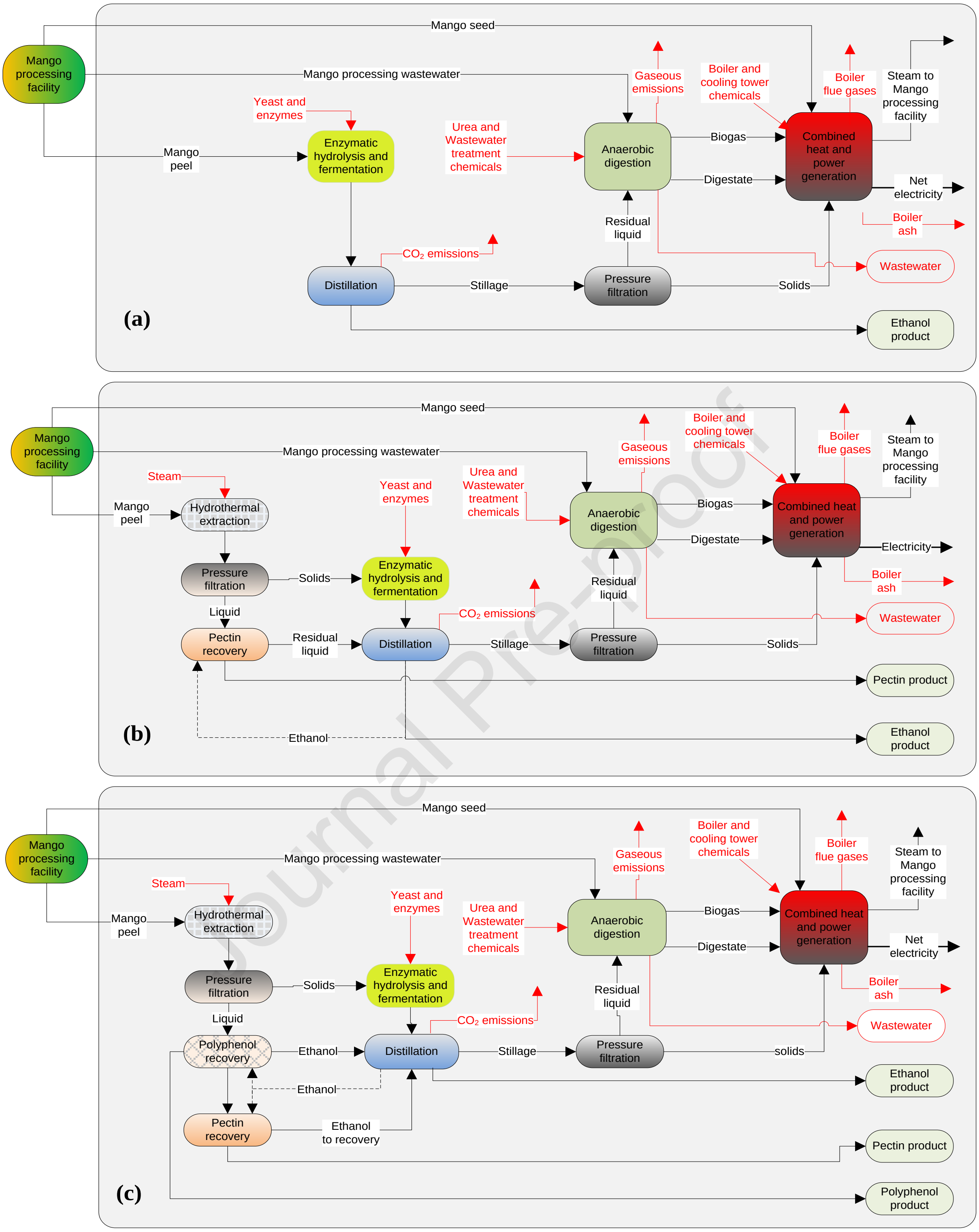

Figure 4: System boundaries for the assessed mango waste biorefineries where (a) is Scenario 1: co-production of ethanol and bioenergy (b) is Scenario 2: co-production of pectin, bioethanol, and bioenergy, and (c) is Scenario 3: sequential recovery of pectin coupled with bioethanol and bioenergy co-production.

2.4 Sensitivity analysis of economic and environmental performance indicators

Fluctuations in market parameters could influence the economic viability of the MWBs. Potential financial risks were, thus, quantified by sensitivity analysis on the NPV for variations within ±10% of the equipment purchase price, feedstock cost, TPC, steam price, electricity selling price, ethanol price, pectin price, and polyphenol product price.

Economic allocation factors used in estimating the environmental impacts of the biorefinery products were calculated using revenue generated from the sale of products. Thus price fluctuations impact the environmental impacts associated with the biorefinery products. Accordingly sensitivities of the GWP, FRS, and WCo of the products were evaluated for variations within ±10% of the prices of steam, electricity, ethanol, pectin, and polyphenols.

3 Results and discussion

3.1 Biorefinery process material and energy flow analysis

The process simulation results for the MWBs are summarised in Table 2. The ethanol product recovered in Scenario 1 is sold as a fuel-grade product while part of the ethanol in Scenarios 2 and 3 is consumed internally for supplementing the ethanol required for the recovery of bioactive compounds. A mass balance on the produced and recycled ethanol streams shows that the ethanol yield in Scenario 1 is 1.6 times that of Scenarios 2 and 3 (279, and 170 kg/tonne of mango peel (dry basis) for Scenarios 1 and 2&3 respectively). The ethanol yields corroborate well with the results obtained with orange peel where ethanol yields were 25-35% higher with *E-coli* compared to *S.cerevisiae* (Grohmann et al., 1996b). However, the predicted values are higher than those obtained with other fruit wastes, for example, 134 kg/tonne apple pomace (Magyar et al., 2016), 155 kg and 156 kg/tonne citrus peel (Joglekar et al., 2019; Lohrasbi et al., 2010). This can be attributed to differences in cellulose content between apple pomace (17%) (Ma et al., 2019) and the mango peel (21%) (supplementary Table A.1). Also, the use of yeast strains that are reportedly unable to ferment galacturonic acid and pentoses in the referred literature, versus the *E. Coli*-based fermentation simulated for Scenario 1 could have caused the differences. When the peel is dedicated to ethanol production only (Scenario 1), the ethanol yield is higher and this accountable to the removal of pectin which is a fermentable component in Scenario 1.

A total polyphenol yield of 12.4 kg/tonne of mango peel (dry weight) was estimated. Higher polyphenol yields have been reported for other fruit wastes including apple pomace (Jin et al., 2021; Martinez et al., 2016) and pomegranate peel (Talekar et al., 2018). The differences could be attributable to the lower polyphenols content assumed for mango peel (0.08% compared to 0.24% for apple pomace (Schieber et al., 2003) and 10-20% for pomegranate (Talekar et al., 2018)). The low yield could also be attributable to the selected process conditions. Reports on sub-critical water extraction of polyphenols from pomegranate seed and apple pomace demonstrate a significant increase in the yield with time (0 – 30 minutes) and temperature (80 – 220°C) (Aliakbarian et al., 2012; He et al., 2012). Thus, opportunities to optimize the polyphenol recovery from mango peel prior to implementation at industrial scale exist.

With a pectin yield of ≈272 kg/tonne peel (dry weight), the proposed process for pectin recovery has an average ethanol consumption of 5 kg ethanol/kg pectin. Owing to the higher pectin content (26.5%) assumed in this study, the pectin yield is slightly higher than values reported for citrus peel and apple pomace using subcritical water extraction (Wang et al., 2014). Reported ethanol consumption values of 161.5 kg/kg pectin for orange peels (Casas-orozco et al., 2015) are in contrast with the referred finding, attributable to the use of 96% (v/v) ethanol in a ratio 2:1 versus the 1:1 used in this study. Furthermore, the evaporation process removing 50% water, prior to the pectin precipitation, contributed to lower ethanol consumption in this study.

Table 2: Summary of output streams from the Aspen process simulation models for the assessed mango waste biorefineries

Scenario	**1**	**2**	**3**
Pectin, kg/h	-	438.70	438.70
Polyphenols, kg/h	-	-	20.09
Total Steam produced, kg/h	32 889	27 887	25 286
Steam consumed within the biorefinery, kg/h	9 401	13 985	16 354
Total recovered ethanol, kg/h	491	2 386	3 559
Ethanol for pectin recovery, kg/h	-	2 133	2 133
Ethanol for polyphenols recovery, kg/h	-	-	1 425
Net ethanol product, kg/h	491	253	122
Gross electricity, MWh	3.58	3.52	2.49
Electricity consumed within the biorefinery, MWh	4.00	2.68	3.15
Net electricity for export/import, MWh	0.42 (import)	0.84 (export)	0.84 (import)

Energy production and consumption analysis (supplementary Table A.3) revealed that only Scenario 2 can potentially meet internal electricity and heat demands and supply the requisite steam for mango drying in the host plant. However, the net electricity available for export is insufficient for the electricity demand from the host plant, meeting ≈7.4% of the demand. Although capable of meeting the steam demand for the biorefinery as well as the host plant, Scenarios 1 and 3 are not fully energy sufficient with electricity deficits of ≈0.42 and 0.84 MWh, respectively. Ethanol production, distillation, and utilities sections are the major electricity consumers with EH and fermentation in Scenario 1 consuming 2.7 times more electricity than in Scenarios 2 and 3. In Scenario 3, distillation consumes 1.6 times more electricity than in Scenario 2 and this is attributable to the higher volumes of ethanol that need to be separated. While it was assumed that the electricity deficit in Scenarios 2 and 3 is supplemented with coal-derived grid electricity, this has environmental repercussions (section 3.3). Thus, alternatives to supplement the biogas + seed fuel in all three scenarios with other biomass feedstock should be explored for total electricity supplies for both the MPF and MWB scenarios (1 - 3).

An analysis of the thermal energy consumption within the biorefineries was carried out to identify the major consumers. The distillation section consumed 6.9, 4.6, and 2.4 kg steam/kg recovered ethanol in Scenarios 1 to 3, respectively. Steam consumption corroborates well with the reported ranges for cane molasses-based ethanol (4.05 - 7.35 kg steam/kg ethanol) (Patil et al., 2015). The decreasing steam consumptions from Scenarios 1 to 3 could be explained by the relatively high ethanol compositions from the mixing of the ethanol streams recovered from the pectin and polyphenols recovery sections (2 & 3) with the fermentation broth prior to distillation.

3.2 Economic analysis

The capital costs increase from Scenario 1 to 3 owing to the recovery of more products. The TCI for the mango waste biorefineries are 77.1, 85.2, and 87.5 million USD for Scenarios 1 to 3, respectively. Contributions of the biorefinery sections to the TCI (supplementary Table A.3) show similar feedstock handling costs (USD 2.10 million) for Scenarios 1-3 due to the similar plant capacities and feedstock handling processes. For the three scenarios, the highest contributor to the TCI is the CHP section, contributing ≈38.5%, 38.0%, and 31.6% in Scenarios 1 to 3, respectively. Other significant contributors are AD & WWT, EH & fermentation, and ethanol recovery. The capital costs per kW of electricity are within reported ranges for other power plants.

The predicted capital costs for the CHP sections range between and USD/kWh and these results corroborate well with other findings on capital cost per unit of power produced.

A summary of the operating costs and profitability indicators for the MWBs is presented in Table 3. An increase in the operating costs can be observed from Scenarios 1 to 3, attributable to the corresponding increase in plant sections, and hence increasing labor, and utilities such as process water. A significant contribution to the annual operating cost is feedstock cost contributing more than 90% of the total variable costs in all three scenarios.

Table 3: Operating costs and profitability indicators for mango waste biorefineries

Scenario	1	2	3
Total operating cost, million USD[a]	11.2	11.0	12.2
Net Present Value, million USD	-142	238	311
Internal Rate of Return, %	0	45.3	53.6
Ethanol MPSP, USD/kg	3.29	*	*
Pectin MPSP, USD/kg	-	3.99	0.77
Polyphenols MPSP, USD/kg	-	-	*
Heat MPSP, USD/kg	0.17	*	*
Electricity MPSP, USD/kWh	-	*	-

***Negative minimum selling price. MPSP = minimum product selling price**

[a]Total operating costs exclude Annual income tax and equipment depreciation

Scenario 1 is not economically attractive with an NPV<0, and an IRR<0%. The co-production of ethanol, electricity, and heat with bioactives (Scenarios 2-3) from MPW is economically favorable compared to the production of bioethanol and bioenergy only but has higher capital costs. Co-production of bioenergy with pectin (Scenario 2) improves the NPV to USD 239 million, IRR to 45.3% at an ethanol MPSP<0. A similar trend is observed with the sequential recovery of pectin and polyphenols prior to ethanol production (Scenario 3) wherein the NPV increases to USD 311 million, IRR to 53.6% and an ethanol MPSP<0. Co-production of bioenergy and bioactives provides affordable clean energy (heat and electricity in Scenario 2 and heat only in Scenario 3) to the host plant with MPSPs<0 in Scenarios 2-3.

3.3 Sensitivity analysis for the Net Present Value

The sensitivity of the NPV in response to fluctuations in selected economic parameters for the MWBs (i.e., feedstock cost, products prices, capital, and operating costs) demonstrate that Scenario 1 is uneconomic under all the varied parameters (Figure 5a) and Scenarios 2 and 3 remain economically feasible (Figure 5b-c) with NPVs>0 at all conditions. For Scenario 1, TPC has the highest impact on the NPV (±7%) with a 10% fluctuation in the feedstock alone having an impact of 4% on the NPV (Figure 6). The pectin price bears the largest impact on the NPV of Scenarios 2 and 3 (Figure 6Figure *6*). However, the profitability of Scenarios 2-3 is driven by revenues from the sale of pectin whose prices is dependent on product purity. Although the predicted MPSP for pectin is lower than the current market price (Table 3), improved revenues could potentially be achieved by further processing of the bioactives for higher purity. However, cost-benefit and environmental impact analysis for further processing will be necessary.

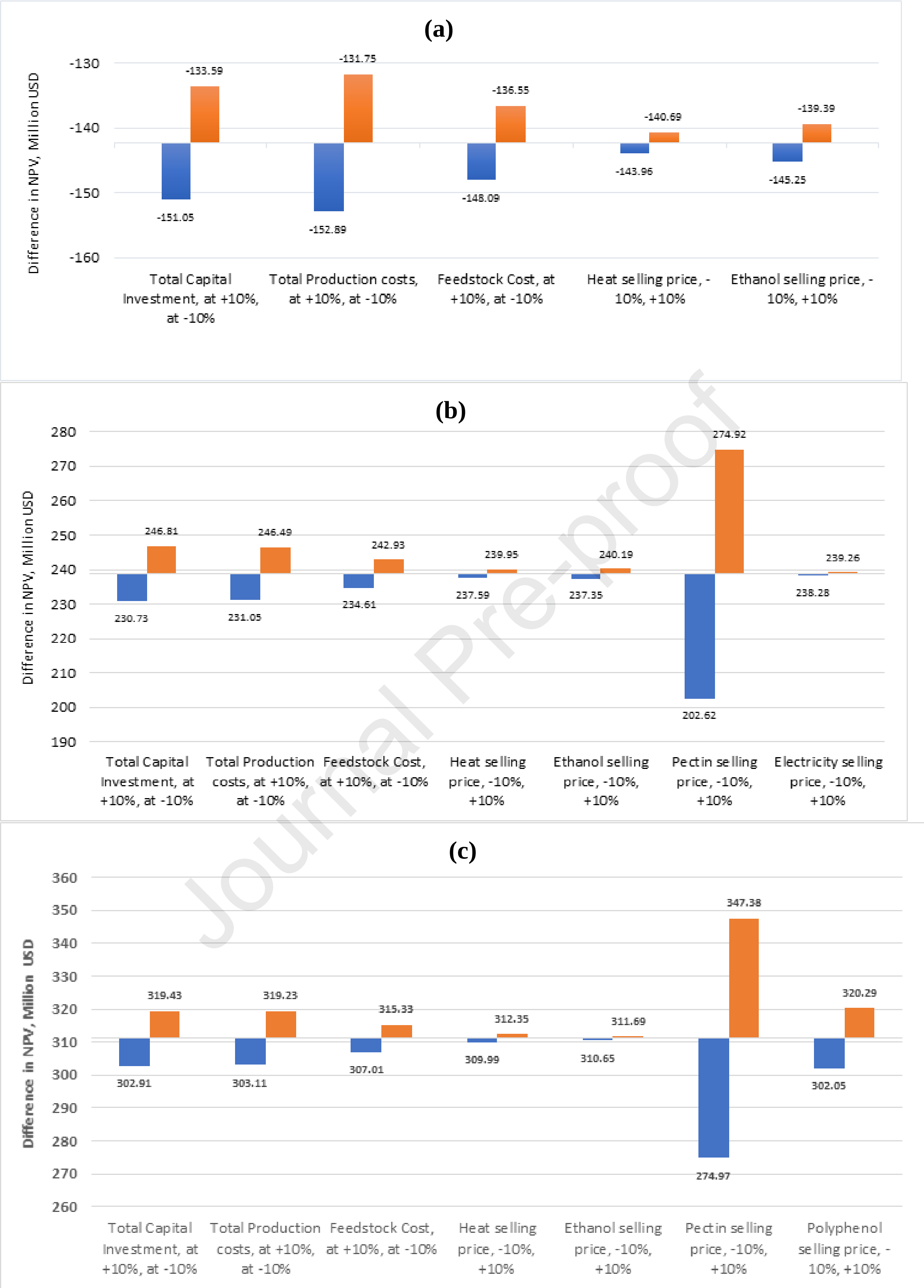

Figure 5: Sensitivity analysis of the Net Present Value to variations in selected economic parameters, where a) is Scenario 1, b) is Scenario 2, and c) is Scenario 3.

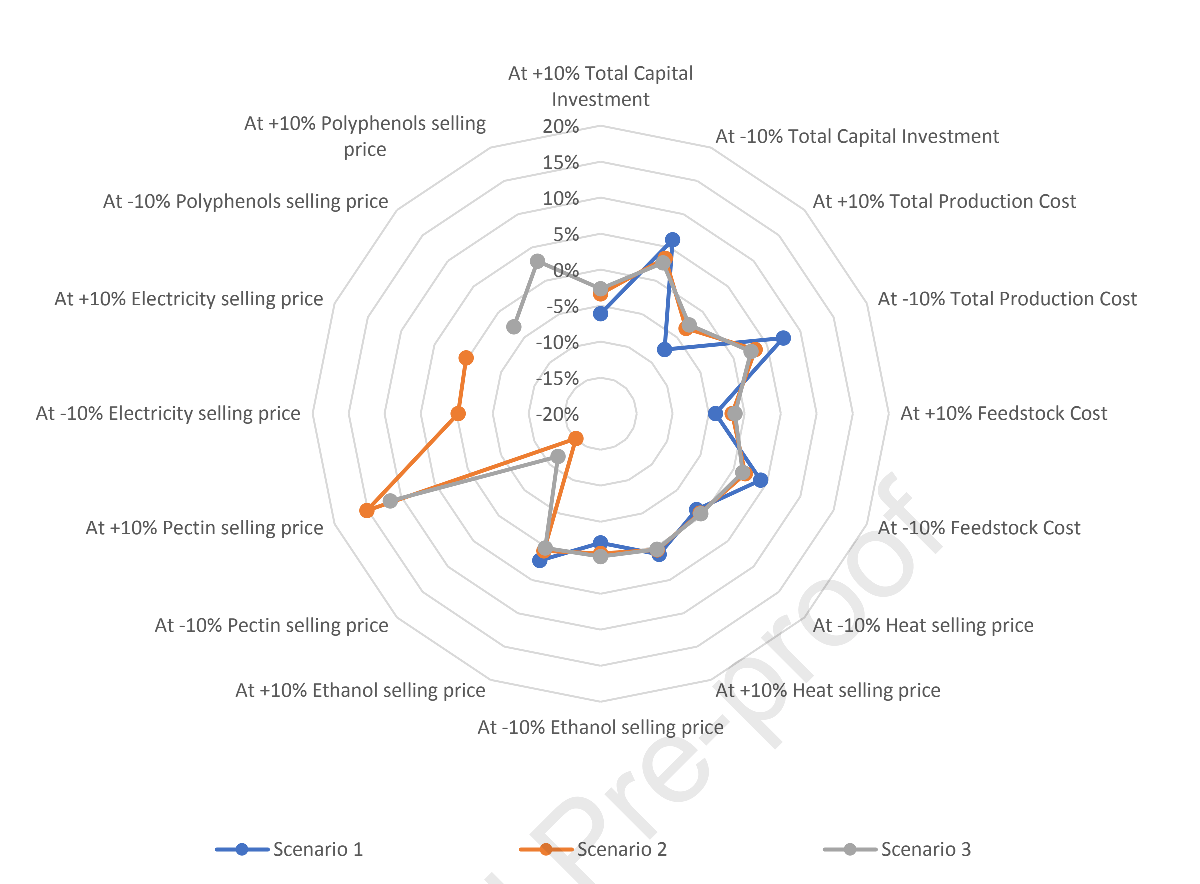

Figure 6: Impact of variations within 10% of selected economic parameters on the Net Present Value

3.4 Life Cycle analysis

The environmental burdens were assessed using 18 midpoint impact categories (supplementary Table A.5). Scenario 2 has the least impact on the environment, followed by Scenario 1 and Scenario 3 has the most impacts. GWP, FRS, and WCo were discussed, and are summarised in Figures 6 and 7. Figure 6 was generated from an analysis of the contributions to the environmental impacts made by various biorefinery unit processes in the form of chemicals consumed at each stage while Figure 7 derives from products contribution according to the economic allocation method used. The environmental burdens for each biorefinery product were allocated by economic value according to the revenue generated from the product sales.

Generally, Scenario 2 presents the least environmental burdens (GWP 16.34 kg CO_2 eq./FU, FRS 5.05 kg oil eq. and WCo 1.07 m^3) compared to Scenario 1 (GWP 21.76 kg CO_2 eq./FU, FRS 6.63 kg oil eq. and WCo 0.89 m^3) and Scenario 3 (GWP 35.52 kg CO_2 eq./FU, FRS 10.91 kg oil eq. and WCo 1.22 m^3). A higher GWP was reported for a biorefinery co-producing ethanol and biogas from citrus peel (Joglekar et al., 2019). Considering that the set system boundaries approximate well with those set in this study, the differences are attributable to the use of fossil-based steam and electricity in the referenced study compared to onsite heat and power production assumed in this study.

Compared to Scenarios 1 and 3, the lower GWP and FRS for Scenario 2 are attributable to energy self-sufficiency, wherein the other scenarios have electricity deficits supplemented by coal-derived grid electricity. Electricity consumption contributes 34% to both GWP and FRS in Scenario 1 (Figure). In Scenario 3, electricity consumption makes up 46% of the GWP and 44% of the FRS. Looking at electricity consumption, the AD & WWT section is a major hotspot for global warming and fossil resources consumption with electricity consumptions of 27% and 31% in Scenarios 1 and 3, respectively (supplementary Table A3). Other potential hotspots are the ethanol production (EH & fermentation), Utilities, and Distillation sections. The contributions to global warming and consumption of fossil resources due to fossil-based electricity consumption could be minimized by supplementing electricity with renewable alternatives (solar or hydropower) or supplementing the boiler fuels with other biomass forms such as wood.

In addition to electricity consumption, the AD & WWT section is a major hotspot for global warming and consumption of fossil resources due to the use of urea and caustic which have significant contributions to both GWP and FRS in all three Scenarios (Figure 7). The contribution of enzymes and ferementation nutrient supplements to both GWP and FRS also make EH & fermentation a hotspot.

Owing to the addition of unit processes with the recovery of products, the WCo increases from Scenario 1 to 3. While the major contribution to the WCo is attributable to process make-up water, urea, caustic, and fermentation nutrient supplements also contribute considerably to WCo. Thus, it can be concluded that the AD & WWT, and ethanol production sections are hotspots for water scarcity. Water consumption within the biorefineries could be minimized by further treating the water to acceptable quality for reuse within the process instead of discharging it for use as irrigation water. However, the economic benefits of such alternatives need to be assessed.

Negligible contributions to GWP and FRS by the biorefineries are attributed to the assumption that carbon dioxide and carbon monoxide emissions are biogenic and there is no direct consumption of fossil fuels within the biorefineries. Electricity consumption values per tonne of waste processed in the assessed biorefineries were predicted to be 64.0, 44.2, and 50.4 kWh and part of this was met by onsite CHP generation. Co-production of high-value products with electricity can be perceived as an attractive venture considering that the environmental burdens could have increased if electricity demands for the biorefineries had been supplied by fossil fuels. Nonetheless, comparative assessments on the environmental savings should be considered in future research.

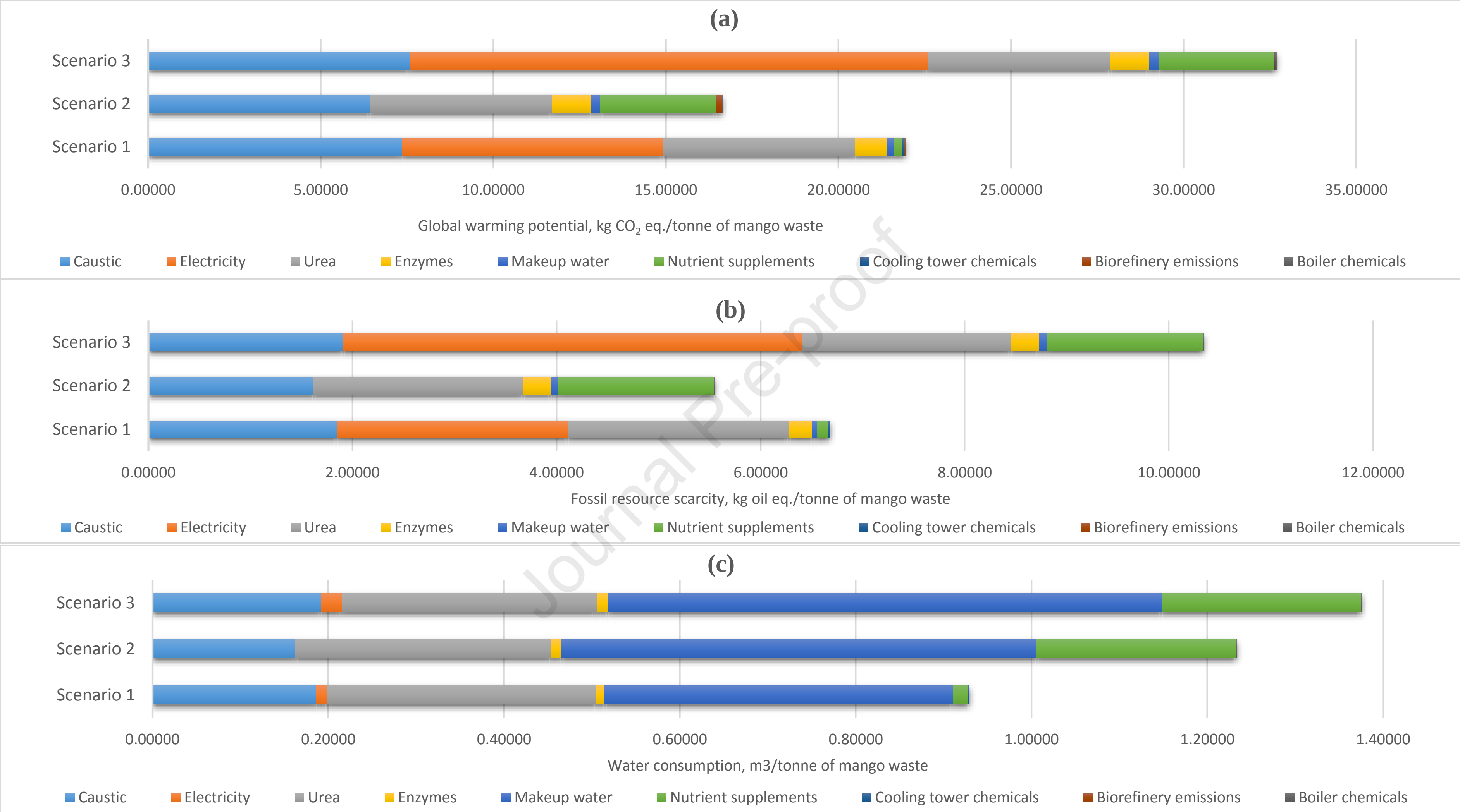

Figure 7: Mango waste biorefineries environmental impacts by source - (a) Global Warming potential, kg CO_2 eq./FU of mango waste, (b) Fossil resource scarcity, kg oil eq./FU (c) water consumption, m^3 water/FU.

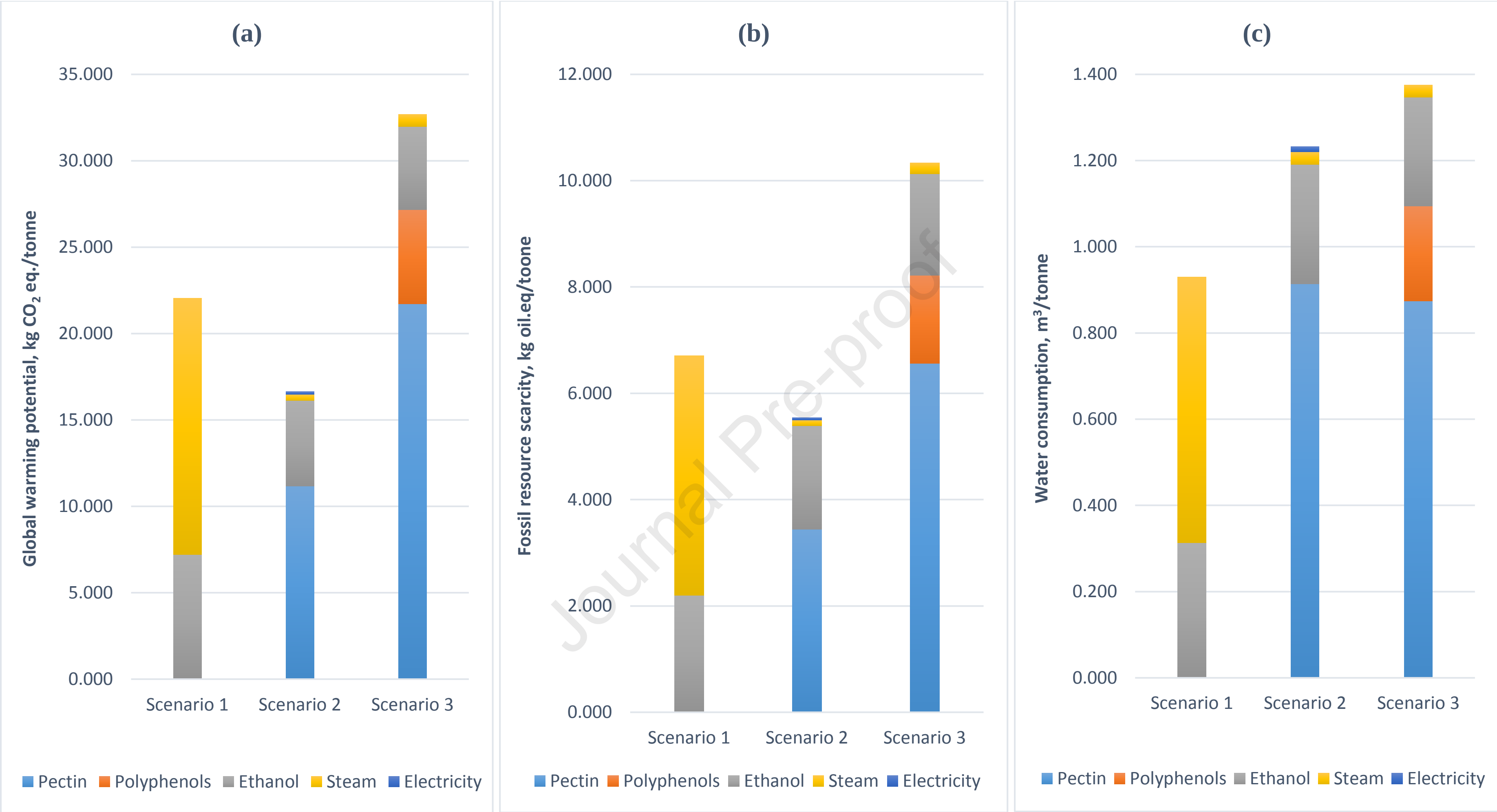

Figure 8: Environmental life cycle analysis results for mango waste biorefinery products based on economic allocation - (a) Global Warming potential, kg CO_2 eq./FU, (b) Fossil resource scarcity, kg oil eq./FU (c) water consumption, m^3 water/FU.

With a GWP value (0.2 g CO_2 eq./kWh) for Scenario 2 comparable to other values reported for biomass-derived electricity, it can be argued that mango waste-based electricity is attractive compared to coal electricity which has GWP between 0.98 and 1.7 kg CO_2 eq./kWh (Bauer et al., 2018). The contribution of heat to the GWP decreases when bioenergy is co-produced with higher value products. While this is attributable to the adopted allocation method which relied on product revenue to estimate the contribution by each product, the GWP for heat in Scenario 2 is higher than that in Scenario 3. An analysis on the GWP values for bioethanol also suggests that co-production of bioethanol and CHP with pectin (Scenario 2) is the most environmentally favourable route, presenting a GWP of 0.89 kg CO_2 eq./kg ethanol compared to 1.82 and 1.86 kg CO_2 eq./kg ethanol in Scenarios 1 and 3, respectively.

The predicted bioethanol GWP is less than that for bioethanol products from rye (3.62 kg CO_2 eq./kg ethanol), potatoes (2.81 kg CO_2 eq./kg ethanol), and maize, (3.13 kg CO_2 eq./kg ethanol) but more than that for sugarbeet-based bioethanol (0.694 kg CO_2 eq./kg ethanol) (Ecoinvent, 2018). The differences are attributable to system boundaries differences. A similar trend is observed with the ethanol contributions to FRS and WCo, implying that while the co-production of bioethanol and bioenergy with high-value bioactive products is attractive, there is need to select/limit co-products in terms of their contributions to the environmental impacts in general. Alternative products with lower resource demands mainly, ethanol and electricity, need to be considered in future research on valorization of mango and fruit processing waste in general.

Without the recovery of polyphenols, the pectin product contributes 12.2 kg CO_2 eq./FU whereas this increases to 24.1 kg CO_2 eq./FU in Scenario III. Converted to a different functional unit, the GWP values per kg of pectin are 1.74 and 3.54 kg CO_2 eq./kg of pectin for Scenarios 2 and 3, respectively. A similar trend is observed with FRS, attributable to the increased energy consumption mainly due to the increasing size of the ethanol recovery section with the recovery of polyphenols. An increase in the energy consumption in Scenario 3 translated to an increase in the demand for grid electricity which, as mentioned before, increased the GWP and FRS for MWBs.

The GWP per kg of polyphenols has been estimated at 21.9 kg CO_2 eq. The contributions to FRS impact per kilogram of pectin are 0.63 and 0.66 kg oil eq. for Scenarios II and III, respectively while the contributions to water consumption are 0.13 and 0.10 m^3 for Scenarios II and III, respectively. Although literature has reported on the LCA of bioethanol, pectin, and polyphenols recovery processes, meaningful comparisons are constrained due to the differences in system boundaries, geographical location, feedstock, and biorefinery product combinations. A combined TEA-LCA study on recovery of polyphenols demonstrated higher environmental impacts (Vega et al., 2021). Thus, there is need for further research aimed at comparing the environmental impacts of alternative recovery methods for the products to the conventional acid/alkali or organosolv-based methods.

3.5 Sensitivity analysis of the environmental impacts

Since an economic allocation was used to assess the biorefinery products environmental impacts, the sensitivity of GWP, FRS, and WCo to price fluctuations were assessed within 10% of the product prices. Price fluctuations affect all impact categories in the same way. For example, in Scenario 1 (Figure 9a), a 10% change in the bioethanol price effects a 6.1% change in the GWP, FRS, and WCo for bioethanol and a 3.4% change in the heat impacts. Similarly, a 10% fluctuation in the heat selling pressing causes a 6.7% change in the bioethanol impacts and 3.1% change in environmental impacts of the heat product.

In Scenarios 2 and 3, the environmental impacts associated with bioenergy products (steam and electricity) are the most sensitive to product price variations with the greatest impact on the environmental impact indicators caused by variations in the pectin price.

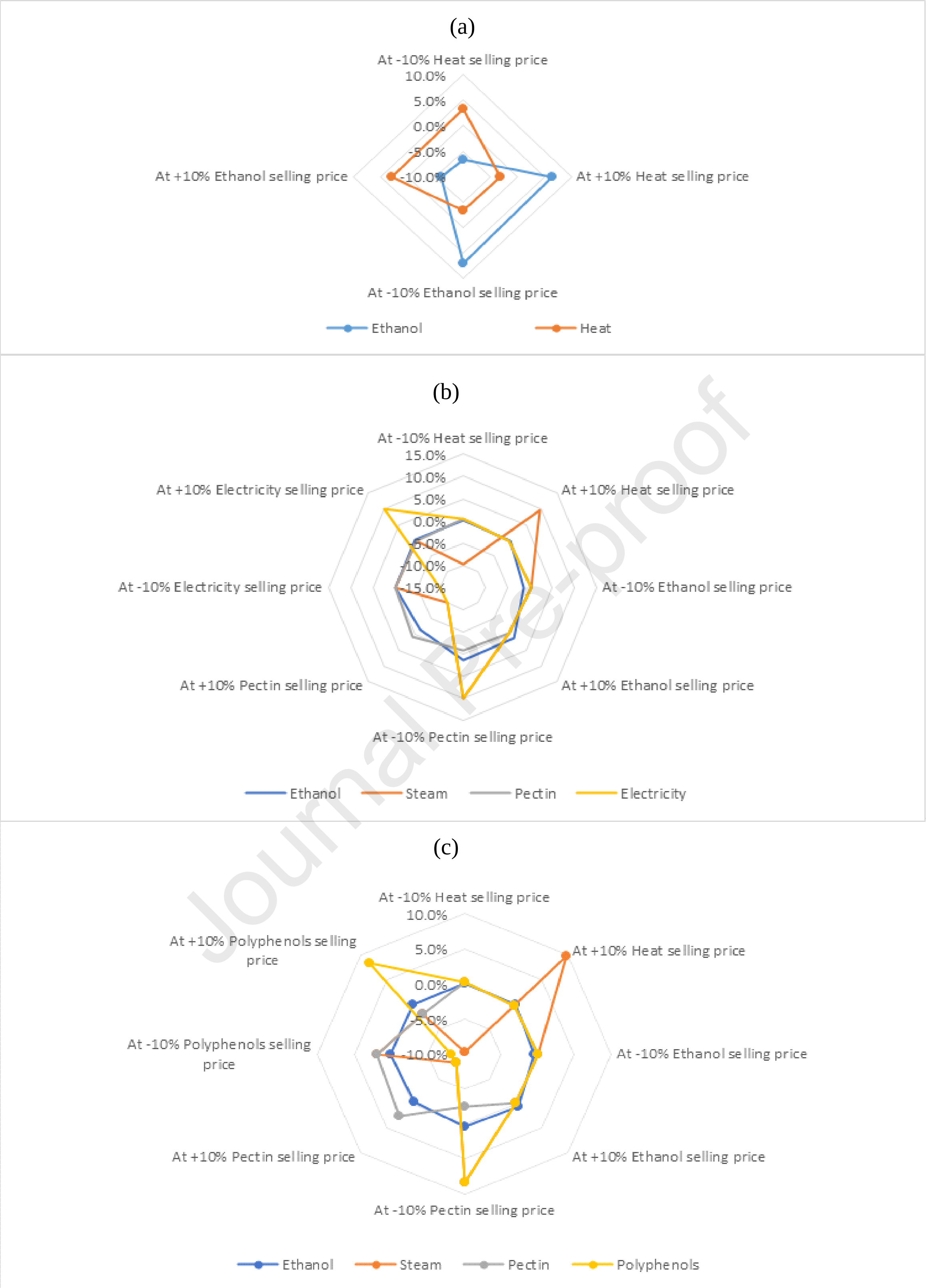

Figure 9: Sensitivity of environmental impact indicators with product price fluctuations; a) is Scenario 1, b) is Scenario 2, and c) is Scenario 3

4. Study limitations and sources of uncertainty

The use of data from different literature sources, for feedstocks that were assumed to have comparable compositions at approximate industrial conditions and yields for mango waste, could pose limitations for implementation at an industrial scale. For example, fermentation conditions for mango peel were adopted from a study on citrus peel, and fermentation of solid residues in Scenarios 2 and 3 was based on results for pomegranate residues. Although the compositions are comparable, variations in the actual product yields are possible thus affecting the predicted environmental and economic performances. Also, the lower lignin content of the mango peel could have adverse effects on the overall ethanol yield, which is not the case with the adopted studies. Accordingly, there is need for more research to determine the actual yields and optimum conditions at the pilot scale for mango waste, prior to implementation.

Sensitivity analysis revealed that variations in the market prices of inputs and products are a source of uncertainty as they have an impact on revenue generation thereby impacting economic viability and product environmental impacts. Product prices, particularly for pectin and polyphenols are influenced by the final product purity thus research aimed at assessing the impact of further processing for maximum purity of products should be considered. Also, studies on alternative processing routes for the products should be explored to enable a wider comparison of biorefinery pathways.

The environmental sustainability of the MWBs was assessed using an attributional life cycle approach. Although the method is useful for comparing scenarios and identifying process hotspots that need improvement, the comparison of results with conventional methods and reference systems is enshrouded by uncertainties. For example, differences in system boundaries or functional unit definitions between studies could limit the comparison of results. Further, the generation of the life cycle inventory from process models that derived data from various literature sources could be a source of uncertainty. Although these limitations have been addressed by sensitivity analysis, more comprehensive studies incorporating multi-decision criterion analysis including emergy, exergy could provide more reliable results for comparison of the assessed scenarios.

5. Conclusion and directions for further research

Biorefining of mango processing waste is an attractive alternative waste management strategy with the benefits of clean energy provision, product diversification, and improved economic performance for mango processing facilities. Replacing the current fossil-based energy with mango waste-based bioenergy will contribute towards mitigating the gradual depletion of non-renewable fossil fuels in support of the bioeconomy.

Basing on the economic performances and energy analysis of the assessed mango waste biorefineries, the valorization of mango waste to co-produce bioethanol and bioenergy only is neither energy self-sufficient nor profitable. However, co-producing the bioethanol and bioenergy with pectin is more profitable and presents lower GWP and FRS but the capital costs, and water consumption increase. Incorporating polyphenols recovery further increases the profitability but at the expense of higher environmental impacts and failure to meet both the biorefinery and host plant’s energy demands. Thus, prospects towards real-world applications of MWBs should explore alternative process routes that minimize capital costs, water, and energy consumption. Also, scenarios that supplement boiler fuels to meet the energy demands, for example, using wood waste, should be evaluated.

In terms of capital expenditure, Scenario 1 is the most favorable followed by Scenario 2, and Scenario 3 is the least attractive. However, Scenario 3 is auspicious basing on profitability (IRR and NPV). While investors could favor Scenario 3 because of the high profitability, Scenario 2 which has the lowest GWP and FRS will be more preferable from an environmental point of view. Accordingly, investment decisions must take into cognizance, the need to balance out economic benefits and environmental emissions prior to implementation of mango waste biorefineries.

Alternatively, more reliable decisions could be made with advanced sustainability assessment tools such as exergetic, exergoeconomic, and exergoenvironmental analysis (Aghbashlo et al., 2018, 2016; Rosen, 2018). Compared to the combined TEA and LCA methodology applied in this study, exergy-based evaluations will unveil hotspots for mass and energy conversion inefficiencies (Aghbashlo et al., 2018, 2016). For example, exergy analysis is critical in identifying specific thermodynamic improvements that could boost profitability and improve environmental performance (Aghbashlo et al., 2021; Soltanian et al., 2020). Thus, exergonomic and exergoenvironmental studies are critical for analysing the proposed biorefineries to identify specific unit processes that are sustainability hostspots and inform the derivation of decisions for commercialization.

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Highlights

- Economic viability & environmental impact of mango waste biorefineries was assessed.
- Production of bioethanol, heat, and power (Scenario 1) is not economic (NPV<0).
- Co-production of Scenario 1 products with pectin & polyphenols improves economics.
- Scenario 2 is has the least GWP (16.6 kg CO_2 eq.) and FRS (5.55 kg oil eq.).
- Trade-offs between economic and environmental performance must be established.

Declaration of interests

☒ 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.

☐The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: