An assessment of the utilization of waste apple slurry in bio-succinic acid and bioenergy production

Highlights

- The production of bio-succinic acid from apple pomace was assessed.
- Two pathways for bio-succinic acid production involving different co-products were assessed.
- Uncertainty assessments of the economic performances of the processes were undertaken.

Abstract:

Recognizing the importance of succinic acid as one of the most relevant platform molecules, the present study assesses the production of succinic acid from waste apple slurry/pomace (WAP) as a sustainable and renewable feedstock. The assessment has been undertaken by incorporating technical and economic considerations in the analysis while also comparing two succinic acid production scenarios. The aforementioned considerations have been applied by utilizing process simulation results, generated from ASPEN Plus software, as input data to undertake economic assessments using classic economic correlations. Employing well-defined system boundaries, scenarios (1 and 2) to produce bio-succinic acid with either bioelectricity or biogas as co-products, were therefore comparatively accessed. This study was able to demonstrate that waste pomace as a feedstock has the potential to generate low cost succinic acid while scenario 2 constituted the preferred pathway overall. This study results may provide valuable information to policy makers, to enable better decisions regarding the viability, design and execution of large-scale bio-succinic acid production projects based on WAP as the preferred feedstock.

Keywords: biochemicals; economic assessment; waste valorization; apple waste slurry; biogas; biorefinery

1. Introduction

It is now well established that the utilization of fossil resources for energy and petrochemical production constitutes the major contributor to net greenhouse gas generation, leading to an intensification of existing climate change and global warming issues (Ahorsu et al. 2018). In response to the associated unfavorable environmental outcomes of fossil resource utilization, researchers have identified the utilization of renewable biomass as an alternative carbon resource for biochemical and(or) bioenergy production (Okoro et al. 2017). This utilization of biomass as a feedstock for producing valuable energy or chemicals reflects the application of the biorefinery concept (Okoro et al. 2017). While the environmental benefits of utilizing biomass as a resource are well documented, the production of cost-effective alternative to fossil products remains a challenge with E4tech et al. (2015) proposing the utilization of inexpensive biomass feedstocks as one way of enhancing process economics. This is because, for most biorefinery processes, the cost of the feedstock constitutes the dominant influencer of overall economic performance (E4tech et al. 2015). This implies that the utilization of abundant biomass (i.e organic waste) as feedstock for biochemical production may lead to enhanced economic performance of biorefineries. Therefore, in line with the need to enhance the economics of biochemical production systems, the current study seeks to explore the utilization of waste apple pomace as a feedstock for sustainable production of bio-succinic acid as a high-value platform chemical. Apple pomace has been considered as a viable biomass resource due to its undisputed global abundance. Apple pomace accounts for approximately 25% of the original mass of fruit and has a moisture content ranging from 40 wt.% (Sun et al. 2007) to 82.7 wt.% (Gustafsson et al. 2019) containing residue that is typically generated as a waste stream from the apple cider and juice processing industries (Gustafsson et al. 2019; Kosseva 2013a; Kosseva 2013b). Due to its low content of proteins, vitamins, poor nutritional value, and high acidic characteristics, apple pomace remains unsuitable as an animal feedstock and disposal in landfills respectively (Gustafsson et al. 2019). Indeed apple pomace is typically discarded to the environment and is recognized as being capable of leading to significant pollution issues (Shalini and Gupta 2010). These associated unfavorable environmental outcomes associated with the disposal of apple pomace are exacerbated by the magnitude of the waste generated annually with as much as 800,000 tons (Vendruscolo et al. 2008), 1 million tons (Shalini and Gupta 2010), and ~540,000 tons (Gramm et al. 2019) in Brazil, India and Italy respectively. In fact the European Union is reported to generate ~ 4 million tons of apple pomace annually (Lin et al. 2013). Notably, waste apple pomace may serve as a rich source of carbohydrate, with the carbohydrate content existing mainly as starch, sucrose, fructose, glucose, cellulose and hemicellulose (Gustafsson et al. 2019). This important observation may be indicative of the feasibility of employing waste apple pomace in the production of high-value sugar-derived biochemicals such as bio-succinic acid. Bio-succinic acid ($(CH_2)_2(CO_2H)_2$) is a four-carbon aliphatic dicarboxylic acid and water-soluble crystal, identified as one of the top value-added chemicals that can be produced from biomass (Jansen and van Gulik 2014; Werpy and Petersen 2004). Its importance is highlighted by its projected 2025 annual market size of over 115000 tons (MarketWatch 2019). This high market share projected is due to the capacity of bio-succinic acid to be employed in a variety of high-value specialized applications such as in the pharmaceutical industry and food industry and in large volume applications such as in chemical industry in the production of plasticizers, polyurethanes, and useful chemical intermediates (Ferone et al. 2019). Interestingly, in spite of the notable opportunity to produce bio-succinic acid as a high value platform chemical from waste apple slurry, at the time of preparing this manuscript, only the study by González-García et al. (2018) assessing (life cycle assessment) the waste apple slurry to bio-succinic acid process has been reported in the literature. In the study undertaken by González-García et al. (2018), the life cycle assessment of the waste apple slurry to bio-succinic acid process was undertaken. The study was able to establish that the utilization of enzymes constituted the most significant parameter responsible for the highest environmental burdens, due to associated energy cost required in generating the enzymes. The purification step for bio-succinic acid constituted the next most significant impact concern, due to the large mass of organic solvents employed in downstream bio-succinic acid recovery operations. More importantly, to our knowledge, no study has thus far explored the economic performance/feasibility of such a bio-succinic acid production process, while using waste apple pomace as the feedstock. Clearly, therefore, the development of an economically feasible process for the bio refining waste apple pomace to bio-succinic acid process will serve to resolve existing waste management issues while simultaneously providing an additional revenue source for apple farmers and apple processing industries. The present study will therefore explore the economic performance of employing apple pomace as a feedstock for sustainable bio-succinic acid production. For clarity, the novelty of the study is highlighted by the observation that the present study will constitute the first study that explores the techno-economic assessment of bio-succinic acid production from waste apple pomace in the literature. The novelty of this study if further reinforced by the unconventionality of the feedstock employed in the proposed biorefinery as a carbon source more so as apple pomace is yet to be extensively explored as a feedstock for large-scale bio-succinic acid production, and the complexity of the proposed production pathways.

2. Methodology employed in the study.

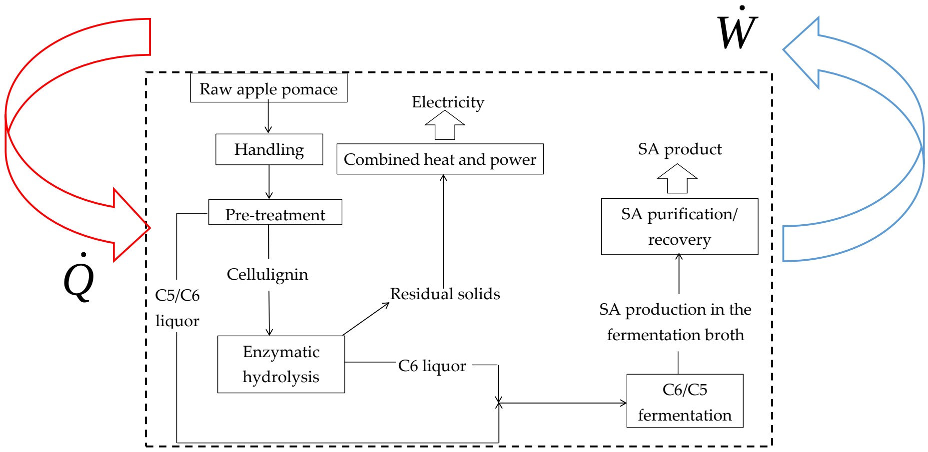
2.1. Process modelling

The present study has employed Aspen Plus® V11 to design, model and simulate the production of bio-succinic using waste apple pomace as feedstock. Aspen Plus® V11 has been selected as a sufficient process modelling and simulation tool for the determination of mass, energy and utility as a basis for undertaking the techno-economic analysis. This is because of its capability to invoke sequential modular and equation oriented modelling strategies in resolving a large number equations (mass and energy balance equations) simultaneously (Okoro et al. 2019b). Suitable processing conditions and configurations have been obtained from literature pomace to facilitate the proposed modeling operation (Hijosa-Valsero et al. 2017) (Hong and Hong 2000; Hong and Hong 2005; Humbird et al. 2011; Kim 2018; Nielfa et al. 2015; Pérez et al. 2008; Song et al. 2007). Thermodynamic property estimation involved appropriate selection steps outlined in the literature (ASPEN 2018; Carlson 1996; Edwards 2008). Based on the guidelines, the non-random two-liquid (NRTL) thermodynamic property method has been specified as the model for predicting corresponding phase equilibrium compositions of chemical species at low pressures (<1000 kPa) and moderate temperatures (2-202 °C) (ASPEN 2018; Carlson 1996; Edwards 2008).

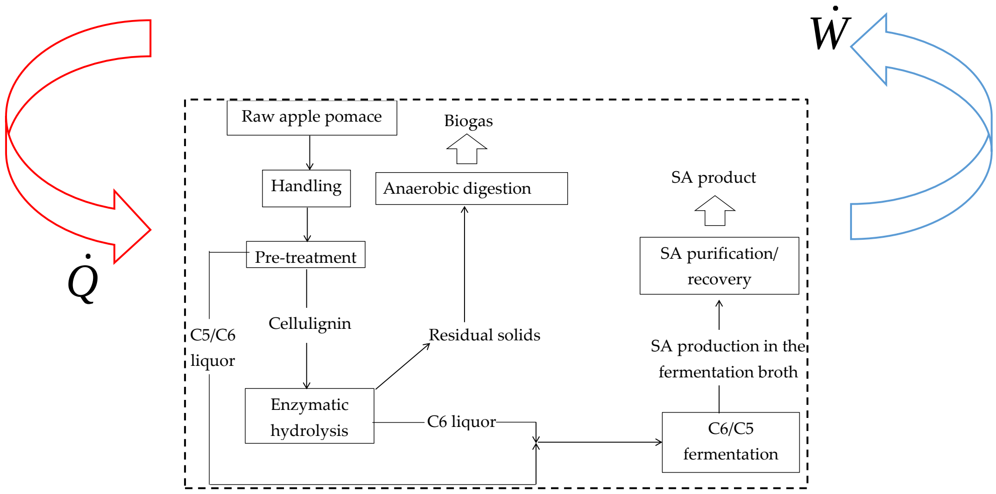
2.2. Process description

Mass and energy balances for the processes shown in Fig. 1 were undertaken. Fig. 1 is schematic illustration of the apple pomace biorefinery for bio-succinic acid production with useful bio-succinic acid and electricity production (scenario 1Fig. 1(a)) or biogas production ((scenario 2 Fig. 1(b)). Given that existing demonstration scale facilities, such as plants by BioAmber, Myriant, Reverdia, are characterized by production capacities ranging from 10 ktons -30 ktons, bio-succinic acid production in this study will be set within this range to enhance practicability (Pais et al. 2016). Fig.1(a) and 1(b) show that initially waste apple pomace (composition summarized in the Table S1 in supplementary document) (Gustafsson et al. 2019) is handled via crushing, at a pressure and a temperature condition of 1 atm and 25 ^{o}C respectively, for further size reduction and to enhance recovery of soluble sugars present in residual juices in the pomace. An electricity consumption of 1.5 kWh per ton of apple pomace (Zimmer 2017) crushed was assumed and introduced in ASPEN plus using Fortran commands in calculator blocks.

The now crushed feedstock is pumped to a pretreatment reactor. In the present study hot water pre-treatment for the solubilisation of hemicellulose has been considered sufficient, since the method facilitates minimal formation of inhibitory compounds such as furfural and minimal losses of useful carbohydrate forms (Kim 2018; Pérez et al. 2008). The hot water pre-treatment has been modelled as occurring at a temperature and pressure of 142.4 ^{o}C and 1 atm, according to the experimental data reported for the pretreatment of waste pomace in the literature (Hijosa-Valsero et al. 2017). Under this condition, a sugar recovery of ~65 % is achieved via cellulose and hemicellulose conversion to C6 and C5 sugars of glucose ($C_6H_{10}O_5$) and xylose ($C_5H_{10}O_5$) respectively. It has been assumed that any sucrose forms present are completely converted to glucose (*G*) and fructose (*F*) forms. Sugars constituting the pre-treatment liquor are subsequently pumped to the fermenter.



(a)



(b)

Figure 1: Flowchart for bio-succinic acid production from apple pomace. In Figure 1(a) and 1(b) solids are employed in electricity and biogas generation respectively (adapted from (Junqueira et al. 2017)). $\dot{Q}$ is the net heat transfer flow rate into the control volume; $\dot{W}$ is the rate of net work done by the system in the control volume.

Residual insoluble fractions of residual cellulose and lignin referred to as cellulignin for simplicity, are then subjected to additional hydrolysis under the action of enzymes which are assumed to be dosed at 20 mg enzyme/g cellulose at a temperature and pressure of 48 °C and 1 atm for 84 h (Humbird et al. 2011). The concentration of solids in the hydrolysis reactor has been maintained at 20 wt.% (Humbird et al. 2011).The enzymatic hydrolysis serves to enhance the mass of useful sugars available for conversion to bio-succinic acid via subsequent fermentation reactions. Having concluded the enzymatic hydrolysis operation, the resulting sugar containing liquor is recovered using a centrifuge and then mixed with the initial sugar liquor generated from the initial pre-treatment process. Fig. 1(a) shows that the solid residue obtained after undertaking the centrifugal separation is made available for electricity generation using a boiler system. The electrical work required by the centrifuge has been assumed to be 1 kWh per m^3 feed and incorporated using calculator blocks in ASPEN plus (Szepessy and Thorwid 2018). The utilization of solids for electricity generation via a combined heat and power (CHP) system will be investigated in scenario 1. The CHP system is based on a Rankine cycle, which is characterized by steam superheating. In this study, the water is initially pressurised using a pump (0.9 efficiency) the pressurised water is subsequently heated using waste heat generated from the combustion of solids (reactions presented in the supplementary document) via the employment of heat exchangers to generate superheated steam. The superheated steam is then transferred to an isentropic turbine, for the generation of useful electrical work via the expansion of the pressurized superheated steam to 1 atm. The resulting hot water is available for reuse within the system. Scenario 1 will have the addition cost constraint of treatment of the wastewater streams in a water treatment plant. Such additional waste water treatment cost are assumed to be avoided in Scenario 2 since, the waste streams containing digestible solids are employed as a feedstock for anaerobic digestion for biogas production (scenario 2 Fig. 1(b)). The AD process has been modelled as occurring under mesophilic temperature conditions of 37 ^{o}C with biogas generation assumed to occur according to Boyles equation (Nielfa et al. 2015). It is acknowledged that biogas productivity will depend on several factors such as the substrate-loading rate and microbial population. Thus, the biogas estimate may vary. The effects of such biogas yield variations on the viability will be assessed. The approaches employed are discussed in section 2.4 below. Further upgrading of the biogas stream was not undertaken in the present study. Fig. 1 shows that the sugar liquor containing both C5 (pentose) sugar and C6 (hexose) sugars is then subjected to oxygen free fermentation under the action of *Actinobacillus succinogenes*. *A. succinogenes* is a gram-negative facultative anaerobe, which has been shown to demonstrate the native capacity to convert C5 and C6 sugars to bio-succinic acid (Guarnieri et al. 2017). Furthermore, *A. succinogenes* has been shown to be effective in the conversion of sugars to bio-succinic acid with attractive yields of bio-succinic acid attainable (Bradfield et al. 2015). The fermentation operation occurs at the temperature and pressure condition of 30 ^{o}C and 1 atm respectively with associated reactions and conversions obtained from the work of Nieder-Heitmann et al. (2019). At the conclusion of fermentation process, the bio-succinic acid produced and contained in the fermentation broth is cooled then pumped to the purification area. To facilitate bio-succinic acid recovery from the fermentation broth, the reactive extraction method described by Song et al. (2007) was assumed to be sufficient (Hong and Hong 2000; Hong and Hong 2005; Song et al. 2007). According to Song et al. (2007), pure bio-succinic acid (>99 %) is recovered using recovery solvent mixture of 1-octanol (OCTA) and tri-n-octylamine (TOA) with mass fractions of 92 wt.% and 8 wt.% respectively at the temperature of 25 °C, such that a v/v ratio of the solvent mixture to the fermentation broth is 1 [33]. The resulting reaction extraction mixture is then subjected to vacuum distillation (temperature of 75 °C, pressure 0.7 atm), acid crystallization at 4 °C and drying at 100 °C obtain pure bio-succinic acid (>99 %) (Hong and Hong 2000; Hong and Hong 2005; Song et al. 2007). In both scenarios 1 and 2, the following mass and energy balance equations at steady state were used and solved using ASPEN plus for each of the individual processes shown in Fig. 1;

$$\sum_{i=1}^{n} \dot{m}_{in} = \sum_{i=1}^{n} \dot{m}_{out} \tag{1}$$

$$\dot{Q} = \left[\sum_{i=1}^{n} \dot{m}_i h_i\right]_{out} - \left[\sum_{i=1}^{n} \dot{m}_i h_i\right]_{in} + \dot{W} \tag{2}$$

where, $\dot{Q}$ is the net heat transfer flow rate in kJ/h into the system in the control volume of the individual process, per s; h_i is the specific enthalpy of the *i*th stream, in kJ/kg; $\dot{W}$ is the rate of net work done by the system in the control volume of the individual process in kJ/h ; and $\dot{m}$ is the mass flow rate of the *i*th stream, in kg/h.

All heating and cooling duty requirements of the processes have been minimised via heat integration using the ASPEN enabled ASPEN energy analyser® V.11. The ASPEN energy analyser® V.11 facilitates heat integration via pinch analysis technique with a minimum allowable temperature difference of 10 °C, between the 'hot' and 'cold' streams at 'pinch point' in the heat exchanger system has been specified(Okoro et al. 2018; Petersen et al. 2020). The pinch point method is not discussed further in the present study as it is well-known and discussed elsewhere in an engineering text (Sinnot and Towler 2009).

2.3. Economic assessments

In the present study the ASPEN process economic analyzer V11 has been employed in equipment costing and sizing. The purchase costs are based on equipment cost data from 2016 (ASPEN technology Inc., personal communication, 1 August 2017). For purchase cost of equipment not costed in ASPEN such as the cost of the hammer crusher employed in handing of the waste apple pomace and the cost of the boiler employed for combined heat and power generation were sourced from external sources (Alibaba 2020b; ETSAP 2010). These externally sourced purchase costs were subsequently adjusted for the desired capacity as follows (Towler and Sinnott 2008).;

$$C_i = C_{i,vref}\left(\frac{v}{vref}\right)^k \quad (3)$$

where C*i* is the purchase cost for the *i* th equipment with a capacity of *v*, C*i,vref* is purchase cost for the *i* th equipment with a reference capacity *vref,* and *k* is the scaling factor specified as 0.6 in the present study for simplicity(Towler and Sinnott 2008). In this study, the chemical engineering plant cost index (CEPCI) has been utilized in estimating the current equipment purchase based on the estimated equipment cost generated by ASPEN process economic analyzer for the year 2016. The cost of the equipment for the year 2020 were therefore estimated as follows (Okoro et al. 2019b);

$$C_{i,2020} = C_{i,2016}\left(\frac{CEPCI_{2020}}{CEPCI_{2016}}\right) \quad (4)$$

where $C_{i,2016}$ and $C_{i,2020}$ are the purchase costs in the year of 2016 and 2020. $CEPCI_{2016}$ and $CEPCI_{2020}$ are specified as 541.7and 607.5 respectively(Okoro et al. 2020). All estimates are therefore presented for the reference year of 2020. Having estimated the purchase costs, the installed cost for each equipment is estimated by utilizing a multiplying factor for each equipment type (Peters et al. 2003). Other cost components for total capital investment (TCI) estimation (Okoro et al. 2020) , employed in the presented study are summarized in the supplementary document. The total operating (production) cost incorporated both the fixed and the variable production costs components. The estimation methods employed in the total production cost determination are presented in the supplementary document. In undertaking the economic assessment of waste apple pomace conversion to bio-succinic process several economic assumptions have been incorporated to facilitate the study. The assumptions are presented in Table 1 (Okoro et al. 2020).

Table 1: Economic parameters and assumptions

Parameter	Value
Location	USA
Base year	2020

Project lifetime (y)	30
Plant availability (h/y)	7200
Tax rate (%)	30
Debt interest (%)	12
Cost of equity (%)	12
Equity-debt (%/%)	50/50
WACC/discount rate (%)	12
Salvage value (US$)	0
Depreciation	Straight line

Having determined the values of OPEX and CAPEX, the minimum selling price (MSP) for bio-succinic acid production using apple pomace as feedstock was estimated. To estimate the MSP a discounted cash flow (DCF) analysis is undertaken. In developing the DCF table, bio-succinic acid constitutes the sellable product in scenario 1 while in scenario 2, bio-succinic acid and biogas have been specified as constituting sellable products. For simplicity it has been assumed that the selling price of biogas is dependent on its methane content with the methane content having a selling price of US$ 1.121 per kg (Globalpetrolprices 2020). Employing the DCF analysis the cost of bio-succinic acid, expressed in US$/kg, that will result in a zero net present value (NPV) of the project, was estimated. The NPV was calculated as follows (Okoro et al. 2020) ;

$$\mathrm{NPV} = -\mathrm{CI} + \sum_{n=1}^{t} \frac{Net_R}{(1+i)^n} + \frac{V_n}{(1+i)^n} \tag{5}$$

where CI represents the capital investment cost, i represents the discount rate specified as 12%, and n denotes 30 y, which is the assumed project lifetime. V_n is the salvage value, which is zero. Net_R, represents the annual cash flow less the assets, was calculated using

$$Net_R = (R_t - C_t - D_t)(1-T) + D_t \tag{6}$$

where R_t and C_t denote the total revenue before tax and total cost before tax in year t respectively; T and D_t denote the corporate marginal tax rate and the depreciation over the life of the plant.

The bio-succinic acid cost when the NPV is specified as zero was designated as the minimum selling price of bio-succinic acid.

2.4. Uncertainty assessments

Crucially, a review of the discussions highlights several assumptions have been utilized in costing and estimating the MSP of the bio-succinic acid produced from waste apple pomace. This observation implies that the economic performance may be subjective and thus vary with differences in the underlying assumptions. The uncertainties in the results must therefore be investigated. A similar approach was employed in the previous work (Okoro and Sun 2019) (Okoro et al. 2019a). Uncertainties due to changes (-50% to +50%) in the TCI, TOP, WACC, project lifespan and purchase cost of equipment were assessed. Additionally for the biogas production scenario, the added uncertainty in methane content of -50% was also investigated. To assess these uncertainties, a multivariate Monte-Carlo analysis was undertaken and the resulting MSP probability distribution for bio-succinic acid production from apple pomace was presented. In the present study a triangular probability distribution of the determinants was employed (Ou et al. 2015) and the resulting probability density according to the probability density function defined as follows (Okoro and Sun 2019);

$$f(x) = \frac{1}{\sqrt{2\pi} \cdot \sigma} \cdot e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} \quad (7)$$

where x represents the values of the MSP, μ represents the mean value of MSP and σ represents the standard deviation of MSP. The area under the curve of f(x) for the interval (a,b) specifies the probability, β, of MSP and was estimated as follows(Okoro and Sun 2019);

$$\beta(a < x < b) = \int_a^b f(x)dx \quad (8)$$

In the present study the stochastic analysis was performed with 1,000 trials using Minitab® V16 to reduce computational time.

3. Results and discussion

3.1 Simulation outcomes

Employing Aspen Plus the model presented in Fig. 2 and Fig. 3, the mass balance results of major streams are presented in Table 2 for scenario 1 and scenario 2. Fig.2 shows that the apple pomace (stream FEED) is crushed and homogenized in the handling hierarchy (100) after which the resulting stream (stream 2) with a mass flow rate of 99244.17 kg/h (Table 2) is subjected to a pretreatment operation using hot water pre-treatment in the pre-treatment hierarchy (200) discussed earlier above. The reactions occurring during the pretreatment have been modelled using a stoichiometric reactor model in Aspen plus and are presented in the supplementary document. The resulting mixture is cooled to 25 °C and centrifuged to enable the separation of solids of cellulose-lignin from the liquor after pretreatment (200). The stream of solids containing useful cellulose is further hydrolyzed in the pre-treatment hierarchy (200) as discussed earlier above. A stoichiometric reactor model in Aspen plus has been employed in modelling all hydrolysis reactions and are presented in the supplementary document.

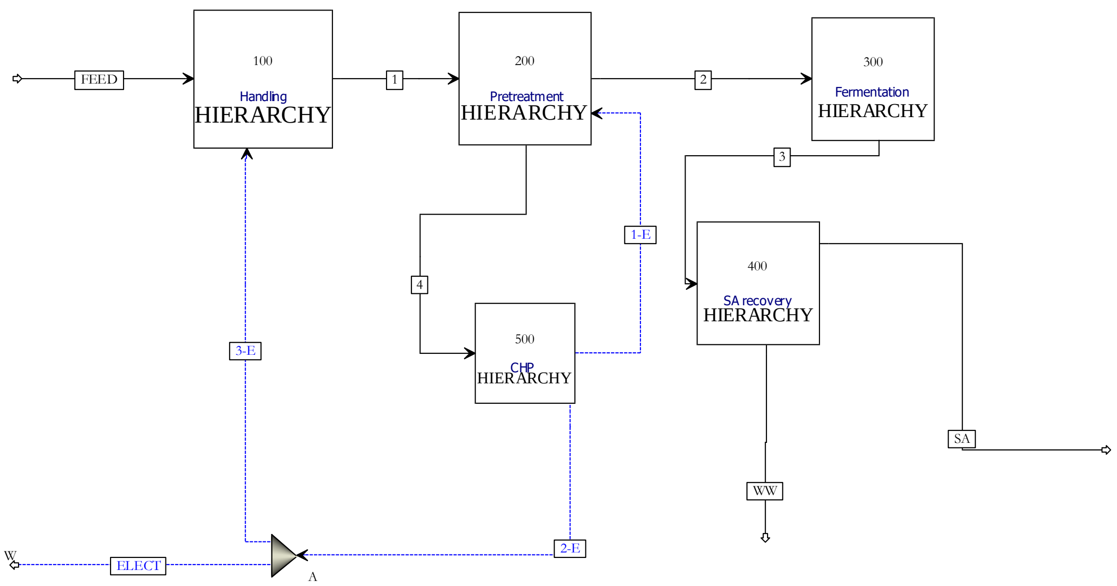


Figure 2: ASPEN plus output for bio-succinic acid production from apple pomace with electricity production (blue-dashed lines denote electricity flow, black continuous lines denote material flow). In the Figure SA denotes bio-succinic acid

Table 2 and Table 3 shows that the sugar constitutes about 5% of the stream (stream 3) transferred to the fermentation hierarchy (300). In scenario 1, all residual solids are transferred to a CHP plant for electricity generation. The liquor containing the total sugar available (stream 3) is then pumped to the fermentation hierarchy (300) to enable bio-succinic acid production. Sugar fermentation has been modelled using a stoichiometric reactor model with the associated reaction equations presented in the supplementary document. For simplicity, CO_2 necessary for bio-succinic acid, production is supplied (purchased) externally. To enhance the completeness of the fermentation reaction, 5 wt.% of the fermentation broth is recycled. The resulting fermentation broth (stream 4) is then transferred to the bio-succinic recovery hierarchy (400) for bio-succinic recovery. In this bio-succinic recovery hierarchy (400), the broth is cooled to 25 °C and mixed with a solvent mixture of 1-octanol (OCTA) and tri-n-octylamine (TOA) with mass fractions of 92 wt.% and 8 wt.% respectively at the temperature of 25 °C, such that a v/v ratio of the solvent mixture to the fermentation broth was 1 (Song et al. 2007). It is assumed that the extractive reaction was sufficient to recover the bio-succinic from the broth mixture. Table 2 shows that the mass of bio-succinic generated is 2063.70 kg/h.

Finally, the residual water stream (WW) containing residual sugars and acid (~3 wt% in Table 2/scenario 1) is transferred to a water treatment plant before reuse. In scenario 2 (Fig 3.), this residual aqueous stream (WW) are transferred to the anaerobic digestion area together with the solids (i.e cellulose-lignin) employed as feed to the CHP in Fig. 2. The mixture is pumped to the anaerobic digestion hierarchy (500) as discussed above with the resulting biogas recovered after cooling to 25 °C.

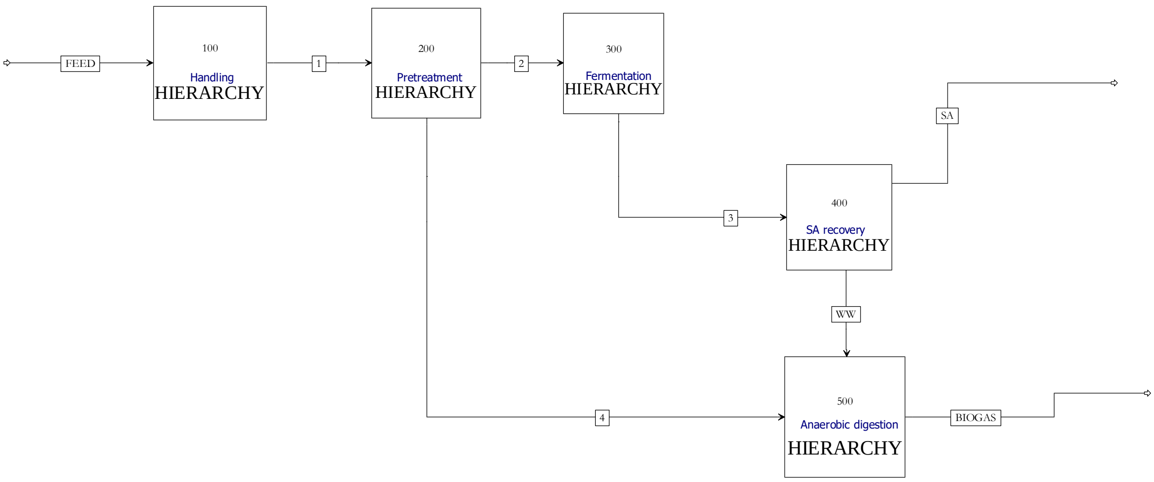


Figure 3: ASPEN plus output for bio-succinic acid production from apple pomace with biogas production (black continuous lines denote material flow). In the Figure SA denotes bio-succinic acid

The post-anaerobic digestion water is assumed to be reusable for other activities such as for apple pomace farming since it contains negligible masses of impurities (0.5 wt.%) as shown in Table 2. Tables 2, and 3 show that ~15 ktons of bio-succinic acid is generated per year which is ~40 % of the annual mean global production volume of 40 kton (Cherubini and Strømman 2011). The minimum heating and cooling utilities as determined in ASPEN energy analyzer® V.11 are also presented in Table 4.

Table 2: Mass balance results for major streams in scenario 1 and scenario 2

	Scenario 1			Scenario 2	
Stream name	SA	WW	Biogas	SA	WW-biogas
Mass Fractions (*x*)					
Glucose	0	0.002	0	0	0
Water	0	0.971	0	0	0.995
CO_2	0	Trace	0.734	0	Trace
Lignin	0	0	0	0	0
Cellulose	0	0	0	0	0
Extract	0	0.003	0	0	0.003
Hemicellulose	0	0	0	0	0
Starch	0	0	0	0	0
Fructose	0	0.021	0	0	0.002
Pectin	0	0	0	0	0
Sucrose	0	0	0	0	0
Xylose	0	Trace	0	0	0
SA	0	0	0	0	0
Acetic acid	0	Trace	0	0	0
Formic acid	0	Trace	0	0	0
SA	1.0	0	0	1.0	0
Methane	0	0	0.266	0	0
Mass Flows (kg/hr)	2063.70	97630.47	3346.676	2063.704	95039.6

WW denotes waste water from scenario 1, SA denotes bio-succinic acid, WW-biogas denotes waste water from scenario 2

Table 3: Summarized mass and energy balance results.

Process result	Value (scenario 1)	Value (scenario 2)
Mass flow of bio-succinic acid (ton/y)	14858.7	14858.7
Heating utility (kW)	55290.0	55290.0
Cooling utility (kW)	46730.0	52920.0
Electricity generated (kW)	385.4	0

Table 4 shows that the total capital investment (TCI) estimation in scenario 1 of MUS$ 12.38 (M indicates a million unit) is slightly greater (0.4%) that the TCI in scenario 2 MUS$ 11.90. The differences in the TCI is due to the differences in the processing pathways employed in the management of the waste stream generated. Table 4 also shows that a lower total operating cost (TOC) is estimated in scenario 1 of ~MUS$ 8.7 compared to the TOC scenario 2 of ~MUS$ 10. The results presented suggest that it may be more economically viable to consider the utilization of the waste solids in the generation of biogas rather than using solids as feeds for electricity generation. This is because of the calculated MSP of bio-succinic acid produced in scenario being ~0.44 times the MSP of bio-succinic acid produced via scenario 1. The estimated MSPs in Table 4 are however, a function of the associated underlying assumptions employed implying that there is a risk of variabilities in the unit cost estimate. The uncertainty of the MSPs for both scenarios was therefore assessed as discussed earlier above in section 2.4. The probability distributions for MSPs in both scenarios are presented in Fig. 4.

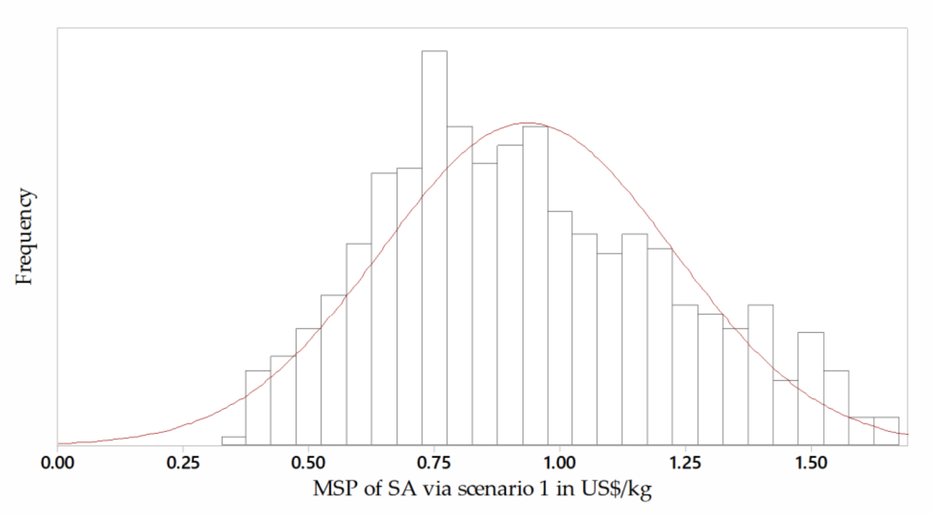
Table 4: Outcome of the economic assessment.

Economic parameter	Scenario 1	Scenario 2
Fixed capital investment(MUS$)	12.38	11.90
Working capital investment(MUS$)	0.62	0.59
Total capital investment (MUS$)	13.00	12.48
Fixed operating cost (MUS$)	2.20	2.19
Variable operating cost (MUS$)	6.45	7.85
Total operating cost (MUS$)	8.65	10.04
Minimum selling price (US$/kg)	0.73	0.33

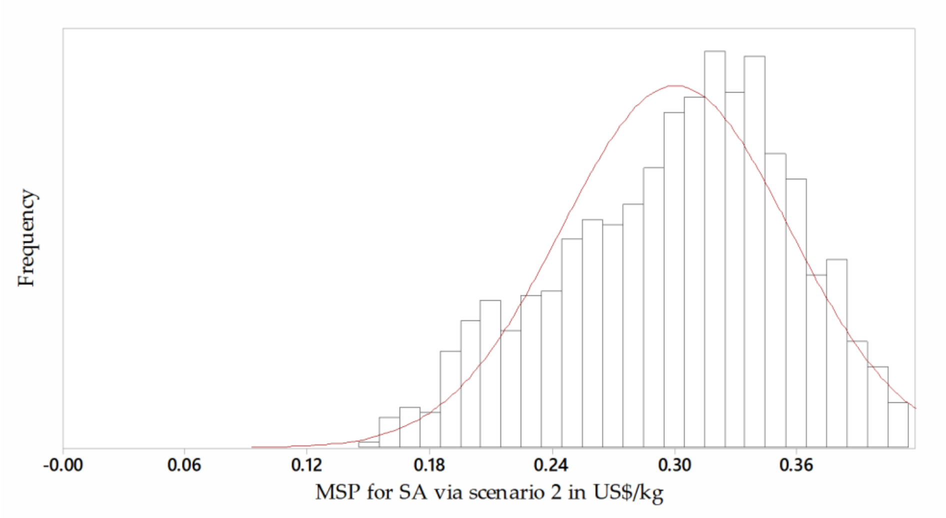
Economic parameter	Scenario 1	Scenario 2
Fixed capital investment(MUS$)	12.38	11.90
Working capital investment(MUS$)	0.62	0.59
MUS$ denotes million US dollars		

Fig. 4 shows that the mean value of the MSP of bio-succinic acid in scenario 1 is US$ 0.94 per kg with a standard deviation of US$ 0.3 per kg in scenario 1 while a mean MSP of bio-succinic acid in scenario 2 is US$ 0.3 per kg with a standard deviation of US$ 0.06 per kg. The lower MSP estimated in scenario 2 is due to the additional revenue from the sales of the biogas product. For completeness, further comparison of the MSPs generated in the present have also been compared to other bio-succinic acid production systems in literature that employed different waste steams as renewable carbon sources (Ghayur et al. 2019; Stylianou et al. 2020).

In the study undertaken by Ghayur et al. (2019) pulp logs were employed in the production of bio-succinic acid. The bio-succinic acid generated was shown to have a MSP of US$ 0.76 per kg. This value is comparable with the MSP of bio-succinic acid (US$ 0.73 per kg) calculated for the scenario 1 production process as investigated in the present study but as expected, higher than the MSP of bio-succinic acid (US$ 0.33 per kg) calculated for the scenario 2. This observation is consistent with our previous discussions above with the additional revenue generation from the sale of the energy dense biogas product, leading to relatively enhanced economics in scenario 2. Notably the study undertaken by Stylianou et al. (2020) showed that the MSP of bio-succinic acid produced from organic waste sourced hydrolysates could be as high as US$ 2.5 per kg, which is higher than the MSPs of both scenarios discussed in the present study. This observation was not entirely unexpected given that the feedstock cost of the hydrolysate was specified as US$ 0.025 per kg. In the present case the assumed feedstock cost of 0 has been assumed. Indeed the high MSP of US$ 0.025 per kg reported in the study by Stylianou et al. (2020) reinforces the role of feedstock cost in determining the overall the economic performance of biorefinery production processes. Nevertheless, both MSPs of the bio-succinic acid generated via the two scenarios considered still on average compare favorably with the selling price of bio-succinic acid in the global market which is ~ US$ 1.6 per kg (high grade)(Alibaba 2020a). As stated earlier above the lower estimated MSPs is due to the utilization of waste apple pomace such that the cost of feedstock is assumed to be US$ 0 per kg. This assumption (feedstock cost of US$0 per kg) is a major concern, with its implication discussion in section 3.2 below. The use of waste apple pomace as a feedstock is therefore of particular importance to the economics of bio-succinic acid production since the feedstock remains one of the most significant determinants of the profitability of bio-succinic acid production (Nghiem et al. 2017)



(a)



(b)

Figure 4: Probability distribution of the minimum selling price of bio-succinic acid from apple pomace.

3.2. Notable considerations and study limitations

The present study has included several assumptions in an attempt to simplify the ASPEN model such as ignoring possibilities of dust/sand impurities in the apple pomace feed, assuming perfect mixing in the reactors for enhanced heat and mass transfer as well as the assumed zero cost of the apple pomace feedstock. The assumption of the absence of dust/sand impurities is because the sand/dust content of apple pomace will vary continuously with location, collection approach etc. Furthermore, the assumption that pomace is freely available (i.e feedstock cost of US$ 0/kg) implies that possible collection and acquisition costs were ignored. This assumption was not incorporated in the study since waste apple pomace may be sourced from numerous locations characterized by varying costing and logistical constraints that may influence the overall performance of apple pomace to bio-succinic acid conversion processes. Additionally, a review of literature suggests that apple pomace composition may vary significantly depending on the generation pathway (Vendruscolo et al. 2008). It must therefore be emphasized that the current study can mainly be considered as an 'initial-level' comparison of two scenarios for apple pomace conversion to bio-succinic acid. Thus while the approach is faultless regarding comparing the two possible pathways, there may be some limitations when the MSPs of the bio-succinic acid products are compared, separately, relative to the selling price of the fossil –succinic acid. It is anticipated that additional studies must therefore investigate supply chain optimization opportunities, in MSP determination, while considering also considering possible logistical cost constraints that may characterize the different collection apple pomace sites.

4. Conclusion

The economics of bio-succinic acid production from apple pomace has been studied in this work. Techno-economic models for the production of bio-succinic acid from apple pomace via two pathways (scenario 1 and scenario 2) were developed such that in scenario 1 pathway all insolubles were employed in the generation of electricity while in the alternative scenario 2 pathway, solids were degraded further for biogas production. The study demonstrated that both pathways had the potential of being economically favorable concerning the minimum selling prices (MSPs) with the base case scenarios 1 and 2 presenting bio-succinic acid MSPs of US$0.73 per kg and US$0.33 per kg respectively compared to existing fossil-succinic acid selling price of US$1.6 per kg . Multivariable analysis however established stochastic variations in the estimates with scenatio2 and scenario 1 projected to present 95 % probabilities of generating bio-succinic acid of MSPs of US$ 0.3 per kg and US$ 0.94 per kg with standard deviations of US$ 0.06 per kg and US$ 0.30 per kg respectively.

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5. Disclosures and declarations

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Conflicts of Interest: The authors declare no conflict of interest in this study.

Availability of data and material: The simulation report has also been provided for the benefit of the reader.

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