Comparative techno-economic assessment of sugarcane biorefineries producing glutamic acid, succinic acid, levulinic acid and xylitol from A-molasses and lignocellulosic biomass

by

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Abstract

The financial sustainability of the South African sugar industry is currently threatened by difficult economic conditions, including external factors such as low sugar prices by new global competitors, and increased production costs. Because of these challenges, some of the sugar mills face potential closure in the future because they are no longer profitable. With this in mind, it has been proposed that sugar mills should valorise by-products to increase profitability.

Molasses and lignocelluloses (bagasse and trash) biomasses are the two by-products of the sugar mill as the potential first-generation (1G) and second-generation (2G) feedstocks, respectively, for valorisation in a biorefinery context. These feedstocks are promising carbon sources for the prominent global bio-based economy, owing to their low cost, high content of the fermentable sugars, and relative abundance. The global demands, technological maturity, and potential to penetrate new markets support the section of the product of interest: glutamic acid (GA), levulinic acid (LA), succinic acid (SA), and xylitol for investigation in a biorefinery context as a way to diversify products in a sugar mill, thereby increasing revenues.

An overall aim of this study was to determine if the profitability of sugarcane biorefineries producing GA, LA could be further improved from the previously attained profitable scenarios that utilised the second-generation (2G) feedstock (lignocelluloses), by further considering 1G feedstock (A-molasses). Considered as a cleaner raw material, 1G results in the elimination of the costly pretreatment and enzymatic hydrolysis processes. Furthermore, the integration of feedstocks (1G and 2G) was investigated to evaluate the economies of scale benefits through a sole production of GA, LA, and SA. Thereafter, multi-production of the aforementioned with xylitol was considered.

Literature data were used to design and develop the process flow sheets for detailed AspenPlus® process simulation models considering feed capacities of 25.4 t/h A molasses and 113.5 t/h of lignocellulose. The generated mass and energy balances data were used for techno economic analysis for a yearly operation if 5000 hours.

With reconfigurations on the sugar mill, 1G biorefineries can benefit from utilising the existing CHP facility or incorporating low-cost, low-pressure boiler in the 1G biorefineries. As a result, 1G biorefineries showed better economic performances than their 2G biorefinery counterpart.

The integration of feedstocks in 1G2G designs showed the economies of scale benefits, compared to 1G-only scenarios. This was demonstrated by the decrease in minimum selling price (MSP) from \$2950/t to \$2102/t in 2G LA and 1G2G LA scenario, \$2237/t to \$1745/t in

2G SA and 1G2G SA, and $2969 to 2205 for 2G GA and 1G2G GA scenarios, respectively. Comparatively, multiproduct facilities achieved lower MSP than the sole product 1G2G configurations counterparts ($2205/t vs $1926/t for GA and $2600/t vs $1133/t for LA). Except 1G2G SA+Xylitol at $1745/t vs $1888/t. This can be accounted for by the reduction in sales for SA from when there was an upgrade from sole product to multiproduct.

Since techno-economic evaluation alone does not fully justify the sustainability and competitiveness of the proposed biorefineries in the eyes of investors or decision-makers, a study on the Life cycle assessment considering the environmental and social impact of biorefineries could be further investigated.

Opsomming

Die finansiële volhoubaarheid van die Suid-Afrikaanse suikerindustrie word tans bedreig deur moeilike ekonomiese kondisies, insluitend eksterne faktore soos lae suikerpryse deur nuwe globale mededingers, en verhoogde produksiekostes. As gevolg van hierdie uitdagings, staar sommige van hierdie suikermeule potensiële sluitings in die toekoms in die gesig omdat hulle nie meer winsgewend is nie. Met hierdie in gedagte, is dit voorgestel dat suikermeule byprodukte moet valoriseer om winsgewendheid te verhoog.

Molasse en lignosellulose (bagasse en afval) biomassa is die twee byprodukte van die suikermeule as die potensiële eerste-generasie (1G) en tweede-generasie (2G) voermateriale, onderskeidelik, vir valorisasie in ’n bioraffinadery-konteks. Hierdie voermateriale is belowende koolstofbronne vir die prominente globale bio-gebaseerde ekonomie, weens hul lae koste, hoë inhoud van die fermenteerbare suikers, en relatiewe volopheid. Die globale vereistes, tegnologiese rypheid, en potensiaal om nuwe markte te penetreer, ondersteun die deel van die produk in belang: glutamiensuur (GA), levuliniensuur (LA), suksiensuur (SA), en xilitol vir ondersoek in ’n bioraffinadery-konteks as ’n manier om produkte te diversifiseer in ’n suikermeul, en daardeur inkomste te verhoog.

’n Algehele doel van hierdie studie was om te bepaal of die winsgewendheid van suikerrietbioraffinaderye wat GA, LA produseer, verder kon verbeter uit winsgewende scenario’s wat voorheen verkry is deur die 2G-voermateriaal (lignosellulose) te gebruik, deur 1G-voermateriaal (A-molasse) verder te oorweeg. Oorweeg as ’n skoner rou-materiaal het 1G die eliminasie van die duursame voorbehandeling en ensimatiese prosesse tot gevolg. Verder, die integrasie van voermateriaal (1G en 2G) is ondersoek om die ekonomieë van skaal se voordele te evalueer deur ’n enkel-produksie van GA, LA en SA. Daarna is multi-produksie van die voorafgenoemde met xilitol oorweeg.

Data uit literatuur is gebruik om die prosesvloeikaarte te ontwerp en ontwikkel vir gedetailleerde Aspen Plus®-prosessimulasiemodelle wat voerkapasiteite van 25.4 t/h A-molasse en 113.5 t/h lignosellulose oorweeg. Die gegenereerde massa- en energiebalanse se data is gebruik vir tegno-ekonomiese analise vir ’n jaarlikse bedryf van 5000 ure.

Met hersamestellings op die suikermeule, kan 1G-bioraffinaderye voordeel trek deur die bestaande Gekombineerde hitte en krag (CHP) fasiliteite of die lae-koste, lae-druk ketel in die 1G-bioraffinaderye te inkorporeer. As ’n gevolg, het 1G-bioraffinaderye beter ekonomiese doeltreffendheid gewys as hul 2G-bioraffinadery eweknie.

Die integrasie van voermateriaal in 1G2G-ontwerpe het die voordele van die ekonomieë van skaal gewys, in vergelyking met die 1G-alleenlik scenario's. Hierdie is gedemonstreer deur die afname in (Minimum Verkoopprys) MSP van $2950/t tot $2102/t in 2G LA en 1G2G LA-scenario, $2237/t tot $1745/t in 2G SA en 1G2G SA, en $2643 tot $2794 vir 2G GA en 1G2G GA-scenario's. In vergelyking het multi-produkfasiliteite laer MSPs teenoor die enkel-produk 1G2G-konfugirasies se eweknieë bereik ($2205/t vs. $1926/t vir GA en $2600/t vs. $1133/t vir LA). Buiten 1G2G SA+xilitol by $1745/t vs. $1888/t. Hierdie kan verduidelik word deur die reduksie in verkope vir SA vandat daar opgradering van enkel-produk tot multi-produk was.

Aangesien tegno-ekonomiese evaluasie alleen nie die volhoubaarheid en mededingendheid van die voorgestelde bioraffinaderye ten volle regverdig in die oë van beleggers of besluitnemers nie, kan 'n studie op die lewensiklusassessering, wat die omgewings- en sosiale impak van bioraffinaderye oorweeg, verder ondersoek word.

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Table of contents

List of illustrations

List of Figures

List of Tables

Nomenclature

Terms, Acronyms, and symbols	Description
1G	First generation
1G2G	Integrated first generation and second generation
2G	Second generation
AD	Anaerobic digestion
BDO	1,4-Butanediol
CEPCI	Chemical engineering plant cost index
CHP	Combined heat and power
COD	Chemical oxygen demand
DA	Dilute acid
EB	Energy balance
FCI	Fixed capital investment
FOC	Fixed operating cost
GA	Glutamic acid
GAC	Granular activated carbon
GHG	Greenhouse gas
IRR	Internal rate of returns
ktpa	Kilo tonnes per annum
LA	Levulinic acid
LLE	Liquid-liquid extraction
MB	Mass balance
MIBK	Methyl Isobutyl ketone
MW	Mega joules
PBS	Polybutylene succinate
PBT	Polybutylene terephthalate
PPM	Part per million
SA	Succinic acid
SBA	Strong base anion
SCB	Sugarcane bagasse
STEX	Steam explosion
TCI	Total capital investment
TCOP	Total cost of production
TDC	Total direct cost
TEA	Techno-economic assessment
TEC	Total equipment cost
THF	Tetrahydrofuran
TIDC	Total indirect cost
TMA	Trimethylamine
TOA	Tri-n-octylamine
TRL	Technological readiness level
VOC	Variable operating cost
WAC	Weak acid cation
WHO	World health organisation

1 Introduction

1.1 Background and motivation

The South African sugar industry is fully developed and continues to act as one of the major agricultural contributors on the country's economy through job creation and revenues. However, the industry is currently facing difficult economic challenges because of numerous external factors such as new global competition with low-cost producers, increased production cost, sugar tax introduced in 2017 and drought that results in low crop yield (Gorgens et al., 2016). With these challenges experienced, there is a threat of closure in the near future for some of the sugar mills that are already economically unviable. To safeguard the financial sustainability of the South African sugar industry, it is proposed that the existing sugar mills should valorise their by-products to increase their profitability, by adopting an integrated biorefinery approach (Mandegari et al., 2017a). Also, supporting this approach is the current plan of the South African government to move towards a green economy because of the binding Paris Agreement to reduce the GHG emissions (Pachón et al., 2018).

Molasses and lignocelluloses (bagasse and harvesting residues, also known as trash) biomasses are the two by-products of the sugar mill as the potential first-generation (1G) and second-generation (2G) feedstocks, respectively, for valorisation in a biorefinery context. These feedstocks are promising carbon sources for the global bio-based economy, owing to their low cost, high content of the fermentable sugars and relative abundance (Hara et al., 2013; Jiang et al., 2017; Taylor et al., 2015). In a sugar mill, molasses is produced during the crystallisation processing and it finds low cost in animal feed or ethanol production (Mbohwa, 2013; Rackeman and Doherty, 2012). Sugarcane lignocellulose is presently used for steam and energy generation in the combined heat and power (CHP) plant, although this is done inefficiently; new biorefinery facilities that process 2G will therefore include installation of a new high-efficiency CHP plant to serve both the sugar mill and biorefinery, and liberate surplus bagasse for biorefinery conversion. Furthermore, by moving away from cane burning before harvesting, substantial additional amounts of harvesting residues ("trash") can be made available, as additional lignocellulose feed to the biorefinery complex (Mandegari et al., 2017a).

The South African industry has been looking into opportunities of diversifying income streams by co-producing biofuels such as bioethanol, or biobutanol with electricity, which is then sold

to the national grid from lignocellulose (Mandegari et al., 2017a; Petersen et al., 2018; Taylor et al., 2015). However, the more recent studies have been focused on the opportunities available for the production of valuable bioproducts other than biofuels (Farzad et al., 2017b; Kapanji et al., 2019; Nieder-Heitmann et al., 2019; Özüdoğru et al., 2019). For this study xylitol, glutamic acid (GA) succinic acid (SA) and levulinic acid (LA) have been selected (hereafter, these products all together are referred to as products of interest), based on their global demands, potential applications and the advancements on the technological maturity of their production processes (Taylor et al., 2015; Werpy and Petersen, 2004).

The estimated 50 million tonnes per annum global production of biobased fuels and chemicals is currently dominated by the well-established products such as ethanol, 1,3-propenediol and lactic acid (Rosales-Calderon and Arantes, 2019; Taylor et al., 2015). However, biobased SA also has the potential to become one of the dominating products due to its fast-growing markets. It currently serves a wide range of applications in a niche market with high value such as food additives and personal care to large volume applications in biopolymers, coating and plasticisers (Dogbe et al., 2020). Currently, it is more expensive to produce biobased SA as compared to fossil-based SA. The biobased price of $2860 per ton is competing with a fossil base one at $2500 per ton (Rosales-Calderon and Arantes, 2019). Moreover, it is expected that the global SA market size will rise to 90 ktpa by 2025 (Gerardy et al., 2020).

On the other hand, xylitol has attracted global interest due to its health benefits when used as a sweetener. As a result, there exists a strong demand for xylitol in pharmaceutical, odonatological and food industries. In 2015, it was reported to have a market volume of 191 ktpa with a market price of $3900 per ton (Rosales-Calderon and Arantes, 2019). Glutamic acid, also being the product of interest, it is used to derive monosodium glutamate (MSG), which is used as a flavour enhancer and food additive in the food processing industry. Currently, its global market size is estimated to be 2900 ktpa with a market price of $3600 per ton (Özüdoğru et al., 2019; Rosales-Calderon and Arantes, 2019). Lastly, the other chemical of interest that is looked at is LA, which has attracted attention to most of chemical industries dues to its potential to replace fossil-derived chemicals (Sinoreta et al., 2019). It currently serves a speciality market, with market prices currently ranging from ~$2000 to 3000 per ton (Gerardy et al., 2020). In 2017 LA market segment was estimated at $267.8 million, and it has been predicted that by the year 2026, it will be at $620 million (Stratistics Market Research, 2019).

1.2 Project Scope and limitations

Integrating sugar cultivation activities with the sugar production process in a sugarcane biorefinery approach, as per global sugar sector development program has a great potential of becoming the producer of renewable energy, biofuels and bioproducts (Pachón et al., 2018). In order to guarantee the South African industry's sustainability, various scenarios of biorefineries utilising 1G, 2G and1G2G feedstocks were investigated. Firstly, sole product 1G2G based on the updated models from previous studies, and 1G2G biorefineries producing GA, SA, LA and xylitol are investigated. Thereafter multi-product biorefineries producing maximum of 2 products are thereof considered, to cater for the changes in demands, fully exploit the presented value of the raw material and to increasing the plant's flexibility. As shown in Figure 1, a typical sugarcane biorefinery, converts the extracted sugars from biomass into valuable bioproducts and utilises the residues for steam and power production in the co-generation system.

To create a self-sustaining biorefinery complex, portion of the lignocellulose along with other by-products such as solids residues and biogas are burnt in the CHP for energy and power generation. Since there is no need further utilisation of bagasse in 1G biorefinery complexes, these processes are designed to incorporate the existing inefficient boilers with deficit in steam demand provided by low pressure boiler for a cost benefit of the process. However, facilities processing 2G feed stock, make use of new efficient high-pressure boiler to ensure that more bagasse is made available for utilisation.

Reconfiguration in the sugar mill by eliminating second and third crystallisation units aimed at high recovery of crystalline sucrose has been recommended by Dogbe et al., (2018), to

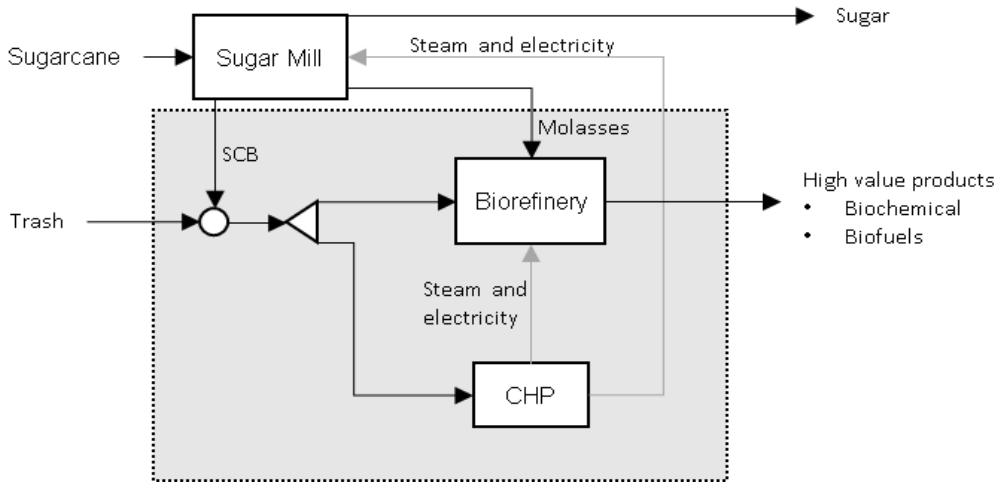

Figure 1: A schematic diagram of scope of this project with the grey area being the area of focus

produces a cleaner A-molasses for use in a biorefinery complex that will omit the further processing before fermentation and yield better product purity. Furthermore, reduction in heating demands from 120 t/h to 104.5 t/h of steam in the sugar mill complex due to this reconfiguration will allow annexed 1G biorefineries to share the existing CHP facility thereby providing the economic benefit (Dogbe et al., 2020).

The integrated 1G2G biorefineries complex are developed based on 1G and 2G configurations. The three concepts: Hierarchy, sequencing, and integration were used. Whereby hierarchy relates to the hierarchical breakdown of raw materials and their relationship with the respective product/s. The sequencing involves synthesising of a logical pathway for obtaining the product. Lastly, integration relates to combining of production technologies, feedstocks, and products (Moncada et al., 2014). It is important to realise that integration stages are directly related to process sequencing and hierarchal breakdown. Therefore, process integration for 1G2G (raw material combination) considered giving best possible product throughput and maximum substrate sugar utilisation for best economic outcome.

The detailed process models are simulated in AspenPlus® V8.8 using literature data and established technologies for production of the products of interest. Subsequently, the mass and energy balances data were extracted to determine the economic performances of each modelled scenarios. The major economic indicators used to assess the profitability, are Internal rates of return (IRR), net present value (NPV) and minimum selling price (MSP).

This study is limited by factors such as literature data for reaction, purification and recovery equipment simulated. In addition, obtaining accurate information for costing process equipment and chemicals cost can be challenging because vendors never divulge prices and acquiring cost processes from literature do not always characterise the true cost. However, the impacts of these limitation are assessed by sensitivity analysis.

1.3 Overall aim and objectives

Previously, 2G-only biorefineries for the products of interest have been considered by Kapanji et al. (2019), Nieder-Heitmann et al. (2019), Özüdoğru et al. (2019) and Dogbe et al. (2020) has considered 1G SA production. However, the production of LA and GA from 1G feedstock in a sugarcane biorefinery has not been considered for the South African context. This study is the first to considered 1G production of GA and LA using A molasses in an integrated sugar mill and biorefinery configuration. Through a study by Dogbe et al., (2020), it was shown that 1G biorefineries significantly improved the economics of biorefineries due to the elimination

of expensive pretreatment and enzymatic hydrolyses process. Moreover, biorefineries combing 1G and 2G raw feeds have been shown to improve the performance due to the shared processing facilities (Fan et al., 2018). The 1G and 2G feedstock integration have been predominantly investigated for biofuels production (Gnansounou et al., 2015; Moncada et al., 2014; Santos et al., 2018). However, no studies have reported feedstock integrations for the production of products of interest. The integrated 1G2G biorefineries are considered in this study to assess the if economic viability could further be improved.

Overall, this work aims to build onto the existing work of (Dogbe et al., 2020; Kapanji et al., 2019; Nieder-Heitmann et al., 2019; Özüdoğru et al., 2019) by improving the process configurations and integrating 1G and 2G feedstocks, evaluating biorefinery scenarios using the most recent research data and assessing the mechanistic and economic viability trends portrayed by integrated 1G2G configurations for both sole and multiproduct. Summary, of the objectives set to achieve the main aim of this study are listed below. Further explanation of the novelty with regards to each objective are presented in Section 2.6.

The objectives of this study are:

1. To design and evaluate the profitability of 1G biorefinery scenarios producing LA and GA.
2. To update existing 2G biorefineries producing LA, GA, and SA as well as 1G biorefinery for SA.
3. To develop integrated 1G2G biorefinery configurations to produce GA, LA, and SA, as we as multi-product biorefinery configurations for production of GA, LA, and SA with xylitol.
4. To compare the economic viability of 1G2G scenarios to the newly built 1G scenarios, existing 1G, and 2G scenarios and 1G2G multi-product facilities.

1.4 Plan of development

The contents of this thesis report are classified into five main sections. Firstly, the report starts with an introduction (1) where the background of the study is discussed. A literature review (2) then follows this to presenting some of the relevance of this research project. Then, the methodology (3) that was used to archive the objectives of this project is outlined. Result and discussions (4) are then present to compare the techno-economic result of different biorefinery scenarios as well as quantification of the developed biorefineries uncertainties by sensitivity analysis. Lastly, conclusions (5) are drawn based on the economic outcome and relations to the objective.

2 Literature review

2.1 Raw materials

Molasses, sugarcane bagasse and trash, are the residual streams resulting from sugar production, with the latter produced from sugar cane harvesting. These substrates are considered to be an ideal raw material for biorefining processes due to their availability, low cost and high content of fermentable sugars (Loh et al., 2013). Also, co-utilisation of these substrates as complementary raw materials in a biorefinery context could bring an economic benefit to the sugar industry.

2.1.1 Molasses

C-molasses is one of the by-products in a sugar mill, along with lignocellulose. It is a dark coloured syrup formed during the crystallisation process for the productions of raw sugar. It is formed by minerals regarded as impurities in raw sugar (Gopal and Kammen, 2009). It contains 50-55% (w/w) of sugars (mostly sucrose with smaller fractions of glucose and fructose), suspended solids, vitamins and nitrogen compounds (Xu et al., 2015). The composition of sugarcane molasses is affected by region, method of processing, soil and climate conditions (Van Der Merwe et al., 2013). Table 1 shows typical sugarcane which is compared with sugar-beet molasses composition to show why it is preferred. The primary sources of molasses are sugar beet and sugarcane molasses with the latter being the primary source for obtaining molasses (Olbrich, 1963). Generally, sugarcane molasses has a lower content of non-sugar and ash, as compared to sugar-beet molasses. Conversely, cane molasses has high sugar content (Olbrich, 1963).

Table 1: Composition of Sugarcane molasses and sugar beet molasses (adopted from Olbrich, 1963)

Constituents	**Sugarcane C-molasses (%)**	**Sugar beet molasses (%)**
Dry Substance	77-84	78-85
Total sugars as invert sugar	50-65	48-58
C	-	28-34
N	0.4-1.5	0.2-2.8
P_2O_5	0.6-2	0.02-0.07
CaO	0.1-1.1	0.15-0.7
MgO	0.03-0.1	0.01-0.1
K_2O	2.6-5.0	2.2-4.5
SiO_2	-	0.1-0.5
Al_2O_3	-	0.005-0.06
Fe_2O_3	-	0.001-0.02
Total ash	4-8	7-11

Both sugarcane and sugarbeet molasses are used as animal feed and in yeast fermentation processes for productions of citric acid, glutamate and ethanol (Gopal and Kammen, 2009; Nikodinovic-Runic et al., 2013). The high concentration of C-6 sugars and fermentable carbohydrates support the fermentation process when processing molasses (Khan et al., 2006). In addition, excess molasses residues in the sugar mill result in cost implications for disposal. Thus, the utilisation as a carbon source for fermentation processes is an excellent substitute for the disposal (Nikodinovic-Runic et al., 2013).

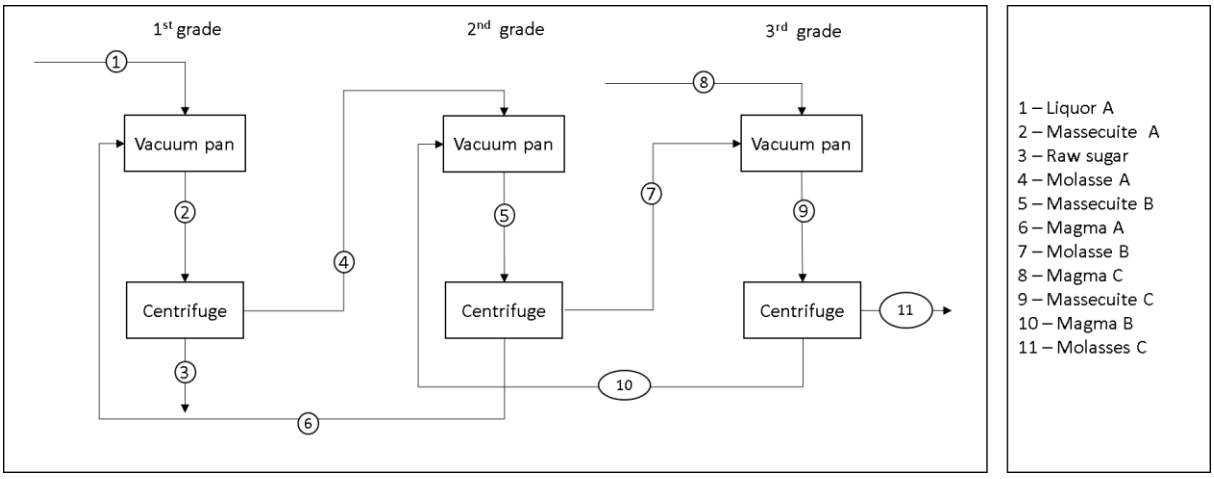

Figure 2: A schematic representation for a crystallisation process in a sugar mill

Within a sugar mill, there are different types of molasses viz. unclarified molasses, A-molasses, B-molasses, C/final-molasses, high test molasses and syrup off (Perez, 1995). However, for this project, only molasses produced during the crystallisation process are discussed (A, B and C-molasses). See Figure 2, for a schematic representation of a crystallisation process in a sugar mill.

A-molasses is an intermediate product obtained by centrifuging massecuite A, a mixture of concentrated sugar juice and magma A (Dogbe et al., 2020). Raw sugar is also produced at this stage and this first centrifugation stage is able to recover up to 75% of sugar (Perez, 1995), A-molasses contain 80 to 85% of dry matter, so if there is a need for end-use, it must be partially inverted or diluted with water before storage to avoid crystallisation. However, if there is immediate use, partial inversion is not necessary (Olbrich, 1963).

B-molasses is also an intermediate product of the second centrifugation. Essentially, it is obtained by centrifuging massecuite B, which is a mixture after boiling together A-molasses and magma B in a vacuum pan. This second stage is able to extract an additional 12% of raw sugar. First and second centrifugation steps recover up to 89% of raw sugar from sugarcane juice fed into the crystallisation process (Perez, 1995). Molasses C, which is the end product

for the crystallisation process, is formed by centrifugation of massecuite C, a mixture of B-molasses and sugar crystals (Magma C).

Molasses A, B and C can be sent out of the boundary limits for end-use in industrial, commercial, and household purposes. For this study, A molasses will be used as feedstock to bioenergy. According to a study done by Castañeda-Ayarza and Cortez (2017), it is best to use final molasses for fermentation processes, because they have no cost implications on the production of raw sugar in the sugar mill. However, not only does using A and B molasses decrease the production rate of raw sugar but also lowers total production cost per unit sugar, while increasing quality. The latter strongly supports the utilisation of A molasses in biorefineries to revitalise the sugar industry.

Furthermore, a change in the current sugar mills' current operation to extract A-molasses for utilisation in the integrated biorefinery provides benefits of energy savings due to the elimination of B and C crystallisation stages. Dogbe et al. (2018), has shown that three stage crystallisation process for a typical sugar mill has the lowest exergy efficiency in an overall sugar mill. Therefore, it was recommended that, to improve the efficiency of the process single crystallisation be used. With this reconfiguration, the steam demand of a typical sugar mill can be reduced from 120 t/h to 104.5t/h (Dogbe et al., 2020). Other vital economic benefit of using A molasses is that it is cleaner in comparison to B and C molasses; therefore, it can eliminate the costs of further downstream processing associated with impurities removal (Dogbe et al., 2020).

2.1.2 Lignocellulosic biomass

Lignocellulose is one of the largest sources of renewable organic material on Earth. It can be found in agricultural residues such as sugarcane bagasse, corn stover, corn rob, rice husk, wheat straw etc., as well as energy crops such as energy tobacco, switchgrass and woody materials (Mussatto and Dragone, 2016). In this project, sugarcane bagasse (SCB) the fibrous matter that is left behind after crushing sugarcane in the sugar mill for juice extraction is used as feedstock to the biorefinery combined with trash, i.e. the brown leaves left after green harvesting of sugarcane. This feedstock contains three major biopolymers, namely: cellulose (40-45%), hemicellulose (20-30%) and lignin (10-25%) (Benjamin et al., 2014). In addition to its constituents, it contains other minor components such as proteins, extractives, inorganic minerals and ash (Mussatto and Dragone, 2016; Sun and Cheng, 2002). It is worth stating that the ratios of these biopolymers vary depending on the biomass type and geographical area of

the biomass. The cellulose and hemicellulose biopolymers of biomass can be hydrolysed to release sugars and subsequently fermented to produce biochemicals and biofuels (Loh et al., 2013).

Cellulose, the main constituent of lignocellulose, is a homopolymer of glucose ($C_6H_{12}O_6$). It consists of ß-1,4 linked D-glucose subunits that are aggregated by hydrogen-bonding and van der Waals forces (Sonil et al., 2015). Cellulose is found in the cell wall and it provides mechanical and chemical stability to the plant (Mussatto and Dragone, 2016). Biomass has cellulose appearing in crystalline and amorphous forms. Owing to the crystalline rigid structure, cellulose need pre-treatment involving a dilute acid, an alkaline and enzymes, after which the amorphous structure in cellulose can be easily hydrolysed to produce hexose sugars (Sonil et al., 2015).

Hemicellulose is a complex polysaccharide mixture containing units of pentose (C5- sugars such as xylose and arabinose) and hexose (C6- sugars such as glucose, galactose and). Along with these sugars, it contains sugar acids such as galaturonic acid and methylglucaronic acid (Hayes, 2013; Sonil et al., 2015). Hemicellulose, unlike cellulose, has a lower molecular weight and has a degree of polymerisation of up to 200 units. This provides the reason why it can be hydrolysed more easily than cellulose and lignin (Özüdoğru, 2018; Hayes, 2013). Generally, hemicellulose has the main polymer with general formula $(C_5H_8O_4)_n$ for pentosans. It consists of D-xylose and L-arabinose with a composition of about 90% and nearly 10% respectively (Mussatto and Dragone, 2016).

Lignin is a shapeless 3D polymer containing phenylpropaniod units such as coniferyl alcohol and *p*-coumaryl alcohol joined by C–C resistant bonds and β-O-4-aryl ether (Mussatto and Dragone, 2016). It combines the cellulose microfibrils and hemicellulose sheath into a structure that forms a plant cell wall in a lignocellulosic material, see Figure 3. It makes the cells resistant to impact and microbial attack. In addition, its polymeric nature makes it insoluble to most solvents except if it goes through chemical or physical treatment for degradation (Mussatto and Dragone, 2016). Lignin along with other fractions (cellulose and hemicellulose) is currently combusted in boilers to produces steam and electricity for sugar mill processes.

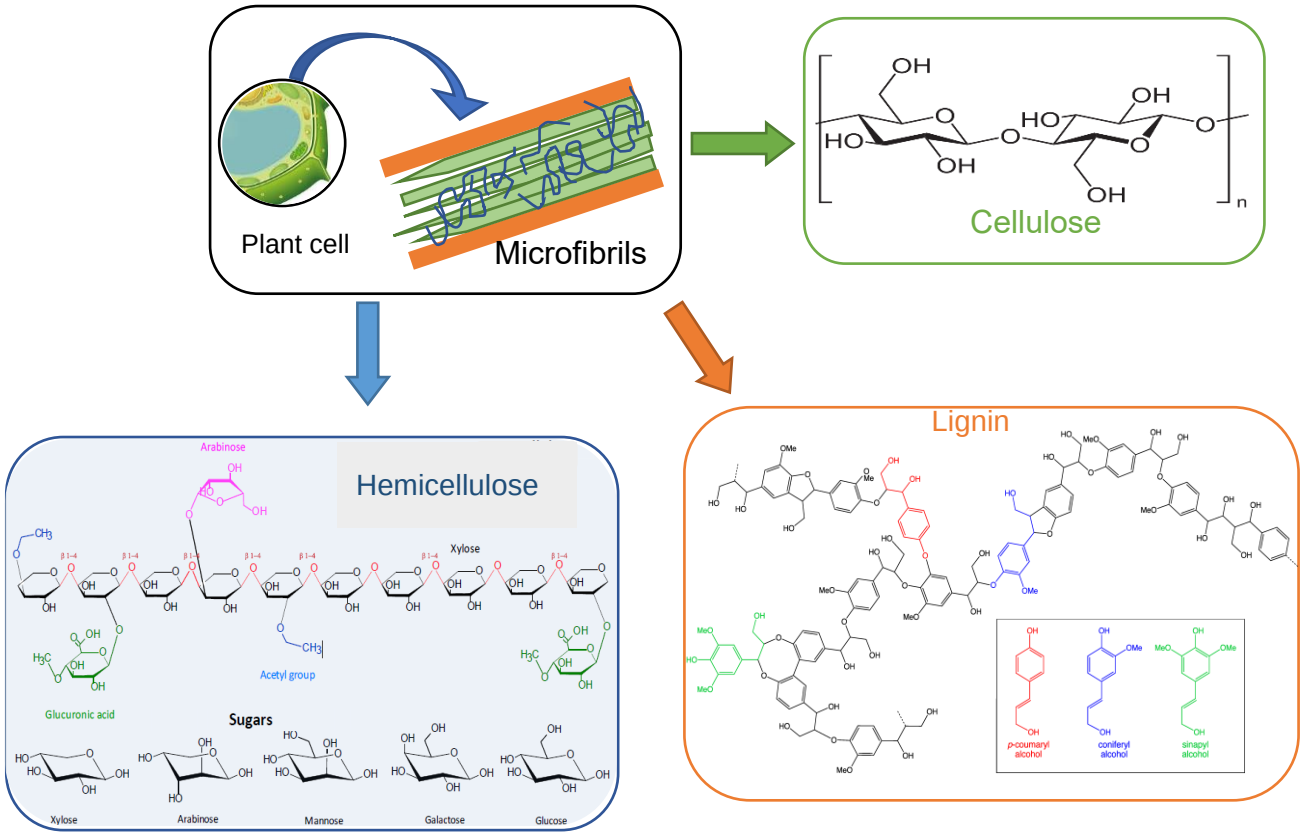

Figure 3: Structure and components of a lignocellulosic biomass redrawn from Mussatto and Dragone, 2016)

After sugar extraction and harvesting, the SCB and trash contain 50% (w/w) and 15% (w/w) moisture respectively (Gorgens et al., 2016; Loh et al., 2013), on a dry basis. The compositions of SCB and harvesting residues are tabulated in Table 2. For a typical 2G biorefinery annexed to an existing sugar cane mill in South Africa, the combined feed of available lignocelluloses is 113.5 t/h (Gorgens et al., 2016). It is worth noting that this total feed available includes the amount of lignocelluloses that has to be bypassed to the CHP system to ensure energy self-sufficiency of both sugar mill and new integrated refinery complex

Table 2: Lignocellulosic biomass composition adopted from (Gorgens et al., 2016)

	SCB		Trash		Mixture (SCB+Trash)	
Components	**Mass fraction (%)**	**Flow (t/h)**	**Mass fraction (%)**	**Flow (t/h)**	**Mass fraction (%)**	**Flow (t/h)**
Cellulose	41.1	18.495	39.8	7.96	40.7	26.45
Hemicellulose	26.4	11.88	28.6	5.72	27.1	17.6
Lignin	21.7	9.765	22.5	4.5	21.9	14.257
Ash	4	1.8	2.4	0.48	6.73.5	2.28
Extractives	6.8	3.06	6.7	1.34	6.7	4.4
Sum of dry matter	100	45	100	20	100	65
Water		45		3.5		48.549
Total (dry+water)		90.000		23.500		113.529

2.2 Pre-treatment

Pre-treatment is the most crucial stage in biorefineries, to avoid process complications and for effective conversion of raw materials into bio-based products. It ensures that sugars are liberated and pathogens in the raw feed and any compounds that might hinder product formation are dealt with, before the fermentation process. Several pre-treatments methods have been studied and developed for different types of raw material and the targeted product. However, for 1G raw feed, fewer pre-treatment methods have been reported. It is only essential to implement these methods when processing crude molasses with high contents of suspended solids and heavy metals (Roukas, 1998). However, since the considered 1G raw feed (A-molasses) is considered clean. It follows a simpler pre-treatment process; after handling, the feed is pasteurised to kill parthenogenic and mesophilic bacteria that might hinder the fermentation process (Salem et al., 2017). Subsequently, it is diluted to the desired concentration.

On the other hand, for lignocellulosic biomass (2G), a vigorous pre-treatment process is always required to overcome its recalcitrance (Mussatto and Dragone, 2016). The subsection below discusses lignocellulosic biomass pretreatment methods in more detail.

2.2.1 Lignocellulosic biomass pre-treatment methods

Lignocellulosic biomass requires a vigorous pre-treatment to improve the digestibility of the substrates, to make lignocelluloses amenable to the subsequent enzymatic hydrolysis to soluble sugars. During pre-treatment the biomass is exposed to process conditions that are sufficiently severe to break down cell wall physical barriers, reduce cellulose crystallinity and increase accessible surface areas (Mussatto and Dragone, 2016). Figure 4 shows how the cell wall of the plant break during pre-treatment. Removing the hemicellulosic biopolymer from lignocellulose results in the substrate having an increased mean pore size. The most crucial aim for pre-treatment is to make the polymeric and crystalline cellulose more accessible to enzymes; in this way, hydrolysis will happen faster and results in high yields (Loh et al., 2013). It is worth noting that pre-treatment methods are chosen in a way that the formation of microbially inhibitory compounds is avoided; if not, then a detoxification step is mandatory (Sasmal and Mohanty, 2017). Inhibitory compounds are formed during lignocellulose pretreatment by the degradation of pentosans sugars derived from hemicellulose, as well

glucose from cellulose and various degradation products from the lignin (Mussatto and Dragone, 2016).

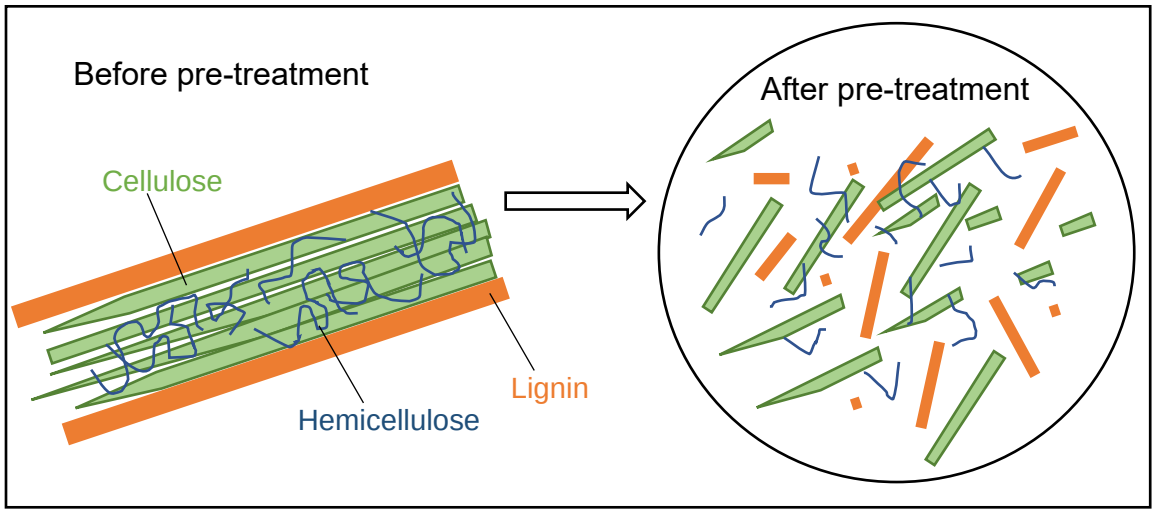

Figure 4: Pre-treatment effects on lignocellulose structure (redrawn from Mussatto and Dragone, 2016)

Numerous pre-treatment methods have been developed for lignocellulosic biomass. These methods can be categorised into 4, namely: physical, chemical physiochemical, and biological.

2.2.1.1 Physical pretreatment

The purpose of physical treatments is to reduce biomass size and crystallinity by milling thereby, improving hydrolysis and mass transfer due to reduced crystallinity and particle size, respectively (Brodeur et al., 2011). Mechanical milling when applied to soft biomass at high temperature (50-70°C), makes the lignocellulose fibre to rupture, resulting in less time required for the subsequent pretreatment (Kucharska et al., 2018). However, this pretreatment method is energy intensive.

2.2.1.2 Chemical pretreatment

Chemical pretreatment methods decompose the biomass into simpler compounds dissolved in aqueous solutions (Kucharska et al., 2018). Dilute acid and alkaline hydrolysis are the most popular owing to their number of advantages overpowering disadvantages (Nieder-Heitmann, 2019). In an acid pretreatment, the rigid structure of the lignocellulosic biomass is broken and fractions of hemicellulose are solubilised into a hydrolysate, resulting in more accessible cellulose fractions (Brodeur et al., 2011). Only the cellulose and lignin fractions remain in the solid state. A notable advantage of the acid treatment is that it can hydrolyse biomass, resulting in hemicellulose to yield fermentable sugars, which can lead to the removal of subsequent enzymatic hydrolysis step in some processes. Operating above the temperature of 110°C results

in inhibitors formation (HMF, furfural etc) (Kucharska et al., 2018; Loh et al., 2013; Sun and Cheng, 2002). However, extensive washing and detoxification can be employed for the removal of inhibitors prior fermentation step for processes that use microorganisms that have a no tolerance to such chemicals (Brodeur et al., 2011).

Alkaline pretreatment, causes the structural changes and partial dissolution of lignin, cellulose partially decrystallises and hemicellulose partial solvation through the use of bases such as sodium, calcium hydroxide, etc. (Kucharska et al., 2018; Sun and Cheng, 2002). Therefore, for the processes requiring relative pure cellulose, the acid pretreatment method followed by alkaline pretreatment method can be employed (Brodeur et al., 2011). The alkaline pretreatment method not only does it use less harsh process conditions but also the capital costs are low in comparison to acid pretreatment method (Nieder-Heitmann et al., 2019). However, acid pretreatment has been proven to be effective for treating softwoods. Additionally, a major drawback for the employment of alkaline pretreatment in biorefineries that utilises lignin in CHP is the cost associated with downstream conditioning.

2.2.1.3 Physiochemical pretreatment

For this pretreatment techniques, biomass is hydrothermally treated with the respective fluids under high temperatures (120 -260 ˚C) and pressure (4-48 bar), to causing a morphological and physicochemical changes to the biomass structure (Bensah and Mensah, 2018). The pretreatment results in the increase pore size and the surface area, leaving cellulose exposed for subsequent enzymatic hydrolysis (Kucharska et al., 2018). Under the physiochemical pretreatment method, steam explosion (STEX) is the positively proven method for the pretreatment of different kind of lignocellulosic biomass with the technological readiness level (TRL) ranging from 6-8 (Taylor et al., 2015).

2.2.1.1 Biological pretreatment

In biological pretreatment method, microbes such as fungi or bacteria are used to partially degrade lignin and hemicellulose in lignocelluloses, whilst cellulose remains intact (Sun and Cheng, 2002). These methods are said to be less energy-intensive and provide an environmental benefit. However, capital costs associated with these processes are high due to slow rate of hydrolysis and long times required for a process to complete as compared to another pretreatment method (Kucharska et al., 2018; Kumar and Wyman, 2009). The efforts in this pretreatment technology have been dedicated to combining with other technologies and

developing engineered microorganism for faster hydrolysis (Brodeur et al., 2011; Sánchez, 2009; Sun and Cheng, 2002)

The selection of the most effective pretreatment method is ultimately based on the requirements of the downstream processing. Also, the upstream (feedstock) can dictate which pretreatment should be applied and vice versa. Therefore, it is a need to establish an effective pretreatment method based on both upstream and downstream requirements. Based on the pretreatment mentioned above categories, physical and biological pretreatment methods have been proven to be less cost competitive in comparison to chemical and physiochemical pretreatment, thus preventing their commercialisation (Brodeur et al., 2011; Nieder-Heitmann et al., 2019).

2.2.2 Hydrolysis

Hydrolysis is a process by which a chemical decomposes to split the chemical bonds in a substance, using water. In biomass, long-chain molecules are catalytically broken into shorter chains and monomeric sugars (Speight, 2017). The two types of hydrolysis are enzymatic and acid hydrolysis. The drawback associated with the latter, such as corroding equipment and yielding to high contents of fermentation inhibitors has led to the former being the preferred hydrolysis method of pretreated lignocellulosic biomass for industrial applications (Benjamin et al., 2014). Additionally, enzymatic hydrolysis requires mild conditions, and it is less energy intensive.

Enzymatic hydrolysis: Cellulose and hemicellulose depolymerisation can be achieved by using highly specific cellulase and hemicellulase enzymes (Sun and Cheng, 2002). These enzymes can be produced using either aerobic or anaerobic culture of bacteria or fungi, for on-site production, such as the one reported by Humbird et al., 2011 for producing ethanol. *Trichorderma reesei* is the widely used commercial source for cellulases (Brodeur et al., 2011). Cellulases are a mixture of various enzymes, the three major types required for cellulose hydrolyses are endoglucanase, which decreases the degree of polymerisation, exoglucanase, which split cellulose to form cellobiose, and β-glucosidases, which produce glucose from cellobiose (Sun and Cheng, 2002). Additionally, several secondary enzymes such as xylanase, acetylesterase and glucomannase attack hemicellulose resulting in the depolymerisation of hemicelluloses to form C5 and C6 monomeric sugars as well as non-sugar acids.

Apart from the quality of the pretreated hydrolysate, the decomposition of cellulose and hemicellulose during enzymatic hydrolysis depends on conditions such as pH, temperature, porosity, cellulose concentration and degree of crystallinity (Sun and Cheng, 2002). Substrate

contents are the major factor that contributes to the hydrolysis rate and yield. Increasing the concentration of the substrate tends to increase the hydrolysis rate. However, at highly concentrated substrates inhibition occurs, as a result, the rate of hydrolysis decreases (Brodeur et al., 2011; Kucharska et al., 2018). One of the factors that lead to the substrate inhibition during the process is the ratio of solid loading to enzymes (Sun and Cheng, 2002). Studies have been conducted to find the optimal enzyme dosage to the pretreated SCB hydrolysate. The reported dosage ranges from 1 to 60 FPU/g (filter paper unit/ gram of substrate) (Brodeur et al., 2011; Gámez et al., 2006; Nieder-Heitmann, 2019; Sun and Cheng, 2002). However, for economical purpose, lower dosages ranging from 10 – 20 FPU/g are used (Benjamin et al., 2014). Above all, the optimal dosage depends on the prior pretreatment's method efficiency and the presence of inhibitory compounds. The optimal temperature for the enzymatic hydrolysis range from 40 -50°C. The temperature higher than optimal, tend to affect the activity of cellulase.

2.2.3 Detoxification

Commonly after pre-treatment of lignocellulosic biomass, the hydrolysate contains inhibitory compounds, which can reduce yields and inhibit microorganisms during bioconversion of liberated sugars. Such inhibitors can be removed by adding the detoxification step prior to the hydrolysis-bioconversion processes. The detoxification process can be either biological, chemical or physical (Singh and Chaudhary, 2017). Below are some of the standard detoxification methods.

- Solvent extraction- employs the use of solvents such as ethyl acetate to remove furfural and acetic acid
- Ion- exchange resin – for acetic acid removal
- Activated carbon adsorption – specifically removes inhibitors obtained from lignin. However, this method is expensive due to activated charcoal powder that cannot be reproduced.
- Alkali treatment – inhibitors are degraded by using $Ca(OH)_2$ to increase hydrolysate pH to 9-10 and subsequently reduced using H_2SO_4 to pH of about 5. However, this process results in loss of fermentable sugars.
- Evaporation – it is used to remove volatile inhibitors such as acetic acid and furfural
- Enzymatic detoxification – employs enzymes to covert inhibitors in the hydrolysate into less toxic compounds (Aresta et al., 2015; Nieder-Heitmann, 2019; Singh and Chaudhary, 2017).

2.3 Integrated biorefineries

In recent years, there has been a substantial improvement in the concept of sugarcane biorefineries to maximise gains of sugarcane utilisation (Hara et al., 2013; Silalertruksa et al., 2015). Also, several researches have shown the need to improve the profitability of sugarcane industry by valorising the residues produced, through integrated co-production of several biobased products in a biorefinery context (Farzad et al., 2017b; Gorgens et al., 2016; Mandegari et al., 2017b; Nieder-Heitmann, 2019).

2.3.1 Biorefining

It has been proposed that green biorefineries will serve as a strong foundation for the new bio-based economy (van der Merwe, 2010). Biorefinery can be defined as a process that integrates the extraction of other materials from biomass and other processing equipment to produce high-value biofuels and biochemicals (Werpy and Petersen, 2004). The concept of a biorefinery is not new; it dates back to the 19th century, where it first started with a steam-driven paper machine (Hingsamer and Jungmeier, 2019). Although the world is dedicated to moving away from a fossil-based economy to sustainable bio-based one, the majority of the chemicals and polymers are still produced from fossil fuels, mostly oil and gas (Navarro et al., 2014). Recent studies are mostly focused on integrated biorefineries, investigating ways of efficiently utilising a broad spectrum of biomass feedstocks into cheaper biofuels, biochemicals and/or bioenergy (Murthy, 2019). Therefore, the world can reduce reliance on fossil-based chemicals due to their severe environmental impact. However, the production costs of bio-based products in many scenarios are much higher than conventional petrochemical production. Correspondingly, the performance of the new products must prove to be the same as their petro-based equivalent and their substitutions and provide better environmental benefit (Navarro et al., 2014).

2.3.2 The current state of the art

Integrated biorefineries make use of novel chemical, biological and mechanical technologies, thereby introducing difficulty in achieving cost competitiveness with fossil fuels products (DOE, 2013; van der Merwe, 2010). However, intensive research is conducted on the development and optimisation of these technologies to achieve profitable production process in comparison to conventional refineries. Moreover, national support on the newly developed integrated biorefineries can significantly lessen both financial and technical risks associated with the implementation of newly developed technologies (DOE, 2013).

Bioenergy Technologies Office works with stakeholders and cost-sharing partners to address major challenges associated with the implementation of these new technologies. Various projects are taken to verify the feasibility of certain raw materials and production pathways. A typical (technological evolution path) lineage progression is followed from research to pilot to demonstration to commercialisation scale. Each level is vital as it approves the production performance of technology, preparing a way for commercial-scale deployment. Figure 5 below shows the technological readiness level (TRL) for the products of interest (Werpy and Petersen, 2004). Despite the hampering challenges for the implementation of new biorefineries such as market and economic viability, meeting environmental impacts standards. An industrial organisation such as Myrant and BioAmber for SA, and GF Biochemicals and Praj for LA have been actively developing their technologies implementation of industrial pilot scale. GA and xylitol are produced in most part of the continent. However, China has been reported to be the major player with a production capacity of 780 ktpa (2015) and 120 ktpa for GA and Xylitol, respectively (Rosales-Calderon and Arantes, 2019).

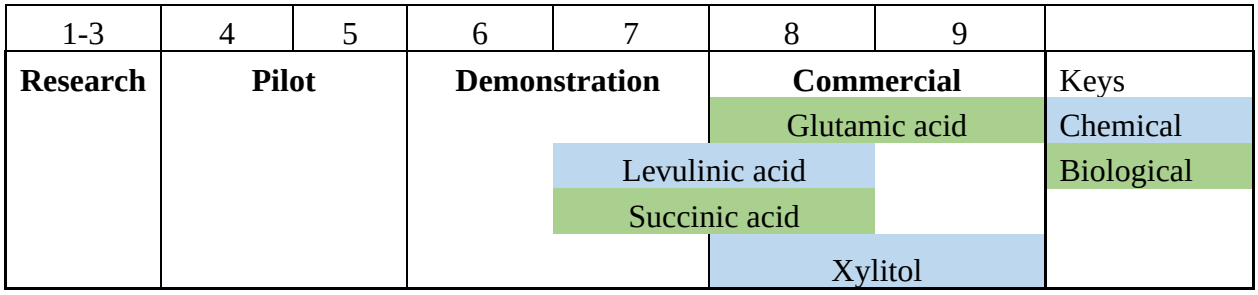

Figure 5: Commercialisation status of the selected 4 bioproducts adopted from (Taylor et al., 2015)

2.3.3 Feedstocks integration in biorefineries

There are doubts regarding the long-term sustainability of 1G biorefineries due to threatened food security as a result of the potential increase cost of crops and competition with over land and water (Gutiérrez et al., 2017). In contrast, the implementation of 2G biorefineries would not form a direct dispute with food security. However, the appraisal of 1G vs 2G biorefineries' sustainability should not be built solely on food security. Aggregated assessments for economic viability and environmental impact should be the principal criterion used for the implementation of these biorefineries (Mohr and Raman, 2015). In this study, only economic performances were used to assess the economic standpoint for their implementation. However, future studies should investigate the life cycle assessment for an environmental standpoint.

Nonetheless, for the South Africa sugar industry, the implementation of 1G biorefineries would not only diversify product range but also, maximise the value presented by the cane juice from

sugarcane (Dogbe et al., 2020). Similarly, 2G biorefineries would maximise the value presented by the waste bagasse.

The integration of 1G and 2G feedstock into a sugarcane biorefinery could improve the viability of production process in comparison to only 2G processes. Moreover, the integrated 1G-2G biorefining provides several advantages compared to 2G stand-alone biorefineries; better economics (capital cost is reduced owing to the shared infrastructure), the use of unutilised solids for cogeneration and cheaper transportation cost as it is readily available on site (Gnansounou et al., 2015). Most importantly, the integrated 1G2G biorefineries are seen as an opportunity to combine different carbon sources/ feedstocks (1G and 2G) for co-utilisation, with the potential to result in inhibitory compounds dilution prior fermentation (Santos et al., 2018). Subsequently, this can eliminate the need for the costly detoxification process.

2.4 Products of interest

2.4.1 Glutamic acid

2.4.1.1 Brief overview

Glutamic acid (GA), also chemically known as (2S)-2-aminopentanedioc acid is non-essential, odourless and water-soluble solid amino acid. It has a chemical formula $C_5H_6NO_4$ and its chemical structure consist of two carboxyl group (-COOH) and amino group ($-NH_2$) as shown in Figure 6 (Sano, 2009). Glutamic acid has a molar mass of 147.13 g/mol, a melting temperature of 199°C and a specific gravity of 1.538 at 20°C (Haynes, 2016). The anion of GA called glutamate is the major molecule for cellular metabolism and removal of nitrogen in the human body. Glutamate functions as an excitatory neurotransmitter of the brain (Dutta et al., 2013).

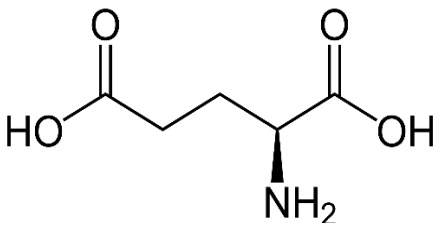

Figure 6: Glutamic acid molecular structure

GA is one of the most important amino acids produced worldwide owing to a variety of industrial applications. Its polymer, poly-γ-glutamic acid (γ-PGA), has properties that has led to its successful commercialisation, such as edibility, biodegradable, dissolvable and non-

poisonous (D'Este et al., 2018). GA is used largely as a flavour enhancer in the food processing. Also, its sodium salt called monosodium glutamate is used as a salt substitute in food industry (D. Zhang et al., 2012). In pharmaceutical industries, it is used as a building block for protein synthesis and precursor to glutamine that can be used for body metabolism or as nutrition supplement to boast immune system (Williams et al., 2005). Lastly, it can be used as animal feed in the poultry farms. The latter industry has been predicted that is likely to experience a significant growth, because of increasing meat consumption and population. In 2015, the global GA production was estimated at 2000 ktpa, with a market volume at $420 million (Rosales-Calderon and Arantes, 2019), Stratistics Market Research, 2019, has reported that by the year 2026, this value is expected to reach $1 billion.

Glutamic acid was firstly discovered in the year 1866 by a German chemist Ritthouse from hydrolysing wheat gluten with sulfuric acid (Shyamkumar et al., 2014). Then in 1907, a Tokyo Imperial University professor Kikuna Ikeda discovered monosodium L-glutamic acid (MSG) as a taste component. Following his discovery GA was then produced industrially from vegetable proteins by hydrolysis with hydrochloric acid (Kinushita, 2010 ;Sano, 2009). However, this method of production posed process challenges due to the production of racemic mixture of (D and L)- GA (Amin and Al-Talhi, 2007). Later in 1957, fermentative process for production of MSG was developed by Kinoshita et al., 1957 where MSG was produced by direct fermentation of carbohydrates and ammonia using *Corynebacteruim glutamicum* as microbial strain. Ever since the fermentative discovery, all industrial GA production have shifted into fermentation method (Sano, 2009; J. Zhang et al., 2012), due to advantages such as environmental benefit and less process costs, as compared to chemical synthesis production (Sano, 2009).

2.4.1.2 Glutamic acid production

The industrial production GA follows a generic biorefinery process such as pre-treatment, fermentation and product recovery and purification. This section will only cover fermentation and downstream process for the GA production.

Fermentation

The fermentative GA producing bacteria's are *Corynebacterium*, meaning that they are gram positive, non-spore forming and non-motile and require biotin for growth (Pal et al., 2015; Sano, 2009). *C. glutamicum* was the first bacteria to be isolated for industrial GA production. This bacteria has the capabilities to utilize different sugar carbon sources such as glucose,

sucrose, galactose, fructose and xylose for its growth and GA biosynthesis (Khan et al., 2018; Kumar et al., 2014; Pons et al., 1996). Although past studies have not fully compiled the stoichiometry for GA synthesis from different carbon sources. The potential pathways have been developed. Glutamic acid biosynthesis follows a tricarboxylic acid (TCA) cycle, the process is done aerobically keeping the oxygen concentration at 7mg/l, to avoid accumulation of lactic and succinic acid (D'Este et al., 2018). It has been proven that, optimum oxygen supply results in the accumulation of α-ketoglutaric acid that subsequently react with NH_3 to form GA. As per these metabolic pathways 1 mole of sugar substrates forms 1 mole of GA. Nutrients supply forms a crucial part of the fermentation process. Introducing nutrients such as yeast extract and inorganic nutrients in the fermentation process results in an increased sugar utilisation, product titre and productivity (Kinoshita et al., 1957).

In addition to these nutrients, biotin is also an important component for GA fermentation. See Figure 8, it promotes biosynthesis of acetyl coenzyme A to oleic acid, which is thereafter converted to phospholipids. However, it should be kept below 3µg/l. Since other feedstock such as sugarcane molasses and beet molasses contain high contents of biotin, penicillin shot method at 8-10 units/l is applied to counteract the limitations of biotin (Kinoshita et al., 1957; Sano, 2009).

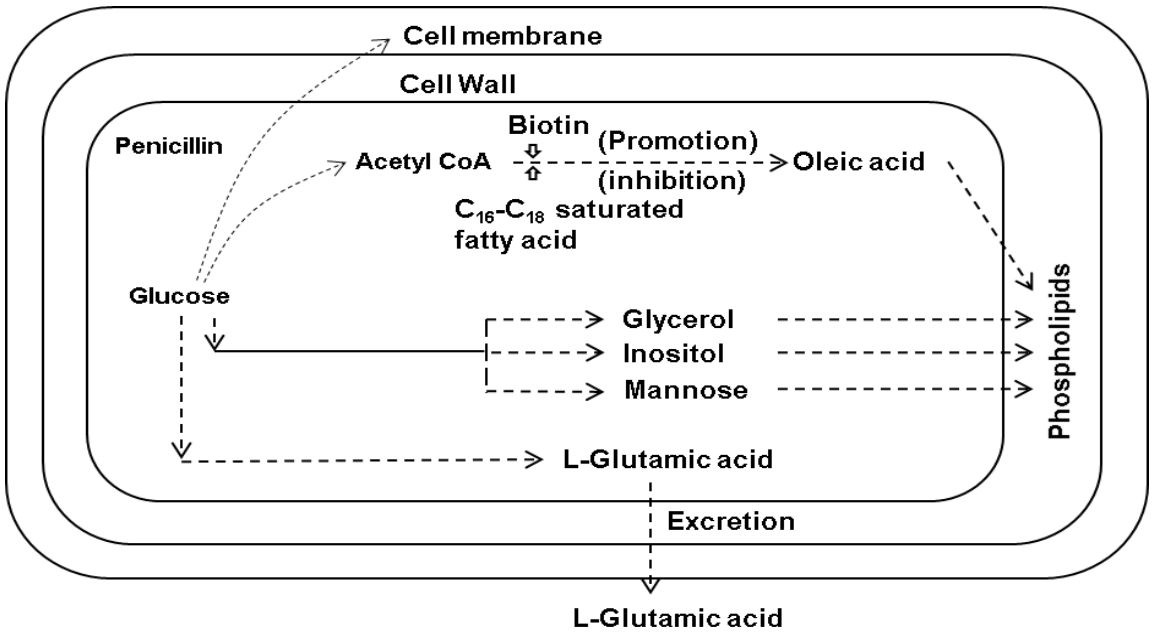

Figure 7: Cell permeability of GA in accordance with phospholipids amount within the microorganism redrawn from (Kumar et al., 2014)

An ideal microorganism for fermentative production of GA should achieve sufficiently-high values for the yield of the products from fermentable sugars, productivity, and final product concentration; it should also tolerate process conditions (pH and substrate concentration) and

be able to ferment both C5 and C6 sugars (Agrimi et al., 2015). It is important to achieve high product yield during fermentation to minimize the waste product and maximize concentration and productivity to reduce the load on the downstream processing. These factors are the key drivers of the economic performance of a production process.

Numerous strains have been investigating for GA fermentation from different types of carbons source. However, only the relevant ones have been reported in Table 3. Pal et al. (2015) has shown that *C. glutamicum* (NCIM-2068) can produce GA from cane juice with yield of 0.95 g/g and 65 g/l titre following continuous fermentation process in an integrated membrane reactor system. The patent, *Brevibacterium divaricatum* NRRL 8-231 can produce high product concentration(100 g/l) consuming up to 91% of glucose to produce GA (Miescher, 1974). Amin and Al-Talhi, (2007), compared batch fermentation to continuous fermentation processes, using *C. glutamicum ATCC 13022* strain to ferment GA from sugarcane molasses. Their results showed that *C. glutamicum ATCC 13022* performs well in a continuous fermentation process, unlike batch processes, obtaining 0.56 vs 0.76 g/g yields, and 3.8 vs 29.1 g/l.h productivity for batch and continuous operations respectively. Employment of the latter for the fermentation process may reduce the capital cost due to high productivity. One study by Jin et al. (2020), attempted to co-utilise xylose and glucose from wheat straw hydrolysate using *C. glutamicum GJ04* strain. Even though GA was produced in reasonable concentrations (62 g/l) sugar utilisation of this process was worse in comparison to the sole substrates that have been reported (Kumar et al., 2014).

Table 3: Glutamic acid producing strains adapted from (Jin et al., 2020; Özüdoğru, 2018)

Strains	**Substrate**	**Process**	**Concentration (g/L)**	**Productivity (g/L.h)**	**Yield (g/g)**
C. glutamicum					
NCIM-2168	Cane juice	Continuous	65	8.3	0.95
ATCC 13022	Sugarcane molasses	Batch	93	3.8	0.56
ATCC 13022	Sugarcane molasses	Continuous	72	29.1	0.76
GJ04	Mixture of glucose and xylose from wheat staw	Batch	62	0.3	0.4
Brevibacterium sp.	Sugarcane bagasse	Batch	-	-	80mg/g
Brevibacterium divaricatum NRRL 8-231	Glucose	Continuous	100	3.51	0.9

Glutamic acid producing strains are grown in a medium containing nutrient such as yeast extract, peptone. Other inorganic minerals such as $FeSO_4$ and $MgSO_4$ are also required to ensure sufficient sugar utilisation of the substrate.

Downstream process

The downstream process for GA production has two sub-steps: cells separations to obtain cells free GA broth and obtaining product from the GA broth. The conventional downstream process for GA has numerous processing steps such as precipitation, crystallisation, evaporation drying etc. (See figure) (Kinoshita et al., 1957). Not only does this process comprise of many processing steps, but also make use of harsh chemicals such as sulfuric acid, that greatly contribute to the economic disadvantage of the process (Kumar et al., 2014).

GA fermentation broth processing using membranes has been investigated to replace the more complicated GA conventional downstream process with more cleaner and greener processes (Kuo and Chiang, 1987; Pal et al., 2016). Membrane separation technologies are employed in biorefineries to reduce the energy demands and chemical consumption of the process (He et al., 2012). A novel route proposed by Pal et al. called integrated membrane integrated reactor system been to proven to be the potential replacement for the conventional process. This is mainly because the process offers less processing steps resulting in both economic and environmental benefits. For these reasons, all GA scenarios will be based on this processing route.

2.4.2 Levulinic acid

2.4.2.1 Brief overview

Levulinic acid (LA), also having the IUPAC name 4-oxopentonic acid or gamma ketovaleric acid is a yellowish liquid after melting with caramellic-odour, having C5-alkyl group (Morone et al., 2015; Signoretto et al., 2019). It is a short chain molecule with a chemical formula $C_5H_8O_2$ and its chemical structure can be seen in Figure 8. LA has a boiling point in the range of 245-246°C with a melting point of 33°C and a specific gravity of 1.1335. It consists of carbonyl (C=O) and carboxylic acid (COOH) functionalities that makes it to have the different reaction pathways with other functional groups. Hence, it is a platform chemical that can be used for wide range of industrial application (Isoni et al., 2018; Khan et al., 2018). Moreover, LA was

listed by the US department of energy biomass program for 2004 as one of top 12 promising bio-based chemicals (Signoretto et al., 2019).

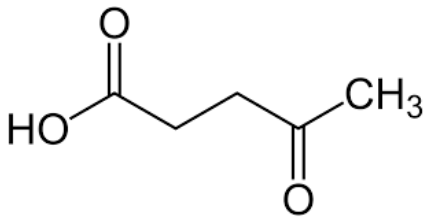

Figure 8: Chemical structure of levulinic acid

Over the past years LA has become a chemical of interest, as a primary biorefinery building block and platform chemical; this is due to the fact that it can be produced with relatively high yield from acid pre-treatment of C6 sugars (Taylor et al., 2015). It currently provides a feasible chemical overlap between biomass and petroleum refining. Numerous of the LA derivatives have been recommended for fuel applications: this includes chemicals such as γ-valerolactone (GVL), ethyl levulinate (EL), and methyl tetrahydrofuran (MTHF) (Signoretto et al., 2019). Moreover, LA can be used as an additive in fuel such as diesel and gasoline, as a member of the valerate ester family. Also, several markets for LA exists in cosmetics, solvent, plasticizer and pharmaceutical industries (Leibig et al., 2011; Morone et al., 2015). In 2017 LA market segment was estimated at $267.8 million, and it has been predicted that by the year 2026 it will be at $620 million (Stratistics Market Research, 2019). Since, obtaining the right market size for LA in open literature is very challenging. The global market can be estimated at 90 ktpa using the fact that the market price for LA is $3000/t (Gerardy et al., 2020), and that in 2017, LA market segment accounted for $270 million (Stratistics Market Research, 2019).

2.4.2.1 Levulinic acid production

There are numerous raw materials that can be utilised to produce biobased LA, this include precursors such as polysaccharides, monosaccharides, furfural, HMF, and renewable resources, such biomasses (Signoretto et al., 2019). In the recent years there has been an extensive research on the acid hydrolysis of 1G and 2G biomasses for LA synthesis. However, research focused on 1G feedstock (molasses) is still limited. It has been shown that, the reaction pathway for LA production from lignocellulosic biomass occurs in 4 steps: 1) firstly, polysaccharides or cellulose are hydrolysed to glucose, 2) glucose is then isomerized to fructose, 3) dehydration of fructose to HMF, and 4) rehydration of HMF to LA, as shown in Figure 9. Moreover, during acid hydrolysis hemi-cellulosic fractions can be hydrolysed to form xylose, which proceed as shown below to form LA. Very little portion of lignin solubilises during LA formation, whereas most of the lignin remains as solid. Presences of lignin residues during formation of LA has

been reported to result in sugar degradation, resulting in reduced LA yields (Hayes et al., 2005).

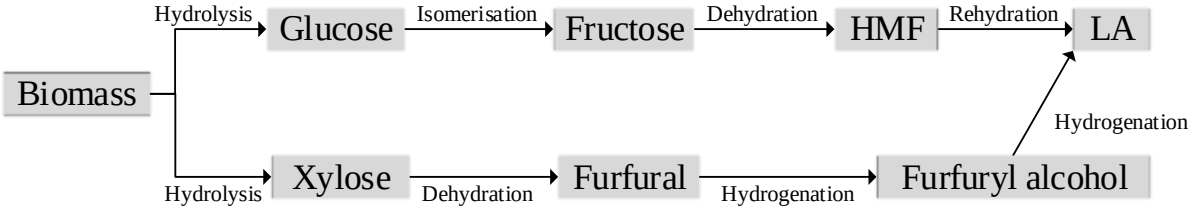

Figure 9: LA synthesis reaction pathway redrawn from (Rackeman and Doherty, 2012)

Levulinic acid from 1G feedstock specifically molasses has not been reported in sufficient detail in literature, nor has there been any technological employment industrially. Table 4, shows different the types of 1G feedstocks that has been studied in literature using different catalyst and different 1G feedstocks to obtained better yields compared to those reported for 2G feedstock and pure sugars (Signoretto et al., 2019). Although, different catalysts have been investigated, H_2SO_4 remains the preferred catalyst for industrial employment. Because heterogeneous catalyst requires longer reaction time to achieve same yields as when acid catalysts are used, whilst HCl poses a potential risk of chlorine gas release in to the atmosphere in the downstream (Brouwer et al., 2017).

Sugar cane molasses has been studied by Kang et al., (2018), where hexose sugars are hydrolysed in a superimposed reaction system to produce LA. The formed LA solution is used in the subsequent hexose sugars hydrolysis to that happens in four reactor stages form more concentrate LA thereby making separations easy. Because it is very challenging to recover LA in a low concentrated aqueous medium.

Table 4: 1G Biomasses for LA synthesis adopted from (Signoretto et al., 2019)

Carbon source	**Catalyst**	**Temperature (°C)**	**LA yield (%)**
Usual corn starch	HCl	165	55%
High-amylose corn starch	HCl	165	55%
Waxy corn starch	HCl	165	55%
kernel sorghum grain	H_2SO_4	200	33%
Cane molasses	H_2SO_4	180	30%
Beet molasses	Amberlyst-36TM	140	70 mol%

The Biofine process developed by Fitzpatrick (1990), has been the most employed process for industrially LA production from 2G biomasses due to high yields of 70-80 mol% (Hayes et al., 2005; Schmidt et al., 2017). In this process, the 2G biomass in processed in series two reactor stages over H_2SO_4 to produce LA along with furfural, formic acid and humins (Leibig et al., 2011). The humins formation remains a challenge in this process, because they lead to clogging

in the reactors hindering the large scale process operations (Schmidt et al., 2017). On contrary, humin residues are a suitable fuel to provide process energy. Their utilisation in CHP, has the potential of resulting in self energy-sufficient biorefinery (Morone et al., 2015).

Numerous studies have been conducted for utilisation of 2G feedstock for LA production and Signoretto et al., (2019) have summarised the progress that has been made thus far. More relevantly, three studies have been reported, that examined the efficient way of utilising sugarcane bagasse for LA synthesis. Due to the energy intensive nature around LA reaction system, Girisuta et al., (2013) optimized the reaction conditions to the temperature of 150°C and residence time of 360 minutes to yield 63 mol% LA. Lopes et al., (2017) and Schmidt et al., (2017), investigated incorporation of pretreatment technologies to obtain high yield from synthesising LA from reducing sugars. Also, to make, the hemi-cellulosic fractions and lignin available for independent utilisation.

Table 5: Recent progress on LA synthesis from sugar cane bagasse

Parameters	**(Girisuta et al., 2013)**	**(Schmidt et al., 2017)**	**(Lopes et al., 2017)**
Pretreatment*	NA	200◦C, 50 bar and 30 min	120°C; 5wt% H_2SO_4;80 min 80°C; 1wt% NaOH;90min
Enzymatic hydrolysis	NA	✓	NA
LA formation conditions	170°C; 360 min	180°C;60 min	150°C;75 min
Catalyst	0.55M H_2SO_4	0.63M H_2SO_4	5 wt% H_2SO_4
Solid loading	10 wt%	18%	6% (w/v)
Yield	63 mol%	67.7 mol%	55%

Typically, LA is recovered from an acid hydrolysate mixture by, firstly, filtering solids residues. Following the filtration stage is acid stripping by liquid-liquid extraction. The extracted LA is then purified in series of distillation columns to obtain 98.5% product purity (Howard et al., 2018).

Seibert, (2010), proposed the use of furfural as an extractant solvent to recover LA and formic acid from an acid hydrolysate mixture. The advantage of using this process is that the self-sufficiency of the biorefinery can be met. As mentioned earlier, furfural is one of the products produced as a result of LA synthesis by Biofine process. Moreover, a study was conducted previously to examine the use of different extracting solvents (Nhien et al., 2016). They showed

that using furfural as extracting solvent can reducing the energy requirement of by up to 25.5% and reduce the manufacturing cost by 30%. However, the selection of the correct solvent remains a challenge since, different feedstock result in different aqueous mixture concentrations. Methyl isobutyl ketone (MIBK) has also been regarded as the most efficient extracting solvent for LA extraction, although it tends to extract furfural along with LA due to relatively high partition coefficient (Alcocer-García et al., 2019).

2.4.3 Succinic acid

2.4.3.1 Brief overview

Succinic acid (SA), the C4-dicarboxylic acid, is an odourless, water-soluble, crystalline solid that is an intermediate metabolite in citric acid cycle (Vaswani, 2010). It has a boiling point of 235°C and molar mass of 118.1 g/mol. Its chemical structure shown by Figure 10, has linear structural features and saturated dicarboxylic acid, which gives it the potential to be used platform chemical for the production of fine chemicals and biodegradable polymers (Cao et al., 2018). It is as one of the top bio-based chemicals that can be obtained from renewable materials with the potential to improve the viability of biorefineries (Taylor et al., 2015; Werpy and Petersen, 2004).

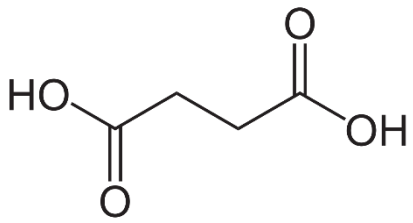

Figure 10: Succinic acid chemical structure

Currently, SA is serving a niche market in food and pharmaceutical industries and large volume market in polymer, plasticiser and chemical intermediates (De Jong et al., 2012; Taylor et al., 2015). The SA global demand was estimated at 40 ktpa in 2012. Again, it has been reported that the demand is expected to reach up to 90 ktpa by the year 2025 (Gerardy et al., 2020).

2.4.3.1 Succinic acid production

The fossil-based SA is produced from maleic anhydride and n-butane oxidation. Whereas its biobased counterpart is synthesised through the anaerobic microbial fermentation of sugars such as glucose, xylose, sucrose and fructose and other reducing sugars (Agarwal et al., 2006; Rosales-Calderon and Arantes, 2019). A typical process to produce SA from biomass includes a pre-treatment, fermentation and product recovery and purification steps (Nieder-Heitmann et al., 2019).

Fermentation

Recent research efforts have been focused on the biosynthesis of SA using different rumen microogranisms such as *Actinobacillus succinogenes*, *Mannheimia succiniciproducens* and *Anaerobiospirillum succiniciproducens* and other types of microbes such as *C. glutamicum and Escherichia coli* (Jiang et al., 2017; Rosales-Calderon and Arantes, 2019).

SA finds its biological production due to its nature of being part in every metabolite of microorganisms (Nghiem et al., 2017). Naturally, all the rumen microorganisms secrete SA via the reductive (anaerobic) TCA cycle. In a TCA cycle, using phosphoenolpuruvate and (PEP) through oxalate steps followed by anaerobic TCA cycle has the potential to theoretically produce 1.71 moles of SA per C6 sugar substrate (Jiang et al., 2017). Because CO_2 is utilised as one to the substrates in this biosynthesis process brings some environmental benefit. Along with the SA product, microbes can also co-secrete product such as ethanol, formic acid and lactic acid (Nghiem et al., 2017).

Currently, for large scale fermentation, *A. succinogenes* has been regarded as the most promising owing to its ability to handle inhibitory compound, acetic acid, to the concentration levels up to 40 g/l, and co-utilisation of different carbon sources such as xylose, glucose, fructose, sucrose, and glycerol for SA production (Nghiem et al., 2017; Vaswani, 2010). Some producers have been deploying *E. coli* due to its fast-growing capabilities in medium with less complicated nutrients (Ahn et al., 2016).

A number of studies have investigated molasses and bagasse for effective SA production (See Table 6). Chan et al., (2012) utilised genetically engineered *E. coli KJ122-pKJSUC* to ferment 150g/l of sugarcane molasses, yielding 56 g/l of succinate within the incubation period of 72 hours to efficiently utilise sucrose. Long incubation period was attributed by the presence of impurities since pure sugars took less time to yield SA. Their results showed a better performance in comparison to Agarwal et al., (2006), who used a low concentration of 26 g/l molasses in 30 hours to produce SA. Pre-treating molasses before fermentation has shown positive results, leading to improve fermentation production and reducing downstream processing complexities (Xu et al., 2015).

A. succinogenes is a robust microbe that has reported over 100 g/l titres to date (Nghiem et al., 2017). However, it tends not to thrive in pH below 6 and requires a complex mixture of nutrients for its growth. Borges and Pereira, (2011), attempted to maximise SA synthesis from bagasse hemicellulose hydrolysate using genetically engineered *A. succinogenes* CIP 106512, while optimising the fermentation nutrients; it yielded 22.5 g/l of SA. Genetically engineered

strain *A. succinogenes* NJ133 showed a better yield of 30.3 g/l (Jiang et al., 2013) results in comparison to NJ114, which was 23.2 (Xi et al., 2013). Results showed low yield due to the use of substrates with concentration below 50g/l. Moreover, *A. succinogenes* NJ114 yielded low SA because the hydrolysate was not detoxified. The pre-treated lignocellulose biomass cannot be applied directly for fermentation due to the presence of inhibitory compound acetic acids, furfural and HMF mixed with sugars (Cheng and Wang, 2013). Typically, a hydrolysate after pre-treatment is subjected to detoxification to remove inhibitors.

Table 6: Succinic acid producing strains adapted from (Jiang et al., 2017)

Strains	Substrate	Process	Concentration (g/L)	Productivity (g/L.h)	Yield (g/g)
A. succinogenes					
NJ133	Sugarcane bagasse (Cellobiose)	batch	30.3	0.84	0.67
NJ114	Sugarcane bagasse	Anaerobic, batch	23.2	0.97	0.87
CIP 106512	Sugarcane bagasse (hemicellulose)	Anaerobic, batch	22.5	1.01	0.43
E. coli					
AS1600a	Mixture of xylose and glucose	Anaerobic, batch	84.26	0.96	0.88
W3110	Cane molasses	Dual phase, batch	26	0.8	0.87
KJ122-pKJSUC	Sucrose cane molasses	Anaerobic, batch	62	1.05	0.96

To maximise product titres, which is required for reducing DSP capacity, initial substrate concentration of about 100 g/l are recommended for *A. succinogenes* (Xu et al., 2015), while *E. coli* has been shown to fermenter substrate with initial concentration up to 150 g/l (Chan et al., 2012). Together with carbon sources, fermentation is usually carried out in nutrient medium containing $NaHCO_3$, 10.0 g /l; $MgSO_4$, 3.0 g /l; yeast extract, 2.0 g /l; KH_2PO_4. 5.0 g / l as optimised by (Borges and Pereira, 2011). However, other carbonates salt can be used, such as $MgCO_3$ and $NaCO_3$ as a CO_2 source (Nghiem et al., 2017).

Downstream processing

The product recovery and purification of SA remain the major capital cost in its process (Nieder-Heitmann et al., 2019). Several studies have investigated SA recovery and purification techniques such as *in situ* separation, direct crystallisation, precipitation, membrane separation, solvent extraction and chromatography (Cheng et al., 2012), to try to come up with economically viable techniques. However, none has proven to be efficient in product recovery acting along. Efficient separation is obtained in the incorporation of these techniques in a separation train that is costly (Nieder-Heitmann et al., 2019; Rosales-Calderon and Arantes, 2019).

Usually, SA downstream processing comprises of three major steps; firstly, cells are removed from the fermentation broth by filtration or centrifugation, followed by SA recovery from the broth by either reactive extraction, evaporation, chromatography, adsorption or electro-dialysis; lastly, it is crystallised and dried to its required specifications for the market (Cheng et al., 2012).

A study by Morales et al. (2016), assessed the economic and sustainability of different DSP technologies for purification of SA and found that reactive extraction is the most economical and efficient in comparison to electro-dialysis and ion-exchange. Moreover, reactive extraction has been reported as the widely used method on an industrial level due to non-severe operating conditions (Ahn et al., 2016).

For an efficient SA extraction and purification, Morales et al., (2016), proposed a 3 consecutive reactive extraction configuration using ternary amines as an extractant. A mixture of 87wt% 1-octanol and 13wt% trioctylamine (TOA) is used. From then, SA is back-extracted into the aqueous phase using a solvent of 25wt % trimethylamine (TMA) and 75wt% water. A process is integrated with solvent recovery and recycling to reduce operating cost (Cheng et al., 2012). The product is then concentrated by vacuum distillation. The volatile TMA is separated and recycled back into the process. Lastly, the product is crystallised by cooling crystallisation and dried sale.

2.4.4 Xylitol

2.4.4.1 Brief overview

Xylitol is a white crystalline 5 carbon sugar alcohol that has been known to the world for almost 100 years (Mountraki et al., 2017). Its chemical structure shown in Figure 12 consist of 5 hydroxyl groups, which makes it highly soluble in water. It has a boiling point ranging from 214-216°C and melting point ranging from 92-96°C (Delgado Arcaño et al., 2020). It is one of the top 12 chemicals that were listed by the US Department of Energy in 2004 of biological origin with the potential to serve as platform chemicals. Even after the revised list it still made to the top 10 chemicals in 2010 (Bozell and Petersen, 2010; Werpy and Petersen, 2004).

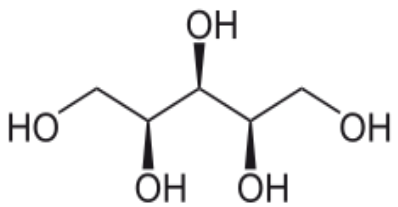

Figure 11: Xylitol chemical structure

Moreover, the European Commission Directorate-General Energy final report of 2015 highlighted it as the high-value product with no fossil-based alternative that shows a notable market (Taylor et al., 2015).

Xylitol was first discovered in 1891 by a German scientist Fischer in the form of a syrup obtained from birch-wood (Rafiqul and Sakinah, 2013). The shortages of sweeteners during the world war II spiked interests in the commercialisation of its productions (Delgado Arcaño et al., 2020). Its industrial production started in 1972 with a production capacity of 6000 t/yr, while in 2003 World Health Organisation (WHO) released a report that promotes the reduction of components such as sugar, salts, and fats in food (Delgado Arcaño et al., 2020). As a result, the search for food alternatives in line with this guideline has been pursued. Providing the same benefits, the xylitol production and demands have been increasing ever since (Mountraki et al., 2017).

Xylitol is commonly used in food and pharmaceutical applications due to its health benefits and sweetening properties. It has sweetness equivalent to that of sugar, however with less calorific value. Also, it is an attractive sweetener for diabetics, because its absorption in the body does not require insulin (Rafiqul and Sakinah, 2013; Rodrigues et al., 1998). The dental benefit has also been recognised: xylitol prevents tooth decay because cariogenic bacteria cannot utilise it to produce harmful acid in the mouth (Delgado Arcaño et al., 2020). Currently, the worldwide common xylitol market is the food industry in confectionery and sugar-free chewing gums (Rosales-Calderon and Arantes, 2019). In 2017, global xylitol demand was estimated at 190 ktpa, corresponding to a market volume of $196.8 million. It is expected to reach $430 million market size by 2026 (Stratistics Market Research, 2019).

2.4.4.2 Xylitol production

Xylitol occurs naturally in nature, more specifically in fruits and vegetables. However, it cannot be extracted directly from these sources because it exists in low concentrations. Moreover, processes associated with its extraction would be costly (Felipe Hernández-Pérez et al., 2019). Currently, xylitol is only produced from lignocellulosic biomass, and it has no fossil-based alternative (Delgado Arcaño et al., 2020). In a search for greener means for xylitol production, biological routes for xylose conversion into xylitol have been studied (Akinterinwa et al., 2008; Rodrigues et al., 1998; Ur-Rehman et al., 2015). Despite the effort of these researches, process efficiencies of the biological route have not matched those of the chemical route. The chemical

route can yield up to 99% of xylitol from pure xylose (Delgado Arcaño et al., 2020), whereas the maximum reported yield for biological process is 65% (Gil-Montenegro et al., 2019).

For the purpose of this study, only the catalytic chemical route is covered in detail since it is the adopted route for investigation. Its chemical synthesis route can be achieved in 4 vital steps shown in Figure 12.

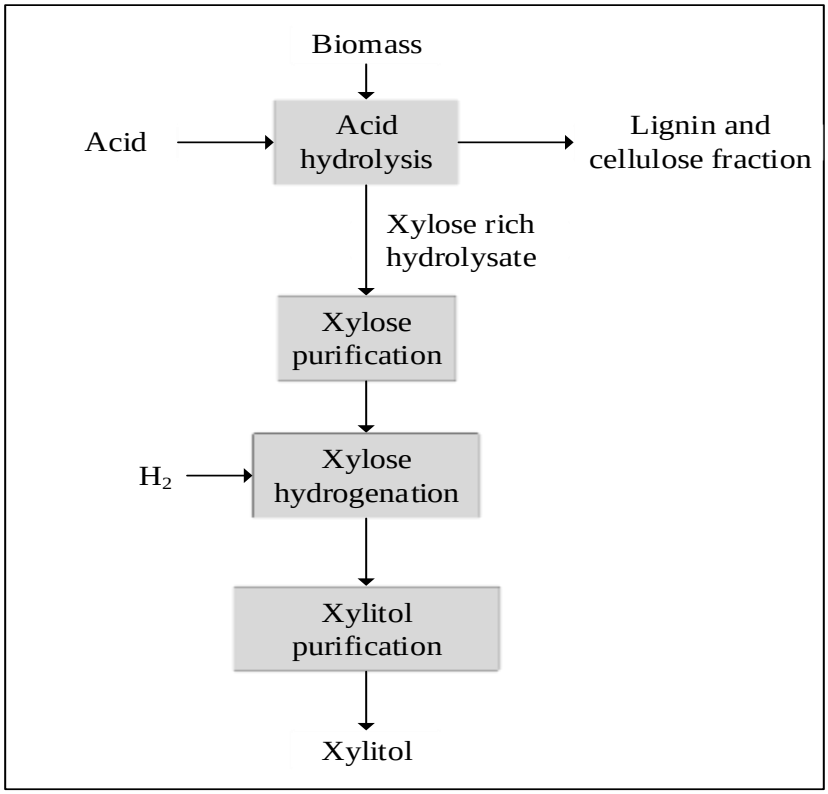

Figure 12: Xylitol chemical synthesis route redrawn from (Delgado Arcaño et al., 2020)

Pretreatment plays a crucial role in lignocellulosic biomass processing. Acid hydrolysis is the most efficient pretreatment method liberating hemicellulose fractions. Despite the drawback of side reaction during acid hydrolysis, it is still considered the most efficient process for the conversion of xylan to xylose (Mesa et al., 2016; Sasmal and Mohanty, 2017). Section 2.2 of this report gives sufficient details of different pretreatment methods and their effectiveness.

To ensure that xylose is at the desired specification prior hydrogenation, it goes through a series of purification steps to ensure that volatiles, the acid catalyst, and undesirable products are removed (Delgado Arcaño et al., 2020). Detoxification and xylose isolation by ion exchange chromatography have been reported as the widely employed techniques industrially, owing to their ability to preserve xylose (Mountraki et al., 2017; Rafiqul and Sakinah, 2013). Hydrolysis and xylose isolation are of great importance, in obtaining pure concentrated xylose (20 wt%) and removal of unwanted compounds that might have detrimental effect (catalyst poisoning

and deactivation) for the subsequent, hydrogenation process. The fractions of other chemicals are acceptable up to 5% (pontoses) and 3 wt % acetic acid (Mountraki et al., 2017).

Catalytic xylose hydrogenation happens at elevated temperatures and pressure, ranging from 110-200°C and 20-100 bar respectively (Delgado Arcaño et al., 2020). At such conditions, all the present sugars are hydrogenated to their respective polyols. By-products such as furfural, xylulose and xylonic acid can also form as a result of polyols degradation (Mikkola et al., 2003). Raney catalysts are employed for the industrial catalytic xylitol synthesis, as they are typically less costly. However, their fast deactivation as a result of the accumulation of inorganic *impurities* on its surface has inspired the investigation for a better catalysts (Yadav et al., 2012). Table 7 shows the effectiveness of employing other catalysts for xylitol production. Research has focused on catalyst development using Ru and Pt as catalyst supports due to their nature to facilitate hydrolysis and hydrogenation reactions (Yadav et al., 2012).

Table 7: Investigations on the different catalysts for better xylitol yield adopted from (Delgado Arcaño et al., 2020; Yadav et al., 2012)

Carbon source	**catalyst**	**Temperature (°C)**	**Yields (%)**		**References**
			Xylitol	**Arabitol**	
Bagasse	Ru(3%)Pt(1%)/C	190	60	-	1
Concentrated C5+C6 mixture	Ru@Duwex-H	120	99	-	2
Xylan	Pt(3.5)Sn(0.43)/Al	130	90	-	3
Xylose	Ru(1%)/NiO-TiO_2	120	99.7	.1	4
Xylose	Ru(1%)/TiO_2	120	96.1	0.1	4
Xylose	Ru(1%)/C	120	94	0.2	4
Xylose	Raney Ni	120	93.7	0.7	4

Yadav et al. (2012)[4], compared three different types of novel Ru supported catalysts with the conventional Raney Ni catalyst for hydrogenation of xylose to xylitol. Among the investigated catalysts, Ru(1%)/NiO-TiO showed the best result for xylitol yield at 99.7%. Yadav et al. (2012), concluded that the addition of NiO enhances the conversion of xylose to xylitol. The temperature was also investigated as one of the factors affecting xylitol yield. It was found that increased temperature of 140°C resulted in an increased xylose conversion, but decreased selectivity due to increased yield of by-products.

Direct synthesis of xylitol from solid lignocelluloses has also been investigated (Tathod and Dhepe, 2014; Yamaguchi et al., 2016)[1&3]. The inspiration behind this xylitol production technique was to try to minimize the conversion, product recovery and purification steps by producing xylitol using cascade catalysis reaction process with no intermediate separations,

thereby resulting in a cost-competitive process. However, with such production method the xylitol yield is lower in comparison to starting with pure xylose as a substrate. Barbaro et al., (2016)[2], investigated the hydrogenation of pentose and hexose sugars for polyols production using a bifunctional catalyst Ru@Duwex-H at 120°C and 30 bar. Xylitol yield of 99% was obtained with no dehydration products formed, however at an increased temperature of 190°C sorbitol was also produced as a result of hydrogenation.

Xylitol is recovered from hydrogenated solution by filtration, ion-exchange chromatography and crystallisation (Rafiqul and Sakinah, 2013). The catalyst is removed from the solution by filtration. Subsequently, ion exchange chromatography is employed to obtain a rich xylitol solution prior crystallisation process. The crystallisation process can yield up to 75% of xylitol crystals at 98% purity (Delgado Arcaño et al., 2020).

2.5 Techno economic assessments of sugarcane biorefineries

The techno-economic assessment (TEA) studies are used as a tool to examine the viability and the technical characteristics of the project, thereby helping in decision making for the investors or required plan of action (Zimmermann et al., 2020). For the South African context, biorefineries annexed to an existing sugar mill have been seen as a way to add value to a diminishing sugar industry (Dogbe et al., 2020). Currently, there are studies ongoing, investigating the implementation of these biorefineries by TEA studies. As one of them, this study builds on the existing work of Dogbe et al. (2020); Kapanji et al. (2019); Nieder-Heitmann et al. (2019); and Özüdoğru et al. (2019). On this section, the progress that has been made and new developments are highlighted.

There are quite extensive biofuels TEA reports in the literature, mainly because there is a motivation to replace the fossil fuels counterpart that constitutes nearly 80% to the world overall energy demands (Cuong et al., 2018). These studies have been looking at different pathways and feedstocks to assess the most profitable pathway for employment in a biorefinery context. In particular, sugar cane biorefineries utilising bagasse and trash have been reported by (Ali Mandegari et al., 2017) who showed that integrating bio-ethanol production to an existing sugar mill can improve the economic performance of such industry. Such configuration benefit from the low-cost raw material. Furthermore, a Brazilian (Dias et al., 2012) and Colombian TEA studies (Moncada et al., 2014) have shown that integrating 1G and 2G for bioethanol production results in better economic performance than 2G biorefinery alone.

Similarly, 1G biorefineries have been said to yield better economic performances compared to 2G biorefineries (Junqueira et al., 2017). A study by Dogbe et al. (2020) for the production of succinic acid from A-molasses showed better results in comparison to a study by Nieder-Heitmann et al. (2019) for the production of succinic acid from sugarcane bagasse and trash. The mandatory pretreatment and enzymatic hydrolysis of the 2G feed is one of the reasons why 1G biorefineries perform better than 2G biorefineries. However, considering different time purview, Junqueira et al. (2017) has shown that in long term 2G production of bioethanol is more cost-competitive than 1G bioethanol production. While the short term for 1G ethanol showed to be more cost-competitive than 2G ethanol.

Özüdoğru, (2018), investigated TEA study for GA production from lignocellulosic biomass. Even though the outcome of the process was deemed profitable, the profitability of such a scenario can be improved by using molasses feedstock which requires no pre-treatment. Pre-treatment can have a massive effect on the profitability of a biorefinery (Nieder-Heitmann et al., 2019). A similar study to this one was done by (Pal et al., 2015), evaluating the economics of producing GA from cane juice using an integrated reactor membrane system. However, in this study, a more detailed A-molasses biorefinery complex, which includes WWT and CHP is considered.

Recently there has been an increasing number of TEA studies for the production LA from sorghum bicolor (Gozan et al., 2018), rice straw (Isoni et al., 2018) and municipal solid waste (Sadhukhan et al., 2016). More relevantly, Kapanji et al., (2019) assessed the production of LA from sugar cane bagasse. Two biorefinery scenarios producing high and low volume LA were compared to determine the economies of scale benefits. From these scenarios, it was deduced that producing LA in high volume will reduce the production cost. However, with all the progress made, there are no TEA reports on the 1G production of LA. This allows an opportunity to explore the production LA from a low-cost carbon molasses in the South African sugarcane biorefinery context.

Even though technologies for xylitol production have been fully commercialised, TEA studies are being done to investigate different carbon sources (Delgado Arcaño et al., 2020). Moreover, Mountraki et al., (2017), compared fermentative and catalytic processes. Their results proved that it is more economically viable to produce xylitol via catalytic than fermentative routes. Özüdoğru et al., (2019), adopted the former process for the TEA case study and showed that it is profitable to produce xylitol by utilising sugarcane bagasse available in the sugar industry.

However, there are no reports on biorefineries producing xylitol along with any of the products of interest.

Table 8, summarises the key results of product of interest from previous studies. Xylitol, GA and SA scenarios were evaluated for a sole product biorefineries whereas LA was evaluated for multi-product facilities co-producing furfural.

Table 8: Summary of existing scenarios

Product	**Raw Feed**	**Production Capacity (t/year)**	**Techno-Economic indicators**			**References**
			MSP (US$/kg)	NVP ($M)	IRR (%)	
Glutamic acid	2G	81648	-	866.5	31.20%	(Özüdoğru et al., 2019)
Levulinic acid *	2G	648	6.5	253	23%	(Kapanji et al., 2019)
Levulinic acid	2G	46656	1.08	139	17.4%	(Kapanji et al., 2019)
Succinic acid	2G	87502	1.50	352	21.60%	(Nieder-Heitmann et al., 2019)
Succinic acid	1G	58000	1.35	422	57.1%	(Dogbe et al., 2020)
Xylitol	2G	37584	3.00	$39.9	12.30%	(Özüdoğru et al., 2019)

* LA and furfural sold for revenues

Multi-product facilities are seen as not only a way to diversifying product range in a biorefinery but only to utilise biomass efficiently. Giuliano et al. (2018) showed that the profitability of production of bioethanol from corn stover can be improved co-producing an added chemical. For the scenarios considered ethanol co-production with xylitol showed better economic viability despite having a high cost of production than ethanol-co production with furfural. The reason the former to yielded better economic performances was due to the high selling price s of xylitol that is significantly higher than of furfural.

In summary, the TEA studies have been predominately used to assess different process configurations, for 1G and 2G production of biofuels and biochemicals. For South African context, the detailed TEA for 2G production of GA, LA, SA, and xylitol have been reported (Kapanji et al., 2019; Nieder-Heitmann, 2019; Özüdoğru, 2018). However, TEA for 1G production of these biochemicals has not been reported sufficiently, with an exception for 1G SA by (Dogbe et al., 2020). According to literature reviewed for 1G and 2G biorefineries, there is still a gap to be explored for TEA studies for 1G production of GA and LA.

Multiproduct facilities utilising lignocellulose have been previously studied. These studies looked at scenarios for methanol, ethanol, lactic acid, furfural and levulinic acid from sugar cane bagasse and trash (Farzad et al., 2017b; Gorgens et al., 2016; Kapanji et al., 2019;

Mandegari et al., 2017b). No TEAs for multi-product facilities have been reported for the integrated 1G2G biorefineries producing GA, SA, LA and xylitol.

2.6 Literature key highlights

Sugarcane bagasse and molasses are considered by-products of sugar production. Their utilisation as both sole and integrated complementary raw materials in a biorefinery context could yield an economic benefit to the sugar industry.

Reconfiguration in the sugar mill by eliminating second and third crystallisation units aimed at high recovery of crystalline sucrose, produces a cleaner A-molasses for use in a biorefinery complex that will omit the further processing before fermentation and yield to better product purity. Furthermore, reduction in heating demands from 120t/h to 104.5 t/h of steam the sugar mill complex due to this reconfiguration will allow annexed 1G biorefineries to share the existing CHP facility thereby providing the economic benefit. On the other hand, 2G biorefineries require the installation of new high-pressure boiler avail more lignocelluloses feedstock for utilisation.

To this end, sugarcane biorefineries are seen as a way to ensure the sustainability of the current diminishing sugar mill through product diversification. The four products (glutamic acid, succinic acid, levulinic acid, and xylitol) of considerably good market opportunities have been selected for investigation in 1G, 1G2G, and 1G2G multiproduct biorefineries configurations. Also, the existing 2G are upgraded.

Considering the gaps in the literature described in section 2.5, the objectives of this study were to:

1. **To design and evaluate the profitability of 1G biorefinery scenarios producing LA and GA.**

Since there are no current reports on TEA for GA and LA production from molasses, the designs of these products are considered using literature data, and their economic viability is compared with updated 2G biorefineries counterparts. Generally, 1G biorefineries result in better economics, primarily benefiting from the eliminations of cost-intensive processing stages such as pretreatment and enzymatic hydrolysis.

2. **To update existing 2G biorefineries producing LA, GA, and SA as well as 1G biorefinery for SA.**

The existing scenarios were developed and assessed under different sets of technical and economic assumptions. However, for a fair comparison, these scenarios are updated to consider

5000 hours of annual operations instead of 6480 hours and the same raw material cost more. For instance, the new costs of feedstock (2G) considering the marginal cost of sugar mill as a result of annexing new biorefineries is updated from $10.6/t to $42.50/t.

3. **To develop integrated 1G2G biorefinery configurations to produce GA, LA, and SA, as well as multi-product biorefinery configurations for production of GA, LA, and SA with xylitol**

There are advantages brought by 1G and 2G feedstocks integration into a single complex such as sharing processing units or infrastructure (CHP, downstream units, and fermentation processes), potential inhibitors dilution in 2G hydrolysate when mixed with 1G liquid, and increased thermal efficiency through heat exchanger network. Through these configurations, the economies of scale benefits, as well as the effect of integration, are assessed. Furthermore, xylose accounts for nearly 30% of sugars that can be derived from lignocellulose and is underutilised in the fermentation process for GA, and SA, and the chemical process for LA. Multi-product facilities are considered to exploit the value presented by the lignocellulosic feedstock and further increase the product spectrum for sugar mills.

4. **To compare the economic viability of 1G2G scenarios to the newly built 1G scenarios, existing 1G, and 2G scenarios and 1G2G multi-product facilities**

To determine which biorefinery configuration gives the best economic viability results. The major economic indicators, such as internal rate of return, minimum selling prices, and net present value. Furthermore, sensitivity analysis is to quantify uncertainties of some economic assumptions and parameters.

3 Methodology

Throughout this section, the methodology and specific steps undertaken to complete the objectives of this project are described. The software, thermodynamic model, process description and rationale followed to develop these biorefinery scenarios are outlined. Numerous scenarios for 1G, 2G and 1G2G biorefineries producing glutamic acid, levulinic acid, succinic acid and xylitol, as well as 1G2G multiproduct facilities producing maximum of two products are investigated in terms of techno-economic assessment, to determine the profitability of each production process and the key driver that influence proditability. Figure 14, shows a summarised research approach that was followed for this project. The processes developed are based on the established technologies and lab scale results for biological and catalytic conversion of sugars. The results obtained from these analyses are beneficial, in providing insights and determining the determinants of profitability for different biorefinery configurations/ scenarios.

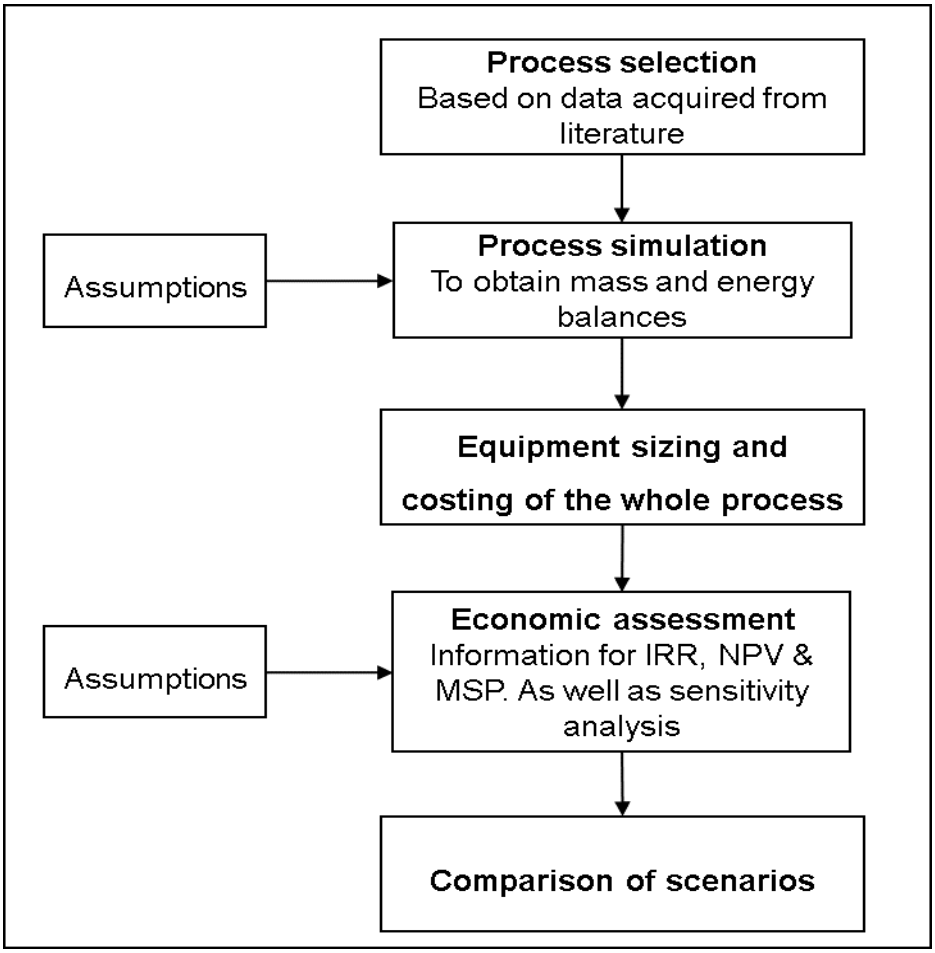

Figure 13: Research approach

3.1 Simulation set-up

3.1.1 Software

All biorefinery scenarios are simulated using AspenPlus® V 8.8 software. This process simulation tool is widely used to model chemical industrial process technologies, such as biorefineries and chemical processes' conceptual designs, and optimisation of processes' technical parameters (Pachón et al., 2018). The process simulation generates mass and energy balances that are used for the subsequent comparisons of the different biorefinery scenarios (Singh et al., 2016).

3.1.2 Property method

Thermodynamic model selection is a crucial part in developing simulation in AspenPlus®, as this can cause a huge impact on the results output. The Biorefinery scenarios are simulated using the activity coefficient model, Electrolyte Non-Random Two- liquid (ELECNRTL). This property method is the most flexible for modelling electrolytes at low and high concentration. Additionally, it can also be adopted for aqueous and combined solvent processes (Aspen Technology Inc., 2013). However, for processes area such as CHP, the STEAM NBS property method is selected owing to its capabilities to estimate the thermodynamic state of pure water using steam table correlations for systems with temperature ranging from 25-1725 ˚C (Özüdoğru, 2018).

3.1.3 Components Selection

AspenPlus® has a wide range of components that are readily available in its databank. However, some components do not exist in AspenPlus® databanks such as humins, biological microbes and some of the lignocellulosic constituents. The simulation was built by specifying lignocellulosic and biological components as non-conventional solids and their properties were adopted form NREL databank produced by Humbird et al. (2011) (Components used for this project are listed in Appendix A).

The stream class for all the simulation models were set to MXISLD. This allows for components entry as either conventional or solids without requiring the solids particle size distribution.

3.1.4 Mass and energy input

The 1G processes use 25.433 t/h of A-molasses feedstock, comprising of 22.07% water, 54.43% sucrose, 11.74 % fructose and 11.74 % glucose on a mass basis (Dogbe et al., 2020).

The 2G feed of 65t/h on dry mass (DM) basis is available for utilisation from atypical sugar mill (Gorgens et al., 2016). It is comprised of 20 t/h DM of trash (brown leaves) and 45 t/h DM bagasse available after sugar extraction. The mixture of trash and bagasse's compositions are assumed to be 40.7% cellulose, 27.1% hemicellulose (3.4% glucan, 17.7% xylan, 3.3% arabinan, 2.2% acetate), 21.9% lignin, 3.5% ash and 6.7 extractives on a mass basis (Gorgens et al., 2016; Özüdoğru, 2018).

Each biorefinery scenario has its power and heating demands which are dependent on the process equipment load and capacity. To close the energy loop, an iterative simulation in was done, in order to determine the amount of lignocellulose that should be bypassed to the CHP to provide heating for both sugar mill and biorefinery. A constant steam supply of 120 t/h is sent to the sugar mill, for biorefineries processing 2G feedstock only. However, when biorefineries processing A molasses are considered steam sent to the sugar mill is 104.5 t/h. This is because there is a reduction in energy demands due to elimination of B and C boils (Dogbe et al., 2020). The heating and cooling demands of each process are determined using utility specifications shown in Table 9.

Table 9: Utility specifications adapted (Gorgens et al., 2016)

Utilities	**Supplied**		**Return**	
	Temperature (°C)	**Pressure (bar)**	**Temperature (°C)**	**Pressure (bar)**
Chilled water	4	2	15	1
Cooling water	28	2	37	1
Cooling air	30	1	35	1
HHPS (for sugar mill)	350	28	90	2
HHPS (for biorefinery) [a]	350	28	260	50
HPS	266	13	192	32
LPS	233	9.5	170	8
LPS from low pressure boiler	180	10	179	9

[a] This is a new addition to the specifications by Gorgens et al., (2016).

The energy system in flowsheet development is one of the significant contributors to the process design's economic outcome, because it affects the bagasse supply and product production rate. In order to design a more rigour energy balances of the process. The return condensates to the boiler have been specified as follows in Table 9 whereby they are mixed in a condensate tank to minimise the heat loss. One of the advantages of returning hot condensates into the boilers includes improved fuel savings in the process and reduced the production cost (Renfrow, 2001). One of the improvements that is done to the existing developed simulations

includes the ovaral energy of the system. The previous simulation models developed by Özüdoğru, (2018) and Kapanji et al., (2019) have assumed total return condensate to the boiler at 90°C and Nieder-Heitmann et al., (2018) have assumed 105°C for the return condensate to the boiler.

The cooling systems (cooling tower and absorption chiller) for provision of cooling utilities are not simulated in this project. However, considerations are made for their respective capital cost by assuming 6.5% of the ISBL total installed cost (Ali Mandegari et al., 2017). The effects of this are quantified through sensitivity analyses on TCI.

3.1.5 Assumptions

Energy

- 10°C minimum temperature approach is used in heat exchanger network design,
- No steam losses around the process,
- High-pressure boiler's temperature is 870°C and 5% energy losses are assumed,
- Existing boiler and cooling tower can operate with 10% excess of their current operation,
- Boilers are supplied with 40% excess air.

Technical

- CEST turbines are set at isentropic efficiency of 85 %,
- Pumps are simulated at 85% and 95%, mechanical efficiency and driver efficiency respectively,
- Fermentation processes are simulated using *RStoic*, using assumed reactions based on yields.

Process considerations

- All 2G processing scenarios assumes replacement of existing boiler with a new efficient high-pressure boiler. As such 45 t/h of bagasse is made available,
- Although not fully simulated, the process is assumed to produce enzymes on-site,
- Nutrients that are not part of the assumed reactions are not simulated. However, their operational cost is considered,
- 50% of the solid catalyst is assumed recyclable.

- All biological tanks are assumed at 950 m^3, with 70% working volume (Humbird et al., 2011). Using these numbers as a basis the number of tanks required is determined using residence times and 12 hours (Assume value time for cleaning and filling the tank).

3.2 Biorefineries block flow diagrams

This section aims to paint a picture for the 1G and 2G /1G2G processes flows configurations. Since the product of interest follows different routes, the more generic block flow diagrams (BFDs) are shown, to illustrate which processing areas are considered for each biorefinery classification.

3.2.1 1G biorefineries process design

Figure 14 shows an overall process diagram for 1G biorefineries. The integrated 1G biorefinery incorporates three major areas: Fermentation/ Reaction (A-100), Downstream processing (A-200) and WWT (A-300), to the existing sugar mill and its energy island. A molasses is extracted from the sugar mill and utilised in A-100 to produce the respective product. The desired product is then purified in A-200 to its required specifications. All wastewater streams are purified in WWT in order to reduce water requirements. Since there is no need to liberate more bagasse for utilisation in the biorefinery complex, the energy and power demands of 1G biorefinery complexes are supplied using the existing boiler in order to reduce the CAPEX associated with the installation of a high-pressure boiler. However, if the power and energy cannot be met using the existing boiler after considering 10% extra capacity. The deficit is then supplied by incorporating a low cost, low-pressure boiler, powered using some of the biogas produced in WWT and excess bagasse's left in the boiler, coal powering can be considered when the heating cannot be met using the available sources of heating.

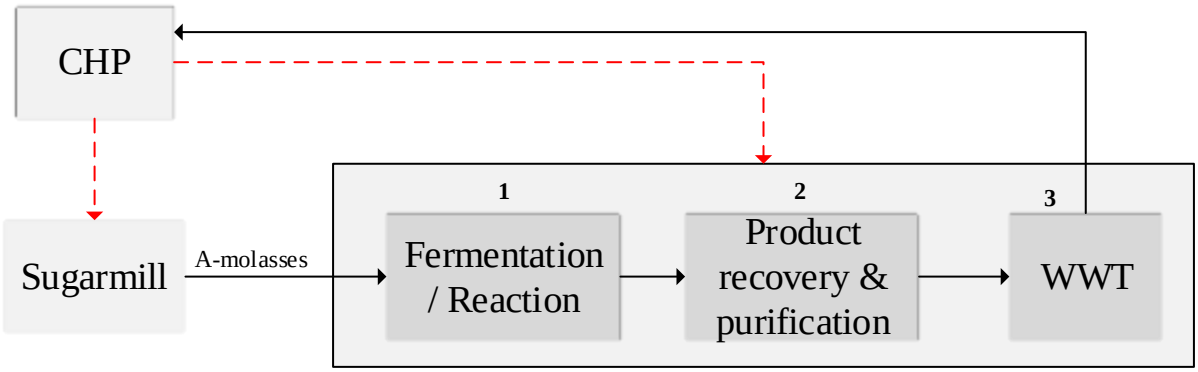

Figure 14: General BFD for 1G biorefinery

3.2.2 2G and 1G2G biorefineries process design

Figure 15, shows the configurations for the self-sufficient biorefinery complex that installs new high-pressure boiler in order to make more bagasse available for utilisation. Herein, the biorefinery is characterised into several areas; Pretreatment (A-100), Enzymatic hydrolysis (A-200), Seed train and Enzyme production (A-300), Fermentation (A-400), Reaction (A-500), Product recovery and purification (A-600), WWT (A-700) and CHP (A-800). The common areas among different scenarios are A-700 and A-800. It is worth mentioning that in this configuration enzymes are assumed to be produced onsite. Though not simulated, the CAPEX associated costs are added in the economics by a plant scaling from NREL.

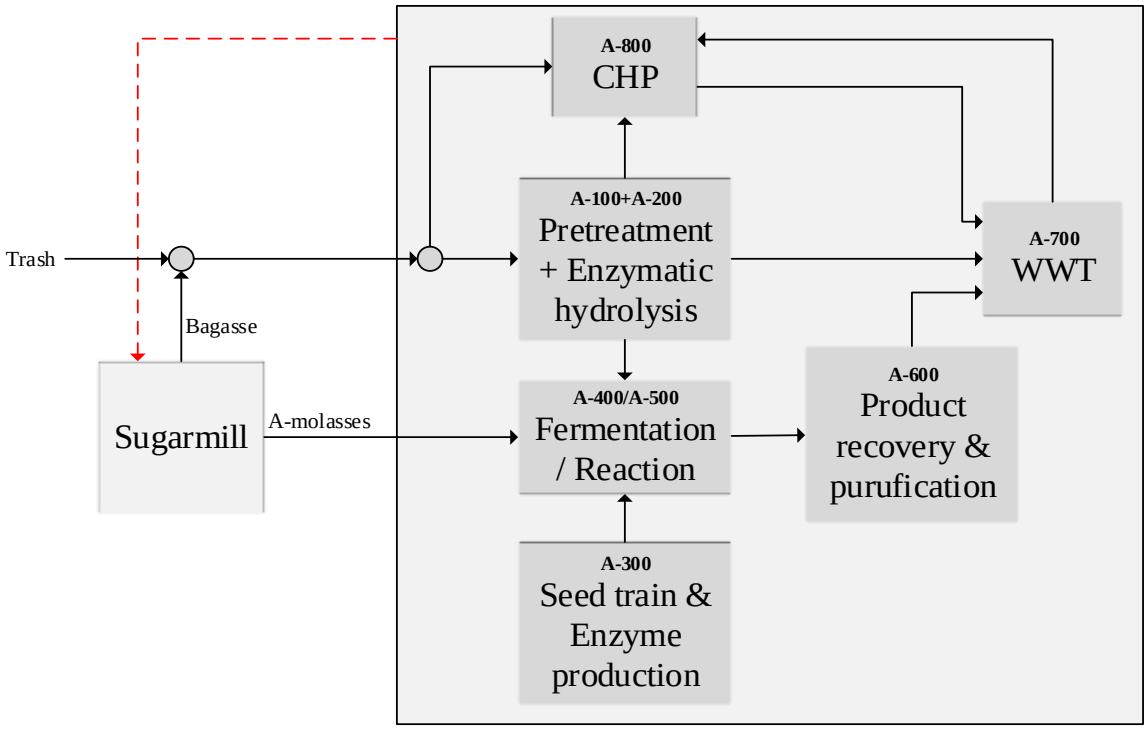

Figure 15: 1G2G biorefineries configurations

3.2.3 Defined biorefinery scenarios

Table 10 shows the codes used to define biorefinery scenarios. The code names: *1G XX, 2G XX and 1G2G XX* are used, where *"XX"* represents an acronym for the product of interest and 1G/2G/1G2G represent the feedstock generation used. Furthermore, 2G scenarios in results and discussions section are referred to as *existing 2G XX* and *updated 2G XX* to distinguish the data the latter from what has been previously done.

Table 10: List of scenarios with their code descriptions

Scenarios	Description
1G GA	Glutamic acid from A molasses
1G LA	Levulinic acid from A molasses
1G SA	Succinic acid from A molasses
1G2G GA	Glutamic acid from A molasses and lignocelluloses
1G2G LA	Levulinic acid from A molasses and lignocelluloses
1G2G SA	Succinic acid from A molasses and lignocelluloses
1G2G GA + Xylitol	Glutamic acid and xylitol from A molasses and lignocelluloses
1G2G LA + Xylitol	Levulinic acid and xylitol from A molasses and lignocelluloses
1G2G SA + Xylitol	Succinic acid and xylitol from A molasses and lignocelluloses
2G GA	Glutamic acid from lignocelluloses
2G LA	Levulinic acid from lignocelluloses
2G SA	Succinic acid from lignocelluloses

3.3 Generic plant areas

3.3.1 Pretreatment

3.3.1.1 Pretreatment overview

The scenarios processing 2G feedstock employ dilute acid pre-treatment technology. Dilute acid is one of the well-established pretreatment methods for lignocellulosic biomass feedstocks. During the hydrolysis reactions, most of the hemicellulose fractions are converted to soluble sugars, i.e. xylose, arabinose, glucan and glucose. Furfural and HMF are also formed as a result of sugar degradation during this process (Humbird et al., 2011). (A detailed PFD of this process is given in Appendix C

After hydrolysis, the hydrolysate is flashed at atmospheric conditions, as a result, a large portion of water is vaporised and fractions of acetic acid and HMF. The cell lignin materials are recovered by filtration and subsequent washing, to ensure that acid and inhibitors are totally removed before enzymatic hydrolysis. For a process where xylose is utilised, neutralisation process is incorporate to remove the acid in the liquid hydrolysate, for further downstream processing, since it can deactivate the catalyst, or hinder fermentation processes (Delgado Arcaño et al., 2020; Wooley et al., 1999).

3.3.1.2 Pretreatment process description and process flow diagram

Lignocellulosic biomass feed enters the process via stream 103, and it gets mixed with water at 95°C in a plug screw conveyer (PS-101), to achieve the solid loading of 30wt% (Humbird et al., 2011). Also, this configuration allows more than 40% of the hydrolysis heating process to be met. PS-101conveys the biomass into a pre-steamer (HX-101), HPS at 266°C is injected

in to preheat biomass to 135°C. After the biomass has been pre-steamed, it is fed into the reactor (RX-101) via blowdown tank (BD-101). The latter act as a seal for the HX-101 and RX-101and has a plug screw feeder that reports biomass into the RX-101. Biomass and 93wt% H_2SO_4 are fed into RX-101 in a ratio of 18 mg acid per g of dry biomass (Humbird et al., 2011). Acid is mixed with biomass in the BD-101 so that it can be diluted by the high-water content available in the latter before it is exposed to the severe conditions of RX-101. HPS is injected in RX-101 to keep its contents at 185°C. The hydrolysis reactions occurring in RX-101are shown in Table 11 (Humbird et al., 2011).

Table 11: Dilute acid hydrolysis reactions adapted from (Humbird et al., 2011; Özüdoğru, 2018)

Reaction	Conversion
Cellulose +H_2O → Glucose	9.9%
2Cellulose +H_2O → Cellobiose	0.3%
Glucan + H_2O → Glucose	9.9%
Xylan+ H_2O → Xylose	90%
Arabinan + H_2O → Arabinose	100%
Acetate→ Acetic acid	100%
Xylose → Furfural+ 3H_2O	4.2%
Glucose → HMF+ 3H_2O	4%
Lignin→ Soluble lignin	5%

The content of the reactor is then flashed (FT-101) at atmospheric conditions. The vaporised stream 129 at 100°C, is used to heat (HE-101) the inlet water stream to 90°C, assuming minimum temperature approach of 10°C. The hydrolysate is then pumped (PU-101) and cooled to 50°C before the being sent to a filter press (FP-101) to remove cellu-lignin solid material from the liquid hydrolysate. The moisture in the filtered solids is then washed (WT-101) with water fed at 1g water per 1 g dry matter in a two-stage wash cycle with an efficiency of 96% (Aden et al., 2002; Dogbe et al., 2020). The washed solids are then pumped (PU-107) to enzymatic hydrolysis. Washed liquid and filtered liquid hydrolysate are mixed (MT-101) and pumped (PU-104) to a neutralisation tank (NT-101). Lime is used to neutralise H_2SO_4 according to the reaction shown in equation *3-1*. This is to avoid catalyst deactivation and microorganism poisoning on the subsequent processing

$$H_2SO_4 + Ca(OH)_2 \rightarrow 2H_2O + CaSO_4 \qquad \textbf{3-1}$$

Lime at 14% excess is conveyed (CB-101) into the NT-101, where 100% conversion of H_2SO_4 to gypsum is assumed (Özüdoğru, 2018; Wooley et al., 1999). The neutralised liquid hydrolysate is then filtered (FB-102), for 99.5% removal of gypsum. Subsequently, it is pumped (PU-106) to the detoxification process.

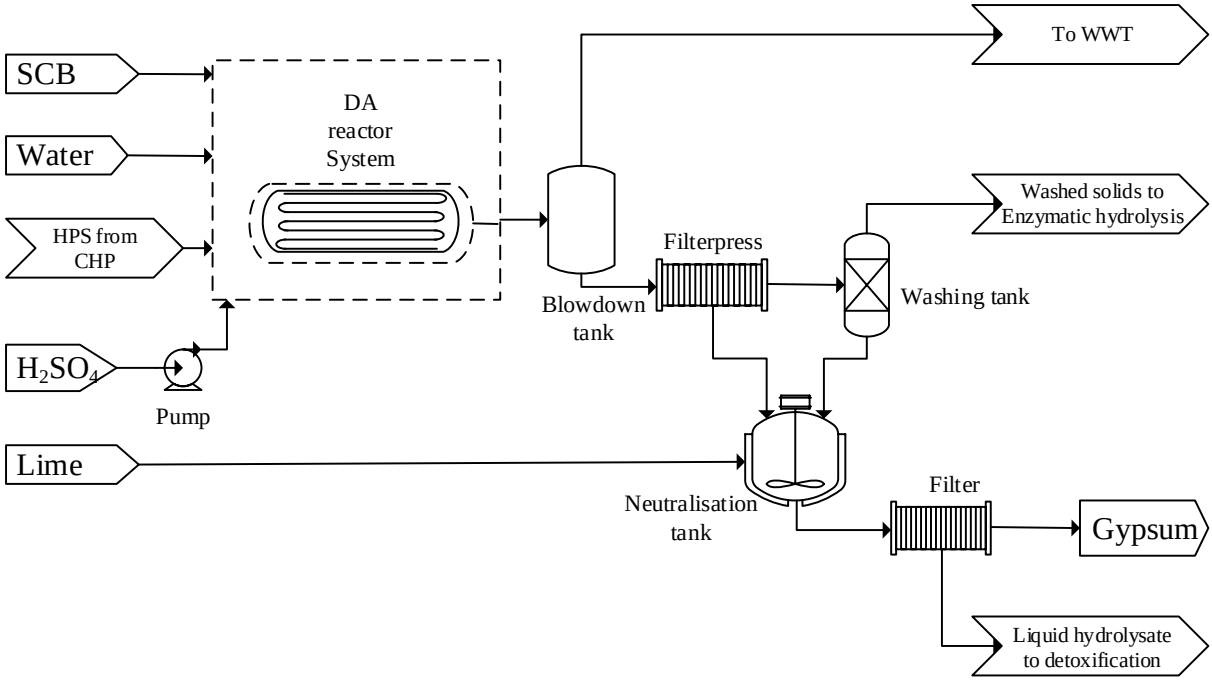

Figure 16: Simplified flow diagram for Pre-treatment section (Humbird et al., 2011; Özüdoğru, 2018)

3.3.2 Enzymatic hydrolysis and detoxification

Enzymatic hydrolysis and detoxification are the two parallel processes considered as the area 200 of this process plant configuration.

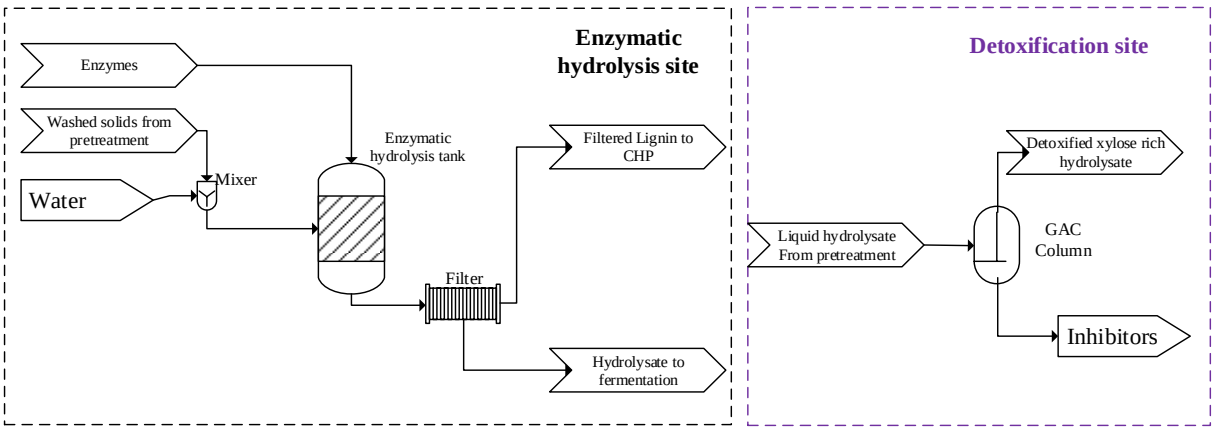

Figure 17: Enzymatic and detoxification flow diagrams (Nieder-Heitmann et al., 2019)

In this process the cellulose present in the solid residues obtained after washing from A-100, are converted into monomeric sugars by enzymatic hydrolysis. The enzymatic hydrolysis reactors are fed a slurry containing 20% solids with enzyme loading 20g protein per kg solid feed. The contents of these reactors are held at 50°C for 3 days to produce a glucose rich slurry containing a solid fraction of lignin residues (See conversion reaction in Table 12). The solid residues are then separated from the hydrolysate by filtration and subsequently sent to the CHP. The obtained rich glucose liquid hydrolysate then taken to the fermentation process (A-400).

Table 12: Enzymatic hydrolysis reactions (Humbird et al., 2011; Özüdoğru, 2018)

Reactions	Conversion
$Cellulose\ (Cisolid) + H_2O \rightarrow Glucose$	90%
$Cellulose + H_2O \rightarrow\ Cellobiose$	1.2%
$Cellubiose + H_2O \rightarrow 2Glucose$	100%

On the other hand, the liquid hydrolysate from A-100, containing fractions of HMF and furfural are passed through a granular activated carbon (GAC) column for complete removal of the former and the latter. Villarreal et al., (2006) has shown that this process can archive complete removal of furans and phenolic compounds and with only 7% of sugars loss. Depending on the process the purified liquid hydrolysate containing pentose sugars is either utilised for fermentation in 2G and 1G2G SA production or utilised for xylitol production. Section 3.6 and 3.7, describes elaborates clearly in this regards.

3.3.3 Wastewater treatment plant configuration

The water requirement in the biorefinery is reduced by incorporating WWT that assumably produce clean water for recycling back into the process. The WWT simulation model is adopted from NREL (Humbird et al., 2011). All the waste-water streams reporting fractions of COD greater than 10000PPM are anaerobically digested to remove 91% of soluble material in the water producing methane at 0.38kg/ kg COD digested. Followed by aerobic digestion to further remove the remaining soluble material, 96% of the remaining soluble material is removed during this process. Subsequently, pure water is then recovered by clarification, filtration and evaporation. The biogas produced by this process, along with sludge, are then combusted in the CHP for energy generation.

3.3.4 Combined heat and power plant configuration

3.3.4.1 1G biorefineries energy island

Heat and power in the 1G biorefinery scenarios are provided by the existing boiler, that is assumed to have 10% extra capacity (Dogbe et al., 2020). A typical sugar mill in South Africa that processes 300 t/h of sugar cane requires 120t/h of steam (Farzad et al., 2017b). However, when the A molasses is extracted for utilisation in the biorefinery complex. The steam requirements in the sugar mill reduce to 104.5 t/h, which leaves a surplus of 30.5 t/h of steam taking into consideration 10% extra capacity (Dogbe et al., 2020). This surplus steam can be utilised for heating in the biorefinery complex. Moreover, the CHP analysed Dogbe et al.,

(2020) under these assumptions, burns 60.5t/h of bagasse on a wet basis (WB) resulting in a surplus 32.3 t/h WB can be spared for utilisation in a low-pressure boiler.

The deficit in steam can be met by installation of a low-pressure boiler. Table 13 shows the technical parameter for a low-pressure boiler (Pertersen, 2018). The low-pressure boiler is not simulated in AspenPlus®. However, the deficit in the steam requirement was determined. Moreover, the costs associated with this process are considered in the economic analyses by assuming the cost of quoted medium pressure boiler.

Table 13:Technical information of low-pressure boiler

Boiler Pressure (bar)	10
Steam Temperature (°C)	180
Latent Heat of Evaporation at 10 bar (MJ/tonne)	2014
Feed Water (° C)	95
Boiler Efficiency	84.70%

3.3.4.2 2G and 1G2G biorefineries energy island

The heat and power demands of both sugar mill and biorefineries are met by burning some of the bagasse in a cogeneration system. Raw bagasse, filtered lignin and humins, as well as CH_4 produced in the WWT unit by anaerobic digestion, acts a fuel source in a burner where these fuels are combusted with oxygen as per reaction shown in Table 14.

Table 14 : Burner combustion reaction and assumed conversion (Humbird et al., 2011; Özüdoğru et al., 2019)

Reactants	**Chemical formula**	**Conversion**
Cellulose	$C_6H_{10}O_5 + O_2 \rightarrow H_2O + CO_2$	98%
Glucan	$C_6H_{10}O_5 + O_2 \rightarrow H_2O + CO_2$	98%
Xylan	$C_5H_8O_4 + O_2 \rightarrow H_2O + CO_2$	98%
Arabinan	$C_5H_8O_4 + O_2 \rightarrow H_2O + CO_2$	98%
Acetate	$C_5H_8O_4 + O_2 \rightarrow H_2O + CO_2$	98%
Extract	$C_6H_{12}O_6 + O_2 \rightarrow H_2O + CO_2$	98%
Lignin	$C_8H8O_3 + O_2 \rightarrow H_2O + CO_2$	98%
Methane	$CH_4 + O_2 \rightarrow H_2O + CO_2$	98%
Humins	$C18H_{20}O_{10} + O_2 \rightarrow H_2O + CO_2$	98%

All 2G and 1G2G biorefineries have the same CHP plant configuration. The existing medium pressure boiler (28 atm) is replaced by the new high-pressure boiler (62 atm). Table 15, summarises the technical parameters of the boiler.

Table 15: Technical parameter for the new high-pressure boiler

Parameter	Value
Deaerator pressure	3.3 atm
Deaerator temperature	137 °C
Boiler feed water pressure	62.2 atm
Boiler feed water temperature	176 °C
HHP steam pressure	62.2 atm
HHP steam temperature	452 °C
Averaged burner temperature	870 °C
Combustion conversion	98 %
Inlet economizer temperature	278 °C
Air preheat temperature	185 °C
Stack temperature	149 °C
Boiler heat loss (total)	10%
Blow down	3%
Air supply	40% excess

CEST section containing four extraction stages receives superheated steam at 452 °C at 62 atm. Firstly, the isentropic turbine operating 29 atm, is used to generate electricity and HHPS (28 atm, 360°C). Here, a portion of the HHPS (23.5 t/h) is extracted for sugar mill turbine. Also, HHPS requirements for LA biorefineries are incorporating extraction here. The remaining HHPS is passed through the next is isentropic turbine operating at 13 atm to produce electricity and HPS (13 atm,266°C). Parts of the steam are extracted, to heat the boiler feed water to 178°C and for injection in the dilute acid reactor system for heating bagasse. The remaining HP steam is passed through another isentropic turbine operating at 9 atm to produce electricity and LPS (9 atm,233°C). Part of the steam is extracted, to provide heating in most of the biorefinery sections. Lastly, the remaining LPS is passed through the next is isentropic turbine operating at 2 atm to produce electricity and saturated steam (2 atm, 130°C, 81.033 t/h) used for evaporative unit and sugar dryer in the sugar production site.

Table 16:Technical parameters for CEST section

Steam and power unit		Sugar mill's steam extraction	27.9 atm
Number of extractions	3	1st extraction pressure	13 atm
Turbine isotropic efficiency	85 %	2nd extraction pressure	9.5 atm
Mechanical efficiency	96 %	Condensate turbine pressure	2 atm

All the condensed steam streams from the sugar mill and biorefinery (See utility specification Table 9 for return conditions) are sent back to the boiler feedwater system incorporated with a makeup waste stream.

3.4 Glutamic acid biorefinery

This section describes the 1G, 2G and 1G2G GA biorefineries. Specifically, the flowsheet design decisions in the seed train, fermentation and downstream processing are rationalised. The generic plant area such as Pretreatment, Enzymatic hydrolysis, WWT and CHP have been described in section 3.3.

Kumar et al., 2014, did a study on the process intensification for GA producing process, in order to reduce the number of processing equipment required and pollutants for GA production processes. As a result, the integrated reactor-membrane system was developed (Pal et al., 2015). This process was seen to have better economies of scale compared to the convectional GA process. The previous study by Özüdoğru et al., 2019, adopted the same process configuration for GA production. So, for this project, the integrated reactor-membrane system configuration is also adopted.

3.4.1 1G Biorefinery (1G GA)

The biosynthesis of GA from A molasses includes major processes such as seed train, sterilisation, fermentation, product recovery and crystallisation.

Seed train

C. glutamicum (NCIM 2168), strain is selected as the fermentation microbe for the process developed, not only because it can achieve nearly 95% yield, but also it was investigated on a similar carbon source (cane juice), which has similar constituents and relatively close composition as molasses utilised in this project. The strain is cultured onsite to avoid the high costs of offsite production. Urea is used as a nitrogen source for both seeding and GA fermentation because it is cost-effective.

Table 17: Nutrients agar slant for sub-culturing *C.Glutamicum* (Pal et al., 2015)

Components	Seed culture composition
Yeast extract	2 g/l
Beef extract	1 g/l
Peptone	5 g/l
NaCl	5 g/l
Agar	15 g/l

C. glutamicum NCIM strain is cultured in a nutrient agar slant of the composition listed in Table 17, at pH of 6.5. Seeding is done in a series of 4 stages to produced 14m^3 of seed culture. The mixture is then transferred to holding tank, where it can be pumped to the fermenter for inoculation.

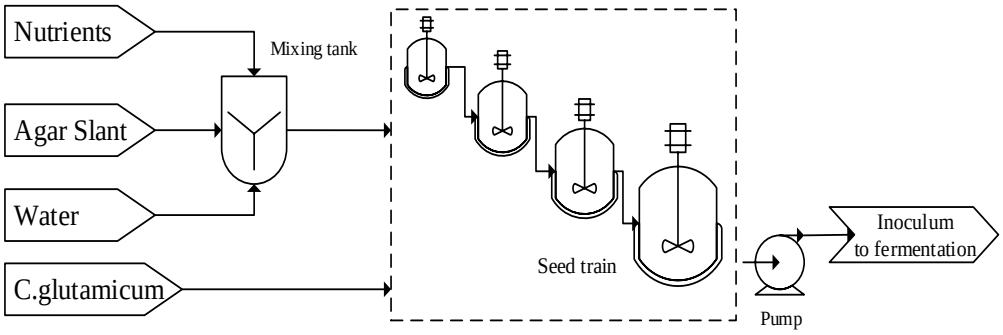

Figure 18: Simplified flow diagram for *C. glutamicum* seeding

Fermentation

Sterilisation of molasses and nutrients is conducted by autoclaving at 120°C for 15 min. Molasses and nutrients are then mixed and subsequently diluted with water to achieve the production media composing of the following: fermentable sugar (110g/l), urea (8 g/l), biotin (1µg/l), K_2HPO_4 (2.5 g/l), $MgSO_4 \cdot H_2O$ (1.5 g/l), $FeSO_4 \cdot H_2O$ (0.5 g/l), $MnSO_4 \cdot H_2O$ (0.02 g/l) and thiamine 80 µg/l (Pal et al., 2015). The production media is then cooled to 30°C using chilled water before is pumped into a fermenter. The feeds to fermenter are inoculum (14 m^3 /hr) and production media (280 m^3/hr), which are fed at the fermenters' conditions 1 bar and 30°C.

Table 18: 1G GA fermenter conditions

Pressure	1 bar
Temperature	30°C
pH	5-6.5
Antifoam agent	tween
Fermentation time	24 hours
Inoculum: Production media	1:15

Table 19 shows how different sugars are consumed to produce biomass cells and product (GA). The respective conversions were determined by iteration until the listed consideration below were met. The assumptions that were made for the entire fermentation process are (Kiefer et al., 2002; Pal et al., 2016, 2015):

i. Product yield is ~0.95g/g
ii. Glucose and fructose are completely consumed in the fermenter
iii. Product concentration is 65 g/l
iv. Biomass concentration in the fermentation broth is 5g/l
v. Unconverted sugar concentration in 20g/l in the fermentation broth

Table 19: Assumed reaction to model GA fermentation

Reaction	Conversion
Urea $+H_2O \rightarrow 2NH_3 + CO_2$	100%
$2Glucose + 2NH_3 + 3O_2 \rightarrow 2GA + 2CO_2 + 6H_2O$	99%
$2Frucose + 2NH_3 + 3O_2 \rightarrow 2GA + 2CO_2 + 6H_2O$	99%
$Sucrose + 2NH3 + 3O_2 \rightarrow 2GA + 2CO_2 + 5H_2O$	56.4%
$3Glucose + 2NH_3 + 8O_2 \rightarrow 2Biomass + 2CO_2 + 14H_2O$	19%
$3Frucose + 2NH_3 + 8O_2 \rightarrow 2Biomass + 2CO_2 + 14H_2O$	15%
$Sucrose + 2NH_3 + 2O_2 \rightarrow 2Biomass + 2CO_2 + 7H_2O$	21%

Once the culture has reached the exponential phase in the fermenters, the continues operation can be maintained by adding the production media at 0.1 per hour dilution rate and continuous removal of the product (Pal et al., 2015). Anaerobic condition of this fermentation process is maintained by sparging air using a compressor.

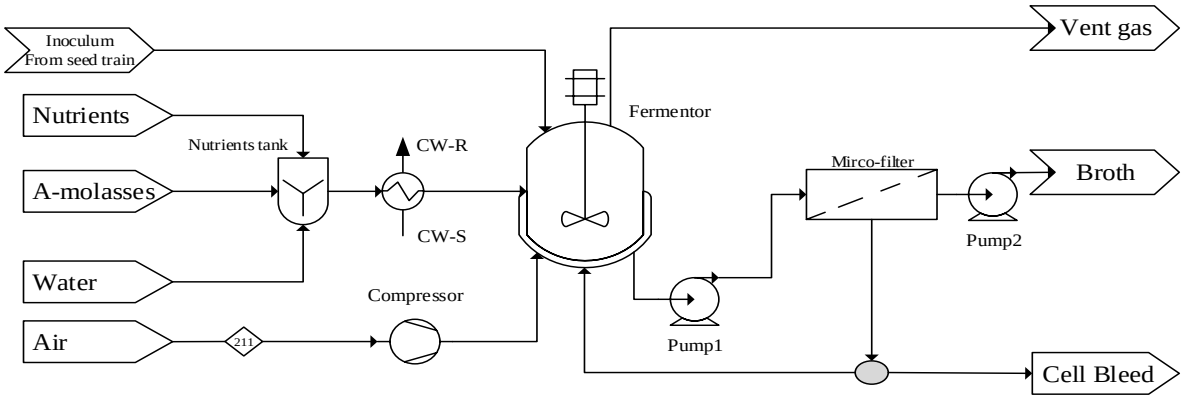

Figure 19:Simplified flow diagram for continuous fermentation of GA

Light gases (CO_2, N_2 and O_2) are vented out in the fermenters. Fermentation broth stream containing 65 g/l of GA is pumped to microfilter operating at 2.5 bar, which separates the cells completely from the fermentation broth; the resultant stream of cells has 10% moisture. 10% of the cells is purges and 90% recycled back into the system, to maintain the steady stated condition and maintain high cell density, respectively. The permeate stream is then pumped into a nano filter system operating at 14 bar.

A-300: Downstream processing

Nanofilter-1 (NF-201) recovers minerals ions (Mg^+, Na^+, etc.), 95% sucrose, 50% glucose (Özüdoğru, 2018) and 15% GA. Then the retentate stream is sent to a nanofilter-2 (NF-202), which forms a concentrated GA stream (~175g/l), by rejecting 85% of GA. Permeate streams from NF-201 and NF-202 containing unconverted sucrose, minerals ions and GA are mixed in a holding tank from then are recycled back into the process for maximum substrate utilisation. However, 10% of this stream is purged to avoid accumulation in the process. The concentrated

GA stream is then pumped to a cooling crystalliser operating at 25°C. Subsequently, the crystals are washed and dried using air dryer. GA crystals at 98% purity are produced that can be sent to storage.

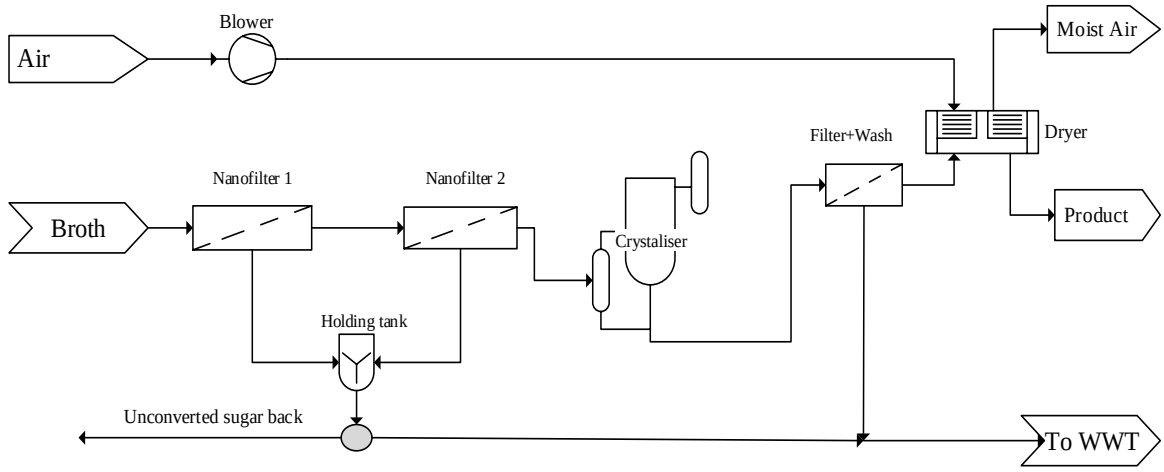

Figure 20: Simplifies product recovery and purification for GA

3.4.2 2G biorefinery (2G GA)

This section covers the seed train and fermentation processes for GA synthesis from the 2G feedstock. The pretreatment and enzymatic hydrolysis are similar, as described in section 3.3.1 and 3.3.2. In this process, hemicelluloses fractions are not considered for fermentation in this scenario, since efficient of hemicellulose and celluloses sugar has not been reported in the literature. Instead, a liquid hydrolysate stream from A-100, containing inhibitors and washed hemicelluloses fractions are sent to the WWT for digestion, while only the glucose from enzymatic hydrolysis of pretreated, washed solids, are used as carbon source for GA production.

Seed train

B. divaricatum NRRL B-2311 strain is cultured in a nutrient and conditions as described in section 3.4.1. Seeding is done in a series of 4 stages to produce 19 m^3 of seed culture. The mixture is then transferred to holding tank, where it can be pumped to the fermenter for inoculation.

Fermentation

The filtered liquid hydrolysate rich in glucose obtained after enzymatic hydrolysis is sterilised by heating the stream up to 120°C for 10 min (Özüdoğru, 2018) and nutrients are sterilised by autoclaving at 120°C for 15 min. Media is then diluted with water to attain a production media concentration comprising of; glucose (120 g/l), KH_2PO_4 (1 g/l), K_2SO_4 (1 g/l), $MgSO_4$(1 g/l),

$FeSO_4$ (6 mg/l) and $MNSO_4$ (6 mg/l) (Özüdoğru, 2018). The production media is then cooled to 37°C using cooling water before is pumped into a fermenter that operates at 1 bar and 37°C for 28.5 hours. The feeds to the fermenter are inoculum and production media which are fed in a ratio of 1:10. Once the culture has reached the exponential phase in the fermenters, the continues operation can be maintained by adding the production media at 0.1 per litre dilution rate and continuous removal of the product (Pal et al., 2015). Aerobic condition of this fermentation process is maintained by sparging air using a compressor. Nitrogen source is provided by feeding anhydrous ammonia into the fermenter in a sufficient amount. Light gases (CO_2, N_2 and O_2) are vented out in the fermenters.

Table 20: Assumed reaction to model GA fermentation adapted from (Özüdoğru, 2018)

Reactions	Conversion
$2Glucose + 2NH_3 + 3O_2 \rightarrow 2GA + 2CO_2 + 6H_2O$	87%
$3Glucose + 2NH_3 + 8O_2 \rightarrow 2Biomass + 2CO_2 + 14H_2O$	9%

The fermentation broth stream containing 100 g/l of GA (See Table 20 for assumed reactions) and 2% of the unconverted glucose, is pumped to microfilter operating at 2.5 bar, which separates the cells completely from the fermentation broth; the resultant stream of cells has 10% moisture. 10% of the cells is purges and 90% recycled back into the system, to maintain the steady stated condition and maintain high cell density, respectively. The permeate stream, it is then pumped to a nano filter system operating at 14 bar.

A-600: Downstream processing

Same as described in section 3.4.1

3.4.3 1G2G Biorefinery (1G2G GA)

The 1G2G GA process configuration was developed by combining the existing 2G GA process developed by Özüdoğru et al. (2019), and the newly developed 1G GA process. In this process, fermentation is conducted separately for 1G and 2G feedstock. Furthermore, each feedstock side has its filtration system; this is to allowed recyclability of unconverted sugars and nutrients. Once the concentrated products are obtained after nanofiller 2, the streams are mixed for the subsequent crystallisation and drying.

Table 21: GA scenarios' overall process configurations summary

Areas	Scenarios		
	1G GA	**2G GA**	**1G2G GA**
Pretreatment	NA	**DA treatment:** 157°C for 10 min, solid loading 20%, 18g H_2SO_4 per kg dry bagasse Solids washing for liquid and solid hydrolysate separation	
Enzymatic hydrolysis + detoxification	NA	**EH:** 20 g protein per kg cellulose added to 20% wt slurry. 48 °C for 3 days.	
	NA	**Detoxification**: No detoxification; liquid hydrolysate to WWT	
Seed train	*C. glutamicum NCIM 2168*	*B.* divaricatum NRRL B-2311	1G site*: C. glutamicum NCIM 2168* 2G site*: B. divaricatum* NRRL B-2311
Fermentation	1G site: residence time 24 h, 30°C, pH 5-6.5, yield 95wt.%, product titre 65 g/l, substrate titre 110g/l	2G site: residence time 28.5 h, 35°C, pH 6.5, yield 80 wt.%, product titre 100 g/l, substrate titre 120 g/l	Separate fermentation of 1G and 2G feedstocks. 1G site: residence time 24 h, 30°C, pH 5-6.5, yield 95wt.%, product conc. 65 g/l, substrate titre 110g/l. 2G site: residence time 28.5 h, 35°C, pH 6.5, yield 80 wt.%, product titre 100 g/l substrate titre 120 g/l
DSP	Microfiltration for cells, nanofiltration for GA concentration, cooling crystallisation 79.7% product recovery, 98% purity.		
WWT	Aerobic and anaerobic digestion, clarification, RO and evaporation		
	Waste effluent:73.9t/h COD: 17.5 g/l	Waste effluent :507.1t/h COD: 45.7g/l	Waste effluent: 579.9t/h COD: 42.1 g/l
CHP	-	High-pressure boiler 62 atm, 452°C steam temperature	
	-	19.9 MW power and 177.4 t/h steam produced	22.4 MW power and 165.4 t/h steam produced

3.5 Levulinic acid biorefineries

This section describes the 1G, 2G and 1G2G LA biorefineries. Specifically, the flowsheet design decisions for conversion reactions and product recovery and purification processes are rationalised. The generic plant areas, such as WWT and CHP have been described in section 3.3. As previously stated, this study considers a novel approach to produce LA from A-molasses (1G LA scenario) based on the concept of Kang et al., (2018). The 2G LA scenario has been studied by Kapanji et al., (2019); these configurations will be adapted for investigations of 1G2G biorefineries.

The downstream processing consists of the flash tank where volatile components such as furfural, forming acid and water are vaporised, to reduce the load on the subsequent, liquid-liquid extraction, solvent stripping and fractionation train.

3.5.1 1G biorefinery (1G LA)

A-100: Reaction

The LA synthesis is accomplished by acid hydrolysis of molasses in a superimposed reaction system, as shown in Figure 21. This configuration is driven by the fact that LA can be produced in concentrated amounts, which can further be isolated and purified easily. LA is highly soluble in aqueous solution when it is in low concentration, which results in a complex separation process (Kang et al., 2018b). However, for simulations purpose, this reaction system is considered as a single unit, but for the CAPEX estimations of the process, three reactors are considered.

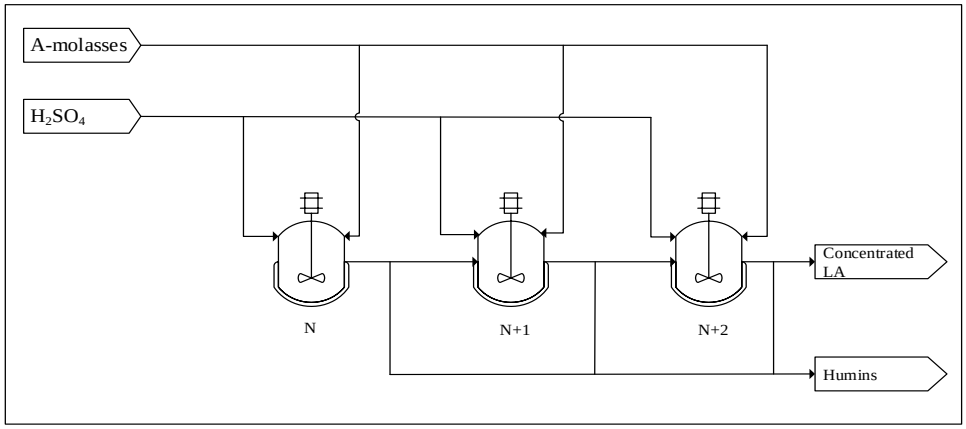

Figure 21: Superimposed reaction system (Kang et al., 2018b)

The catalytic chemical conversion of 1G LA process starts by, diluting molasses to 250g/L using water and subsequently mixed with 0.2M H_2SO_4 in a ratio of 1g feed per 0.08 g of H_2SO_4 (Kang et al., 2018b). The reaction mixture is then pumped and heated to 14 bar and 180°C respectively. Reactors are maintained at 180°C using cooling water. The reaction system was simulated using a single *R-Stoich* unit in AspenPlus®, assuming the reactions shown in Table 22, considering the following (Kang et al., 2018b):

i. 180 g/L of levulinic acid in the solution averaging to about 30% and 10% yields for levulinic acid and formic acid respectively
ii. 30 wt% of humins is formed

Table 22: Assumed LA formation reactions from molasses (Hunt and Attard, 2018; Kang et al., 2018b)

Reaction	Conversion
Sucrose + H_2O → Glucose + Fructose	100%
Glucose → Fructose	90%
Fructose → HMF+ $3H_2O$	95%
HMF+ 2 H_2O→ Levulinic acid + Formic acid	58.7%
8 HMF + Glucose → Humins	100%

A-200: product recovery and purification

Reactor outlets are taken into a flash tank operating at atmospheric conditions to remove some of the formic acid and water to concentrate the stream further. To recover some heat, the vapour stream, from the flash tank, is used to pre-heat the organic stream after extraction to reduce the load in the reboiler of the stripper. The flash liquid stream is then cooled to 45°C using cooling water, before it is sent to a filter press, where humins are removed, a cake with 80wt% and 20wt% solids and moisture respectively is formed (Sadhukhan et al., 2016). This stream is sent to the existing CHP plant for steam generation. LA containing stream is then sent to the extraction column, where is it contacted with MIBK to recover LA. The amount of solvent required was adjusted to recovery 99.4% of LA. The aqueous phase containing fractions of COD is sent to WWT. Organic stream obtained from extraction column is then sent to a stripper column operating at 1 bar and 225°C to strip off the MIBK, the vapour stream is then used to pre-heat the feed to the striper, it is then cooled to 45°C using a condenser, where after cooling is then pumped and recycled back to extraction column. Due to lower volatility LA at 98.8% purity is obtained at the bottom of the stream. This product stream is then cooled before being sent to the storage.

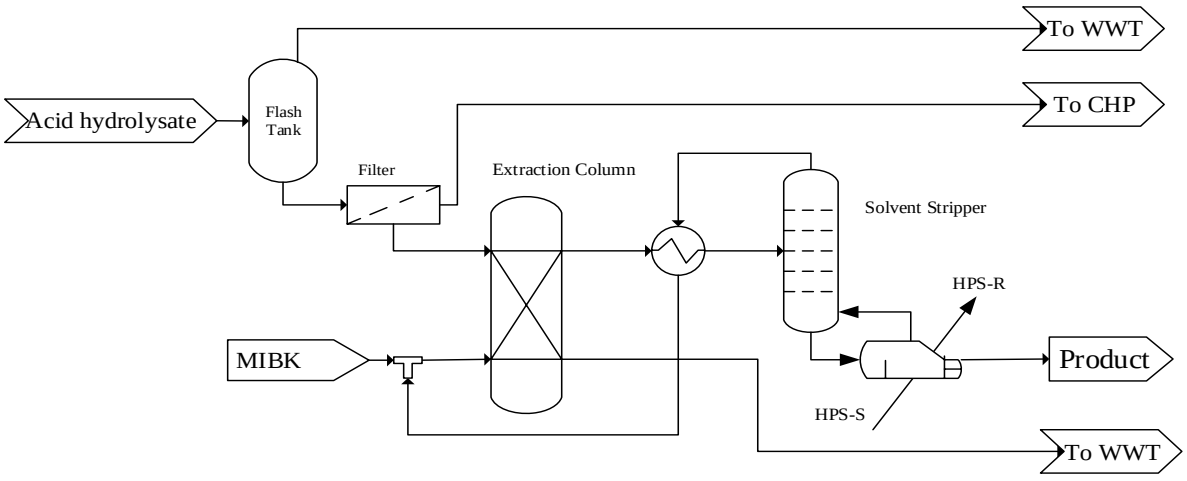

Figure 22: Simplified DSP for LA production in a 1G biorefinery

3.5.2 2G Levulinic acid (2G LA)

The 2G site for LA synthesis is archive by the most industrially employed Biofine process. See the Figure 23 for simplified process diagram.

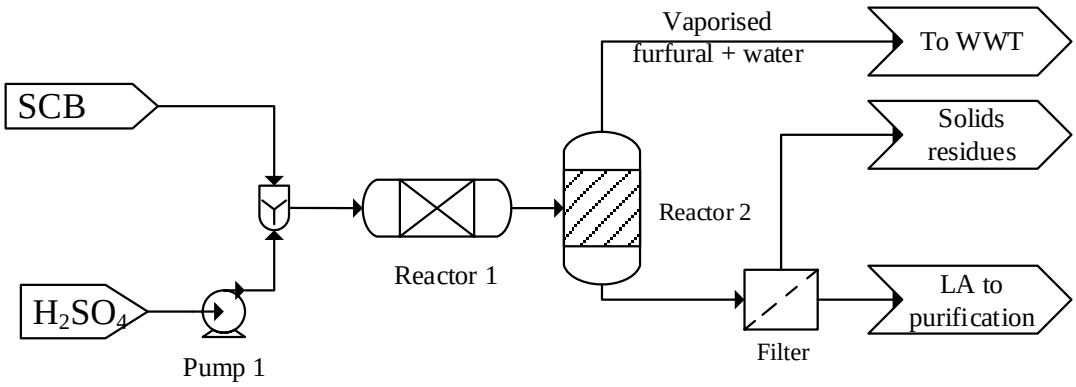

Figure 23: Simplified process diagram for LA production from 2G biomass

2G biomass is acid catalysed in a 2-stage reactor system. In the first reactor, operating at 215°C and 25 bar, lignocellulose and 3wt% H_2SO_4 are mixed and fed into a reactor at a solid loading of 30%. Due to the rapid nature of the hydrolysis reactions that form the intermate product HMF, the reactor contents are held just for 15 seconds (Hayes et al., 2005). From then on, the slurry is transferred into the second reactor operating at 14 bar and 195°C. The contents of the reactor are held for 25 minutes for further hydrolysis reactions occur. Whereby HMF is hydrolysed to LA and co-producing formic acid in equimolar ratio. The assumed reaction that happens in two reactors system are shown in Table 23. The assumed reaction equations take into account the following mass yields (Hayes et al., 2005; Hayes, 2013) :

i. 46% levulinic acid, 18% Formic acid and the balance being primarily humins of the initial cellulose mass
ii. 40% furfural, 35% humins and the balance being primarily water of the initial hemicellulose mass
iii. Majority of the initial lignin mass being humins/lignin in the product stream.

Table 23: Assumed reactions (Hayes et al., 2005; Hunt and Attard, 2018)

Reactions	**Conversion**
Reactor 1	
Cellulose +H_2O → Glucose	9.9%
2Cellulose +H_2O → Cellobiose	0.3%
Glucan + H_2O → Glucose	9.9%
Xylan+ H_2O → Xylose	90%
Arabinan + H_2O → Arabinose	100%
Acetate→ Acetic acid	100%
Xylose → Furfural+ 3H_2O	4.2%
Glucose → HMF+ 3H_2O	4%
Lignin→ Soluble lignin	5%
Reactor 2	
HMF+ 2 H_2O→ Levulinic acid + Formic acid	58.7%
8 HMF + Glucose → Humins	100%

A-200: product recovery and purification

Same as described in section 3.5.1. But in this configuration, there is further LA refining due to presence of some furfural contents. The obtained LA in the bottoms of the stripper is then refined in a distillation column operating at 0.4 bar and 150°C to obtain 98.8% pure

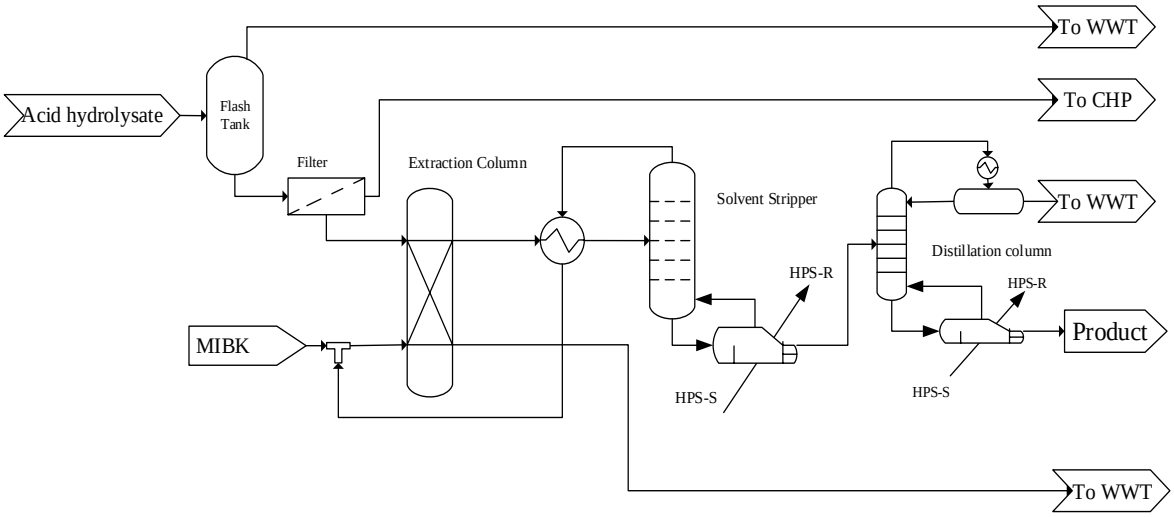

Figure 24: Simplified DSP for LA production in a 2G biorefinery

3.5.3 1G2G Biorefinery (1G2G LA)

The 1G2G LA process configuration was developed by combining the existing 2G LA process developed by Kapanji et al. (2019) described in 3.5.2, and the newly developed 1G LA process described in 3.5.1. In this process, hydrolysis reactions are conducted separately for 1G and 2G feedstocks. Once the product has formed, the crude product from 1G and 2G reactors are combined for shared downstream processing.

The Biofine process is a well-established technology for processing solid feedstock (2G) for LA synthesis. This hinders the possibility to integrate the reaction system for co-utilisation of 1G and 2G feedstocks. Efforts to combine sugar-feedstocks prior the reaction system would mean that the 2G feedstock will have to go through pretreatment and enzymatic hydrolysis process to form a liquid hydrolysate to combine with A-molasses. Furthermore, it is well known that these two processes are expensive (Nieder-Heitmann et al., 2019). As a result, this will constrain the cost-benefit brought about by integration. Moreover, no studies in the literature have reported that combines molasses and bagasse for LA synthesis.

Table 24: LA scenarios' overall process configurations summary

Areas	Scenarios		
	1G LA	**2G LA**	**1G2G LA**
Reaction	180°C for 30 min, Sugar conc. 150 g/l, Acid catalyst; 0.08kg H_2SO_4 per kg dry feed	**R1:** 215°C and 25 bar, 30% solid loading with 3 wt.% H_2SO_4 catalyst, residence time;15 seconds, HPS injection for slurry heating **R2:** 195°C and 14 bar. Residence time 25 min.	Separate reaction system using conditions for 1G and 2G processes
DSP	LLE with MIBK, Distillation for refining		
	1 fractionation column	2 fractionation columns	2 fractionation columns
WWT	Aerobic and anaerobic digestion, clarification, RO and evaporation		
	Waste effluent: 90.1 t/h COD: 48g/l	Waste effluent: 314.2 t/h COD:66.4g/l	Waste effluent: 403.1t/h COD: 62.4g/l
CHP	Low-pressure boiler to supply 15t/h steam deficit	High-pressure boiler 62 atm, 452°C steam temperature	
		26.4 MW power and 288.2 t/h steam produced	29.6 WM power and 318.4t/h steam produced

3.6 Succinic acid biorefineries

This section describes the 1G, 2G and 1G2G GA biorefineries. Specifically, the seed train, fermentation and downstream processing processes' decisions are rationalised. The generic plant area such as pretreatment, enzymatic hydrolysis, WWT and CHP have been described in in section 3.3. The designs for the biosynthesis of SA from 1G and 2G have been presented in detail by Dogbe et al., (2020) and Nieder-Heitmann et al., (2019) respectively. Herein the processes' designs consider the most recent literature data and utilisation of 1G and 2G feedstocks in 1G2G biorefinery scenario.

3.6.1 1G biorefinery (1G SA)

Seed train

A genetically engineered strain *E. coli KJ122* is cultured in a solution containing a portion of diluted A molasses 10% (v/v) in a 5-stage seed train. An AM1 salt is used to supply all the necessary nutrients for the microbes' growth (Dogbe et al., 2020).

Fermentation

A-molasses is diluted to 150 g/l and mixed with 4.2 g/l of AM1 minerals salt supplemented with $NaHCO_3$ as a CO_2 source. The fermenters are kept at 37°C and pH of 7 for 72 hours (Chan et al., 2012). During the fermentation process, 96% are consumed yielding to a product titre of 55.8g/l. These specifications are met by assuming the reactions and conversions in Table 25

Table 25: Assumed SA biosynthesis reactions from A molasses

Reactions	Conversion
Sucrose + H_2O → fructose + glucose	100%
7Glucose + $6CO_2$→ 12SA + $6H_2O$	83%
7Fructose + $6CO_2$→ 12SA + $6H_2O$	79%

Downstream processing

The fermentation broth is filtered to remove solid cell with no recycling. The obtained cells free broth is then treated with an organic solvent of TAO (13wt%) and octanol (87wt%) in a series of three reactive extraction columns operating at 50°C. Each column is fed the organic solvent and aqueous mixture in 1:1 volumetric ratio to archive 87% SA extraction into the organic phase, with just 0.21% loss of octanol into the aqueous phase. The organic phase stream is then taken into a back-extraction column to recover 99.9% of SA back into the aqueous phase. This process is conducted by feeding extraction solvent containing 25 wt% TMA and 75 water at 50°C in a ratio of 2 moles of TMA per model of SA (Mesa et al., 2016). The organic solvent is then recycled back into the process for reuse; however, due to octanol losses, a constant make-up is required. TMA solvent is then recovered back by vacuum distillation and subsequently recycled back into the process. A crude liquid stream containing SA is then sent to a cooling crystalliser operating at 20°C. The crystals are then washed using water-fed in at water solid ratio of 2:1 and dried at 130°C by compressed air.

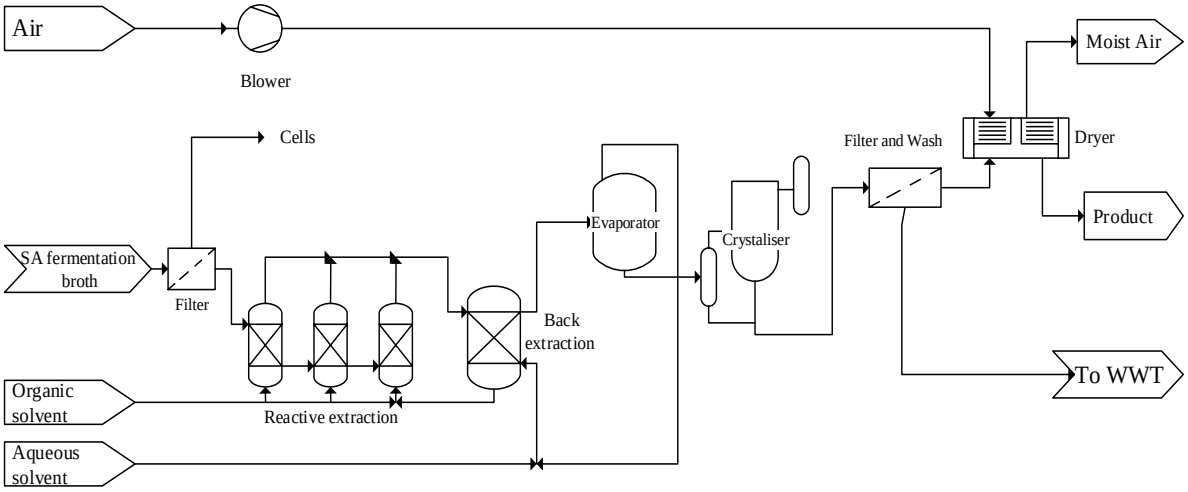

Figure 25: SA downstream processing by reaction extraction (Nieder-Heitmann et al., 2019)

3.6.2 2G biorefinery (2G SA)

This section covers the seed train and fermentation processes for SA synthesis from 2G feedstock. The pretreatment and enzymatic hydrolysis are similar to those described in section 3.3.1 and 3.3.2 . In this process, hemicelluloses fractions are considered for fermentation,

together with the glucose derived from cellulose hydrolysis. The rich glucose hydrolysate from enzymatic hydrolysis and the detoxified liquid hydrolysate from acid hydrolysis are combined for co-fermentation of pentose and hexose sugars.

Seed train

For the 2G site, *A. succininogenes* is cultured in a medium containing $NaHCO_3$ (10g/l), $MgSO_4$ (2 g/l) and K_2HPO_4 (5g/l). The nutrients used in this process are sterilised by autoclaving at 120° for 15 minutes (Borges and Pereira, 2011; Nieder-Heitmann et al., 2019).

Fermentation

Hydrolysate sugar streams are fed into the fermenters with concentration below 100 g/l, supplemented with a nutrient medium containing $NaHCO_3$ (10g/l), $MgSO_4$ (2 g/l) and K_2HPO_4 (5g/l). The fermenters are operated at 38°C and pH of 7 for 36 hours. Table 26. The fractional conversions have been iterated to yield 0.87g/g of SA from sugars consumed.

Table 26: Assumed SA reactions adopted from m pentose and hexose hydrolysate (Nieder-Heitmann et al., 2019)

Reactions	Conversion
7 Glucose + $6CO_2$ → 12SA + $6H_2O$	65%
Glucose + $6CO_2$ → SA + AA + FA	0.3%
3Glucose + $2CO_2$ → 4SA + $2H_2O$ + 2AA	16%
7 Xylose + $5CO_2$ → 10SA + $5H_2O$	30%
7Arabinose + $5CO_2$ → 10SA + $5H_2O$	20%
Cellobiose + CO_2 → 2SA + $2.5H_2O$	97%
6 Xylose + $4CO_2$ → 8SA + $4H_2O$ + 1AA	27%
6Arabinose + $4CO_2$ → 8SA + $4H_2O$ + 1AA	20%

AA – acetic acid, SA – succinic acid, FA – formic acid

Downstream processing

Same as described in section 3.6.1

3.6.3 1G2G biorefinery (1G2G SA)

The1G2G SA process configuration was developed by combining the existing 2G SA process developed by (Nieder-Heitmann et al., 2019), and 1G SA process developed by (Dogbe et al., 2020). In this process, fermentation is conducted separately for 1G and 2G feedstocks. However, DSP integrates both fermentation broth from the 1G site and 2G site.

Table 27: SA scenarios' overall process configurations summary

Areas	Scenarios		
	1G SA[a]	**2G SA[a]**	**1G2G SA [b]**
Pretreatment	NA	**DA treatment:** 157°C for 10 min, solid loading 20%, 18g H_2SO_4 per kg dry bagasse Solids washing for liquid and solid hydrolysate separation	
Enzymatic hydrolysis + detoxification	NA	**EH:** 20 g protein per kg cellulose added to 20% wt slurry. 48 °C for 3 days.	
	NA	**Detoxification**: Detoxification applied to liquid hydrolysate for complete removal of HMF and furfural	
Seed train	*E. Coli*	*A. succinogenes Z130*	1G side*: E. coli* 2G side*: A. succinogenes Z130*
Fermentation	residence time 72hr, 37℃, pH 7, yield 0.96g/g product titre 56 g/l, sub-strate titre 150g/l	residence time 38.8 hr, 35℃, pH 5-7, yield 0.87g/g, product conc. 74 g/l substrate conc. >100 g/l	Separate fermentation of 1G and 2G feedstocks.
DSP	Microfiltration for cell, Reactive extraction, back extraction. 99% product recovery, 98% purity.		
WWT	Aerobic and anaerobic digestion, clarification, RO and evaporation		
	Waste effluent:160.7/hr COD: 47.9 g/l	Waste effluent :482.6/hr COD:35.5 g/l	Waste effluent 551.5/hr COD: 44.5 g/l
CHP	Deficit of 10 t/h of LPS required	High pressure boiler 62 atm, 452°C steam temperature	
		26.1 MW power and 240.0 t/h steam produced	29.1 WM power and 265.6t/h steam produced

[a] adopted from previous studies Dogbe et al. (2020), [#] Nieder-Heitmann et al. (2019), [b] new configuration developed in this study by using technologies from 1G and 2G.

3.7 1G2G Multi-product biorefineries

This section describes the 1G2G multiproduct biorefineries. Specifically, the flowsheet design decisions regarding process configurations are rationalised. The multiproduct facility follows the same configuration as 1G2G biorefineries. Herein the sole product biorefineries that have been considered in 1G2G biorefinery complex are incorporated with xylitol production to form a multiproduct facility producing a maximum of two sealable products.

Incorporation of xylitol process introduces new production site categorised as follows:

i. Area 200: detoxification and xylose isolation

ii. Area 500: catalytic hydrogenation

iii. Area 600: product recovery and purification

Xylitol synthesis is accomplished by catalytic hydrogenation of the xylose rich hydrolysate obtained from lignocellulosic biomass. The xylose hydrolysate after acid hydrolysis is subjected to series of detoxification and xylose isolation steps to obtain hydrolysate containing

78 wt% xylose on dry basis. Özüdoğru, 2018 has already developed a viable process configuration for the catalytic hydrogenation of xylose for xylitol production using a Raney Ni catalyst.

3.7.1 1G2G GA+Xylitol Multi-product biorefinery

Xylose accounts for nearly 30% of sugars that can be derived from lignocellulose. Even so, co-utilisation of xylose along with other reducing sugars remains major challenges in the fermentation process of GA (Jin et al., 2020). So, for the GA multiproduct configuration, it is realised that xylose can be efficiently utilised to produce xylitol instead of being digested in the WWT for biogas production. For this process, the liquid hydrolysate (Pentose sugars stream) from acid pretreatment is detoxified as described in section 3.3.2 then further processed as explained in the next section and the cellulignin material follows process as describes in section 3.4.3.

3.7.2 1G2G LA+Xylitol Multi-product biorefinery

In 2G LA chemical route, hemicellulose fractions are converted into furfural that is not only energy intensive to purify but has a lower market value than xylitol. In this configuration, only 1G feedstock in considered for LA production while the 2G feedstock is used for xylitol production. The 2G feedstock is processed as described in section 3.3.1 for acid pretreatment then the liquid hydrolysate is detoxified as described in 3.3.2, and the filtered cellulignin is used as a heating source in the CHP. The filtered cellulignin is sent CHP to avoid further incorporation of enzymatic hydrolysis to obtain glucose for LA synthesis as such process are costly. However, future studies could evaluate such configuration.

3.7.3 1G2G SA+Xylitol Multi-product biorefinery

The 2G and 1G2G SA scenarios considered xylose for fermentation to ensure maximum sugar utilisation. However, for multiproduct scenario co-producing SA and xylitol, xylose is used to produce the latter, while glucose rich stream obtained from A-200 (Enzymatic hydrolysis) described in section 3.3.2, is combined with 1G feedstock for SA production. The fermentation process proceeds as described in section 3.6.1.

3.7.4 Xylitol production

Area-100 and A-200

Acid hydrolysis and detoxification follow the same process described in section 3.3.1 and 3.3.2. The stream containing water, pentose, and hexose sugars (liquid hydrolysate), taken from

activated carbon adsorption column, is pumped to an ion-exchange chromatography column packed with weak base (WBA) resin to separate hexose sugar from pentose sugars. Due to the high relative separation of factor shown by WBA resin on xylose and arabinose compared to glucose. It is assumed that all the glucose is removed from the liquid hydrolysate along with a small fraction of arabinose. The xylose rich stream after chromatography is then sent to an evaporator to remove a portion of the water to produce a xylose (20wt%) solution for the catalytic hydrogenation process. The xylose rich mixture should be free of hexose sugars, however other impurities such as acetic acid and other pentose sugars are acceptable up to 3 wt% and 5 wt% respectively (Mountraki et al., 2017).

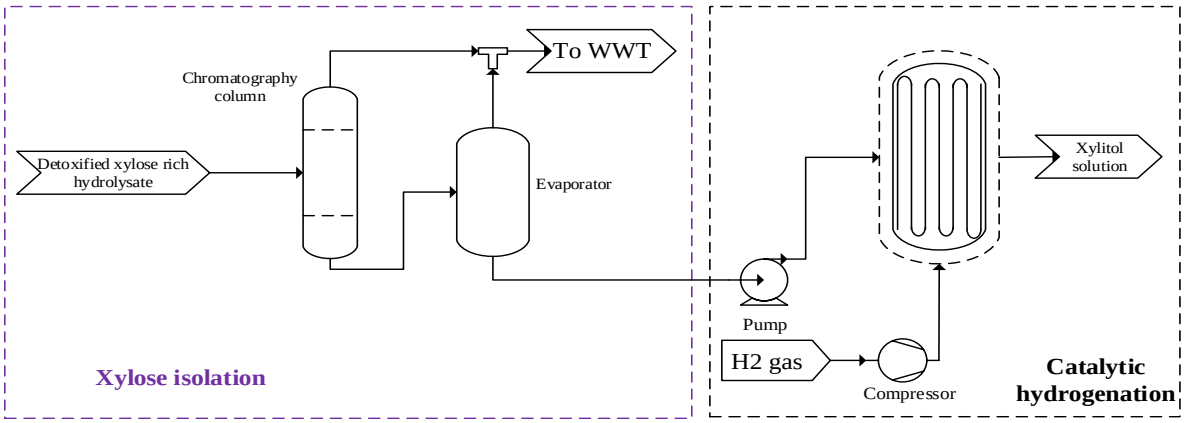

Figure 26: Simplified diagram for xylose isolation and hydrogenation

Area-500

Xylose solution is hydrogenated in the presence of Raney nickel catalyst loaded at 5 % (w/w) of the xylose feed into the reactor (Mikkola and Salmi, 2001). The hydrogen gas (H_2) is used to pressurises the reactor at 40 atm. The reactor is maintained at 135°C for 2.5 hours, within the reactor xylitol is produced by the catalytic hydrogenation of xylose over Raney-Ni catalyst (Mikkola et al., 2003)(reactions happen as shown in Table 28). All the fractions of arabinose present in the xylose solution, as well as a small portion of the xylose are converted to arabinitol (Özüdoğru, 2018).

Table 28: Assumed reaction to model xylitol hydrogenation

Reaction	Conversion
Xylose +H_2 → Xylitol	97%
Arabinose + H_2→ Arabitol	99%
Xylose + H_2→ Arabitol	0.1%

Area-600

The reactor outlets are cooled to 65°C, and the catalyst is recovered by filtration. This process assumed 95% recycling of the recovered catalyst integrated with catalyst reactivation using alcohol (preferably ethanol) containing solution (Mountraki et al., 2017). Once the catalyst has been removed, the liquid stream is taken to an ion-exchange membrane packed with strong acid cation (SAC) resin. The SAC resin shows a high separation factor between xylitol and arabitol. Forthwith, perfect separation is assumed the two, resulting in xylitol rich stream and arabitol rich stream. The former is then concentrated to 900g/l using an evaporator (Mountraki et al., 2017). The concentrated stream is then crystallised by cooling crystallisation, followed by washing and drying to produce 98% pure xylitol crystals.

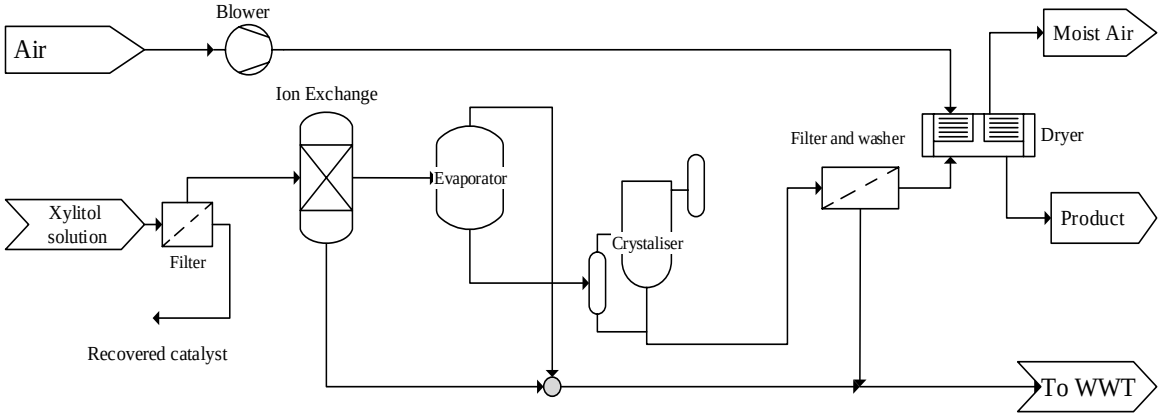

Figure 27: Simplified flow diagram for xylitol purification and recovery

3.7.5 Overall processes summary

Table 29: Multi- products scenarios overall process configurations summary

Areas	Scenarios		
	1G2G GA+ Xylitol	**1G2G SA+ Xylitol**	**1G2G LA+ Xylitol**
A-100 Pretreatment	**DA treatment:** 157°C for 10 min, solid loading 20%, 18g H_2SO_4 per kg dry bagasse Solids washing for liquid and solid hydrolysate separation		
A-200 EH + detoxification	**EH:** 20 g protein per kg cellulose added to 20% wt slurry. 48 °C for 3 days.		No EH, solids hydrolysate to CHP
	Detoxification: Acid neutralisation with lime, Inhibitors removal with GAC, xylose isolation with ion exchange		
A-300 Seed train +EP	1G site*: C. glutamicum NCIM 2168* 2G site*: B. bacterium sp.*	*E. coli*	NA
A-400 Fermentation	Separate fermentation of 1G and 2G feedstocks		NA
	1G site: residence time 24 hr, 30°C, pH 5-6.5, yield 95wt%, product conc. 65 g/l, substrate conc. 110g/l 2G site: residence time 28.5 hr, 35°C, pH 6.5, yield 80 wt%, product conc. 100 g/l substrate conc. 120 g/l	residence time 72hr, 37°C, pH 7, yield 0.96g/g product conc. 56 g/l, substrate conc. 150g/l	
A-500 Reaction	NA	NA	**LA:**180°C for 30 min,

Areas	Scenarios		
	1G2G GA+ Xylitol	1G2G SA+ Xylitol	1G2G LA+ Xylitol
			Sugar conc. 150 g/l, Acid catalyst; 0.08kg H_2SO_4 per kg dry feed
	Xylitol: Residence time 2.5 hr, xylose solution 20% wt 135°C and 40 bar, Raney Ni catalyst 5% loading of xylose		
A-600 DSP	**GA:** Microfiltration for cells, nanofiltration for GA concentration, cooling crystallisation	**SA:** Microfiltration for cell, Reactive extraction, back extraction	**LA**: LLE with MIBK, Distillation for refining
	Xylitol: Catalyst filtration, recovery using chromatography, evaporation and crystallisation Product purity: 98%, product recovery 99.5%		
A-700 WWT	Aerobic and anaerobic digestion, clarification, RO and evaporation		
	Waste effluent 354.9t/h COD: 20g/l	Waste effluent 440.2t/h COD:42.9 g/l	Waste effluent 338t/h COD: 17.2 g/l
A-800 CHP	High pressure boiler 62 atm, 452°C steam temperature		
	31.6MW power and 252.8 t/h steam produced	36.4MW power and 297.4 t/h steam produced	39.4 WM power and 336.1t/h steam produced

3.8 Economic analysis

Economic analysis in a TEA study is used to evaluate the economic viability of the proposed biorefineries on an industrial scale, in particular whether an investor in such a facility has a reasonable chance of securing the desired return on capital invested. Moreover, it can be used to establish which parameters influence the profitability of the biorefineries by sensitivity analysis. The mass and energy balances data obtained from AspenPlus® was used to size equipment and utilities, from which total capital investment (TCI) and variable costs were determined. This section outlines the procedure as well as assumptions made to assess the profitability of each biorefinery scenarios.

3.8.1 Total Capital Investment

Total capital investment also called “Capex” short for Capital Expenditure is the money used or the cost incurred to undertake new projects such as the construction of an industrial plant, until its operation (Kenton, 2019). TCI considers the purchased cost of equipment, installation cost, and direct and indirect cost and working capital (Kumar et al., 2019).

The purchased equipment costs were determined in one of the three ways:

1. Using AspenPlus® Economic Analyser. The AspenPlus® software allows detailed cost estimation of certain equipment by interactive equipment sizing based on the model data (Feng and Rangaiah, 2011).

2. Using correlations or cost curve data. The equipment cost is estimated based on the sizing coefficients a, and b and sizing exponent n according to equation ***3-2***. The respective coefficients are attainable in Appendix C.A; costs are based on the 2010 US Gulf coast basis (Sinnott et al., 2005; Turton et al., 2012)

$$C_e = a + bS^n \qquad \textbf{3-2}$$

3. Quoted cost from vendors or literature. The cost of an equipment (C_1) was estimated from the known cost (C_2) of the respective plant with the known capacity as per capacity ratio exponent equation ***3-3***. Where S_1, S_2 and n are new sizing capacity, referenced capacity and scaling exponents respectively

$$C_1 = C_2\left(\frac{S_1}{S_2}\right)^n \qquad \textbf{3-3}$$

The scaling exponent n in equation 3-3, varies with the type of equipment to consider the economies of scale reliance. Typically, the value ranges from 0.4 to 0.9 as shown in Appendix C.C. For pieces of equipment not listed in Table 46 $n = 0.6$ can be used, which is the average estimate across the entire chemical industry (Turton et al., 2012). Once the purchased equipment cost is estimated, the installed cost is determined according to equation 3-4.where F represents the installation factor. Installation factors of various equipment are listed in appendix B. Subsequently. The cost can be escalated from their based year to the project yeast cost, using equation ***3-5***. CEPCI values

$$C_{installation} = C_{purchased} \times F \qquad \textbf{3-4}$$

$$C_{2016} = C_{base\ year}\left(\frac{CEPCI_{2018}}{CEPCI_{base}}\right) \qquad \textbf{3-5}$$

Once the purchase equipment cost has been computed, the direct costs (warehouse, site development and piping) are calculated at 4%, 9% and 4.5% of the total inside battery limits (ISBL) installed cost respectively. The cost not forming part of the ISBL, the costs are taken as outside battery limits (OSBL). The major areas that form part of the biorefinery are pre-treatment, seed-train, fermentation product recovery and purification sites are considered the ISBL in this project. Summation of the direct cost and total installed cost is computed to obtain the total direct cost (TDC). TDC is used to calculate the total indirect cost (TIC). Indirect costs such as *pro rata* expenses, field expenses, project contingency and other costs (permits, plant start-up, etc) were calculated at 10% of the TDC each. Whereas, home office and construction cost was calculated at 20% of TDC (Humbird et al., 2011). From then, fixed capital investment (FCI) was calculated by addition of TDC and TIC.

Since the cost estimates are based on the US Gulf coast basis, location factor of 1.08 (Gorgens et al., 2016) was implemented to obtain the corrected FCI for the South African context. Subsequently, the working capital is calculated at 5% of the corrected FCI. Lastly, TCI is obtained by addition of working capital and corrected FCI.

3.8.2 Operating expenditure

Operating expenditures (Opex) are the costs incurred for the daily operational activities of the plant and can be categorised into variable operating costs (VOC), fixed operating costs (FOC) and general expenses (Kenton, 2019; Turton et al., 2012). VOC are costs that are directly related to the rate of production. FOC's are not directly related to the rate of production. The costs associated with labour, insurance, maintenance, and general overhead. Table 30 shows the salaries of workers in different positions and numbers workers required in a position for each biorefinery scenario. The salaries were adopted from (Davis et al., 2018), for a typical biorefinery processing lignocellulosic biomass. Salaries were brought to the costing project year of 2018 using the labour cost index of 125.2 and 131.7, for the year 2016 and 2018 respectively.

Table 30: Staff salaries and number of workers per position (Gorgens et al., 2016; Humbird et al., 2011)

Position	Salary ($) 2016	Number of workers per position in scenarios							
		1G GA	1G LA	1G2G GA	1G2G LA	1G2G SA	1G2G GA + Xylitol	1G2G SA+ Xylitol	1G2G LA + Xylitol
Plant manager	168458	1	1	1	1	1	1	1	1
Plant engineer	80218	2	2	2	2	2	2	2	2
Maintenance supervisor	65320	1	1	1	1	1	1	1	1
Maintenance technician	45839	8	8	8	8	8	8	8	8
Lab manager	64174	1	1	1	1	1	1	1	1
Lab technician	45839	2	2	2	2	2	2	2	2
Lab tech-enzyme	45839	0	0	2	0	2	2	2	0
Shift supervisor	55007	3	3	4	4	4	6	6	6
Shift operator	45839	6	6	15	15	15	20	20	20
Shift operator enzyme	45839	0	0	6	0	6	6	6	0
Yard employees	32087	3	3	3	3	3	3	3	3
Clerks & secretaries	41255	3	3	3	3	3	3	3	3

The required number of workers was estimated based on the scale of the biorefinery. For the South African context, salaries are expected to be lower (Gorgens et al., 2016). The uncertainty of this on profitability was investigated through sensitivity analysis. The 90% labour burden was added as part of FOC to account for the benefits of workers (Humbird et al., 2011). General

overhead costs, that include maintenances, and property insurance and tax were also added as part of FOC. Maintenances were calculated as 3% of ISBL and, property and taxes were calculated 0.7% of FCI (Humbird et al., 2011).

3.8.3 Cash flow data

Upon completion of Capex and Opex calculations, a discount cash flow rate of returns analysis was done to assess the profitability of each biorefinery scenario. Table 31 shows all the significant cash flow assumptions parameters. These assumptions have been adopted from the previous work (Farzad et al., 2017a; Gorgens et al., 2016; Nieder-Heitmann, 2019; Özüdoğru et al., 2019).

Table 31: Cash flow assumptions parameters (Dogbe et al., 2020; Gorgens et al., 2016; Mandegari et al., 2018; Nieder-Heitmann et al., 2019)

PARAMETERS	VALUE
Annual operating hours	5000
Project life	25 years
Project cost	2018
CEPCI	603.1
Discount rate	20 % for real term DCF analysis
Income tax rate	28 %
Depreciation	Straight line method applied over 5 years (i.e. 20 %)
Salvage value	0
Construction period	2 years
% Spend in year -2	10 %
% Spend in year -1	60 %
% Spend in year 0	30 %
Working capital	5% of FCI
Start-up time	2 years
First year operation capacity	50 %
Second year operation capacity	75 %
Third year operation capacity	100%
IRR evaluation	Real terms
GA selling price	$3600 /t [a]
LA selling price	$2750 /t [b]
SA selling price	$2500/t[c]
Xylitol selling price	$3900/ t[d]

a) (Özüdoğru et al., 2019) ; b & d) (Rosales-Calderon and Arantes, 2019); c) (Nieder-Heitmann et al., 2019)

3.8.4 Economic indicators

All the major economic indicators are evaluated at a 20% discount rate to cater for the minimum risk premium necessary to attract investors (Dogbe et al., 2020). The location and time affect

the market price, as a result, differing prices ranges are reported in the literature. The main parameter used for profitability comparison is the MSP due to its independence on the product price. The complexities of determining an MSP in multi-product scenarios are solved by determining the MSP of one product, while keeping the other product price(s) at the relevant market price(s). The market prices used to for evaluation of other intensive parameters such as IRR are similar to those used in studies by (Dogbe et al., 2020; Kapanji et al., 2019; Nieder-Heitmann et al., 2019; Özüdoğru et al., 2019). Furthermore, the uncertainty associated with the assumptions of economic evaluations is quantified by the sensitivity analyses on MSP looking at TCI, FOC, VOC, operational hours, and income tax.

3.8.5 Sensitivity analysis

A sensitivity analysis is a method that allows the examination of the changes in a model parameters assumption used to predict the economic viability. This method analyses the effects of sensitivity parameters on the financial results (Brown and Brown, 2013). Sensitivity analyses analysis on this project was investigated by varying the parameters in Table 32. The parameters are varied by making the baseline 30% less and more, to evaluate the effect on MSP.

Table 32: Sensitivity analysis parameters

Parameters	**Baseline (units)**
FCI	Variable ($)
COP	Variable ($)
Feed stock cost	Variable ($)
Operation hours	5000 hr
Income tax	28%

4 Results and Discussion

The results and discussions are presented per product of interest. Under each sub-section of the product of interest, overall mass and energy balances, economic performances and sensitivity analysis results are presented. Then, comparison of biorefineries scenarios across all product of interest is carried out considering an annual operation of 5000 hours for the performance evaluation, all annexed into an existing sugar mill facility with self-energy sufficient concept.

4.1 Glutamic acid

4.1.1 Mass and energy balance

The results for the overall mass and energy balances are presented in this section. This include a bypass ratio, amount of feedstock utilised, products produced, CHP feeds and energy demands (cooling, heating, and power) as main key parameters and indicators of the developed processes. A total of five GA scenarios are presented in Table 33, this includes the 2G GA scenario developed by Özüdoğru, (2018). However, the scenario has been updated to a new technical data and new configurations for the pretreatment section as discussed through this section in detail. Also, newly developed biorefinery configurations for integrated 1G, 1G2G and multi-product facility. The efficiency of these processes in terms of product recovery after fermentation all reported 79.9%. The downstream processing uses the proposed ultrafiltration system for GA recovery by Kumar et al. (2014) and Pal et al. (2015), whereby a two staged ultrafiltration train recovers 94% and 85% GA respectively.

The steam demands reported in Table 33, excludes the needs for sugar mill which are; 120t/h steam when the current configuration in the sugar mill is maintained (no A-molasses extraction) and 104.5t/h steam when there is a reconfiguration to extract A-molasses. It is worth mentioning that all scenarios processing 1G feedstock result in reconfiguration in the sugar mill to extract A-molasses. The bypass ratio for the facilities installing new CHP system was determined through an iterative approach to meet the heating demands of both sugar mill and biorefinery complex considering the amount of biogas produced and solid residues filtered during pretreatment of 2G feedstock as a source of heat.

The existing CHP facility can meet the heating demands of both sugar mill and 1G GA biorefinery complex because only 7.6 t/h of steam is required by the latter. The current capacity of the existing CHP in 120 t/h, however with reconfiguration 15.5 t/h of excess steam can be made available. Which is more than enough to provide the heat demands for the integrated 1G

biorefinery complex (Dogbe et al., 2020). Although the energy demands of this scenario can be provided by only combusting bagasse. The 1.1 t/h of biogas produced in this scenario is combusted along with available bagasse to mitigate the environmental impact. Nonetheless, co-combustion of the produced biogas and bagasse has negligible impact on the steam to bagasse ratio of 2.22 (Dogbe, 2020) for the current CHP, since biogas is composed of mostly CO_2 (69wt%) and less of CH_4 (30.1wt%), with the balance being other impurities such as moisture. 1G GA scenario has an economic advantage compared to scenarios that process 2G feedstock (2G GA, 1G2G GA and 1G2G GA+xylitol) because they make use of the expensive high-pressure boiler.

Table 33: Overall mass and energy balances for the GA biorefinery scenarios

Parameters		**GA scenarios**				
		2G GA*	**Updated 2G GA**	**New 1G GA**	**New 1G2G GA**	**New 1G2G +Xylitol**
Bypass ratio		35%	-	-	-	48%
1G feed (t/h)		-	-	25.4	25.4	25.4
2G feed (t/h DM)		42.2	65.0	-	65.0	33.8
Product (t/h DM)		12.6	15.1	11.1	26.1	21.4[a]
						6.4[b]
Product recovery	1	79.9%	79.9%	79.9%	79.9%	79.9%[c]
	2	-	-	-	-	99.5%[d]
Heating (MW)		40.6	39.5	3.9	49.0	69.5
Cooling (MW)		24.4	73.5	30.1	106.9	117.5
Power (MW)		1.7	5.5	0.5	5.7	10.6
Steam Demand (t/h) *		73.6	57.1	7.6	61.2	118.0
CHP feed (t/h DM)	Bypass	39.7	-	-	-	54.5
	Lignin residues	22.0	37.1	-	37.1	17.9
	Biogas	5.1	18.5	1.1[e]	19.7	4.9
Power produced (MW)		14.5	24.6	-	26.4	31.6
Residue remains (t/h)		0.0	8.6	-	7.3	0.4
Surplus power (MW)		4.2	10.5	-	12.2	12.4

[a] Glutamic acid production rate; [b] Xylitol production rate; [c] Glutamic acid recovery after fermentation; [d] Xylitol recovery after reaction, [e] Biogas fed to an additional low-pressure boiler; *exclude steam for the sugar mill; *Özüdoğru et al. (2019)

The 2G GA simulation developed by Özüdoğru (2018) required a bypass of 35% bagasse bypass to the CHP plant. In the updated scenario, the bypass was reduced to zero by reducing the steam demand of the process by replacing an evaporative crystallisation unit that contributed 60% to the total of steam demand of the process, with a cooling crystallisation unit. An evaporative crystallisation is widely known that, is an energy intensive process (Wu et al., 2018). While cooling crystallisation provides energy saving benefits due to elimination of heat input. Furthermore, in the updated GA scenario there is 18.5 t/h biogas that is sent to the CHP,

which is higher than 5.1 t/h reported for the existing 2G GA scenario. The main reason for these differences in biogas production is discussed in section 4.4.1.

The integrated 1G2G multi-product facility (1G2G GA+Xylitol) required the highest bypass of 48%. This is due to the integration of an energy intensive xylitol production process. Furthermore, the steam demand is the highest (118 t/h) compared to other sole product biorefineries. Not to mention, in multiproduct biorefinery complex xylose is utilised for xylitol production, and therefore not available for biorefinery energy supply, through anaerobic digestion of hemicellulose fractions to biogas. As can be seen in Table 33, the amount of biogas sent to CHP is higher for sole products facilities (18.5 t/h and 19.7 t/h 2G GA and 1G2G GA respectively) compared to multiproduct complex (4.9 t/h).

The integrated 1G2G GA scenario show the highest production rate (26.4 t/h), primarily benefiting from separate fermentation of 1G and 2G feedstocks that yield 96 wt% and 88 wt% from sugars (Özüdoğru, 2018; Pal et al., 2015) and inclusion of unconverted sugars recycle. While, 2G GA scenario's production rate improved from 12.6 t/h to 15.1 t/h due to decreased bypass ratio (34% vs 0%).

Considering an estimated global market volume of 2900 ktpa for GA, the current scenario only captures, 1.9% (1G GA), 2.6% (2G GA), 4.4% (1G2G GA) and 3.7% (1G2G GA+Xylitol). On the other hand, co-production of xylitol in 1G2G GA+ xylitol scenario result in 16% of the market size considering a xylitol global demand of 200 ktpa.

The specific energy requirements of the GA scenarios in MW per tonne of product are shown in Figure 28. The energy requirements of GA processes are compared with a 2G GA process developed by Özüdoğru (2018) (Presented as the "existing 2G"). It is worth noting that, these energy requirements exclude those of a sugar mill. In terms of heating, the overall process performance was improved by removing the energy intensive crystallisation units and incorporation of the new heat integration network. As can be seen by a decrease from 3.22 MW/t to 2.62 MW/t in Figure 28. However, the specific cooling demand of the process increased from 1.94 MW/t product in the existing 2G(Özüdoğru, 2018) scenario to above 2.71 MW/t product in new developed scenarios. This is mainly because of the applied cooling crystallisation that happens at 20°C.

As further presented in Figure 28, it can be seen that integrating xylitol production process in 1G2G facility increased the heating demand of the process from 1.9 MW/t to 2.5 MW/t. The multi-product complex showed highest electrical demand (0.38 MW/t). This is attributed to the

operation of xylitol site at more severe conditions (pressure of 40 bars) in the reactor. Also, blowers are contributing to this high electrical demand because voluminous amount of air required to dry the xylitol product to its specifications of 98% purity.

Lastly, the 1G biorefinery scenario is more energy efficient (lowest heating, cooling, and power demands at 0.35 MW/t, 2.71 MW/t 0.31MW/t respectively) compared to 2G and integrated biorefinery 1G2G complexes. This is due to the elimination of a pretreatment section in the process. Incorporation of 2G feedstock in a biorefinery complex increases the energy demand of the process because of mandatory pretreatment that is required to liberate the sugars (Nieder-Heitmann et al., 2019).

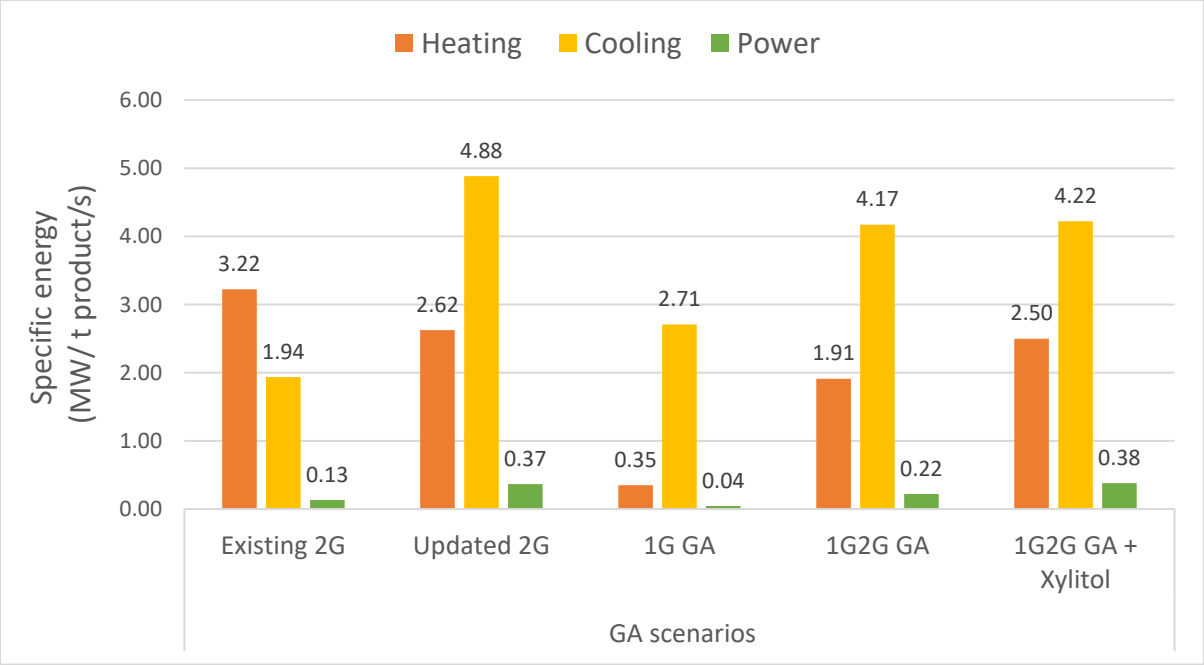

Figure 28: Specific energy demand of GA biorefinery scenarios

4.1.2 Economic performances

4.1.2.1 Capital and Operating cost

The mass and energy balances results were used for economic assessment of different scenarios. This involved Capex and Opex estimations to determine the production cost of biorefineries considering all the marginal costs as a result of annexing new biorefineries into an existing sugar mill. Table 34, shows the summary of the TCI cost breakdown including Total equipment cost (TEC), Total direct cost (TDC) and total indirect cost (TIDC) of the new scenarios that have been developed through this study.

As presented in Table 34, For the 2G GA scenario, the obtained results are comparable with past studies (Özüdoğru, 2018). However, the cost for WWT (A-700) is high due to a different

WWT process adopted for treating waste streams. The WWT technology for treating waste effluent and biogas production adapted in this study is similar to that developed by Humbird et al., (2011). The installed cost for this technology in 2011 was $44 million for a plant that treats 411t/h of waste effluent. In addition, processing 2G feedstock in Area 100 and 200 contribute nearly 30% on the total installed equipment cost which is comparable with the result of Nieder-Heitmann et al., (2019).

Unlike scenarios processing 2G feedstock, 1G scenario benefited from the absence of cost intensive areas, such as CHP and pretreatment. Since the steam demands (7.2 t/h) of the 1G GA process can supplied using the existing boiler, no boiler cost was included in the TCI. Therefore, the 1G GA scenario requires the lowest capital investment of $ 145 million in comparison to 2G and 1G2G scenarios. On the other hand, processing 2G feedstock result in a mandatory pretreatment and enzymatic hydrolysis introducing Area 100-300 in the process.

Table 34: Capital cost breakdown for the GA scenarios

Area	**Installed cost ($ million)**			
	1G GA	**2G GA**	**1G2G GA**	**1G2G GA +Xylitol**
Area 100: Pre-treatment	-	56.71	56.71	47.10
Area 200: Enzymatic hydrolysis +detoxification	-	32.98	32.98	32.33
Area 300: Seed train+ Enzymes production	1.18	19.42	20.85	15.40
Area 400: Fermentation	29.51	42.51	71.90	67.35
Area 500: Reaction	-	-	-	8.42
Area 600: Downstream processing	20.23	22.19	39.41	55.67
Area 700: WWT	20.31	64.57	69.94	52.10
Area 800: CHP	-	72.30	69.58	79.61
Area 900: Storage (5% of ISBL)	2.55	8.69	11.09	11.31
Area 110: Utilities (6.5 % of ISBL)	3.31	11.30	14.42	14.71
ISBL Total	**50.92**	**173.82**	**221.84**	**226.27**
Total Equipment Cost	**77.09**	**330.68**	**386.88**	**383.99**
Warehouse (4% ISBL)	2.04	6.95	8.87	9.05
Site development (9% ISBL)	4.58	15.64	19.97	20.36
Additional piping (4.5% ISBL)	2.29	7.82	9.98	10.18
Total Direct Costs (TDC)	**86.00**	**361.09**	**425.70**	**423.59**
Proratable Expenses (10% TDC)	8.60	36.11	42.57	42.36
Field Expenses (10% TDC)	8.60	36.11	42.57	42.36
Home Office and Construction (20% TDC)	17.20	72.22	85.14	84.72
Project Contingency (10% TDC)	8.60	36.11	42.57	42.36
Other Costs incl. start-up, permits etc. (10% TDC)	8.60	36.11	42.57	42.36
Total Indirect Costs (TIDC)	**51.60**	**216.66**	**255.42**	**254.15**
Fixed Capital Investment (FCI = TDC + TIDC)	137.60	577.75	681.12	677.74
Working Capital (5% FCI)	6.88	28.89	34.06	33.89
Total Capital Investment (TCI = FCI + WC)	**144.48**	**606.64**	**715.17**	**711.62**

The integrated 1G2G GA scenario requires the largest TCI ($ 751.17 M) compared to a multi-product facility ($711.6M). Primarily due to plant capacities, 1G2G GA scenarios processes 100% lignocelluloses to produce GA whereas 1G2G GA+xylitol only 52% is processed for GA and xylitol production. Integrated 1G2G GA scenario has the highest total installed equipment costs due to parallel processing (fermentation and DSP) of 1G and 2G feedstocks. Unlike the production of bioethanol that can be produced by co-fermentation bagasse's hydrolysate and molasses (Gutiérrez-Rivera et al., 2015), there is no report for co-fermentation 1G and 2G feedstocks for GA production. As a consequence, through integration of 1G and 2G feedstocks for GA production, there was no reduction in installed cost in Area 300 and 600. As can be seen, area 300 and area 600 in 1G2G GA are more or less the summation of 1G GA and 2G GA processes.

Figure 29, shows the total operating costs breakdown for the GA scenarios. Overall, it can be seen that raw materials and nutrients are the major contributors to the TCOP. As can be seen nutrients cost more in 1G GA scenario than 2G GA scenario. The multi-product scenario has the highest TCOP per product. This is due to the use of expensive Raney Ni catalyst used for hydrogenation of xylose to produce xylitol and activated carbon for removal of toxic compounds (HMF and furfural) that can cause catalyst deactivation.

Comparably, the total cost of productions obtained for this study are much lower than $4300/t reported by Pal et al., (2015) for a 1550 t/yr GA producing plant from cane juice. The reason for higher TCOP by the latter can be attributed to the expensive cane juice cost ($157/t), higher than an average price of $102/t used for A-molasses in this study and the economies of scale. The more detailed Opex calculations are presented in Appendix E.A.

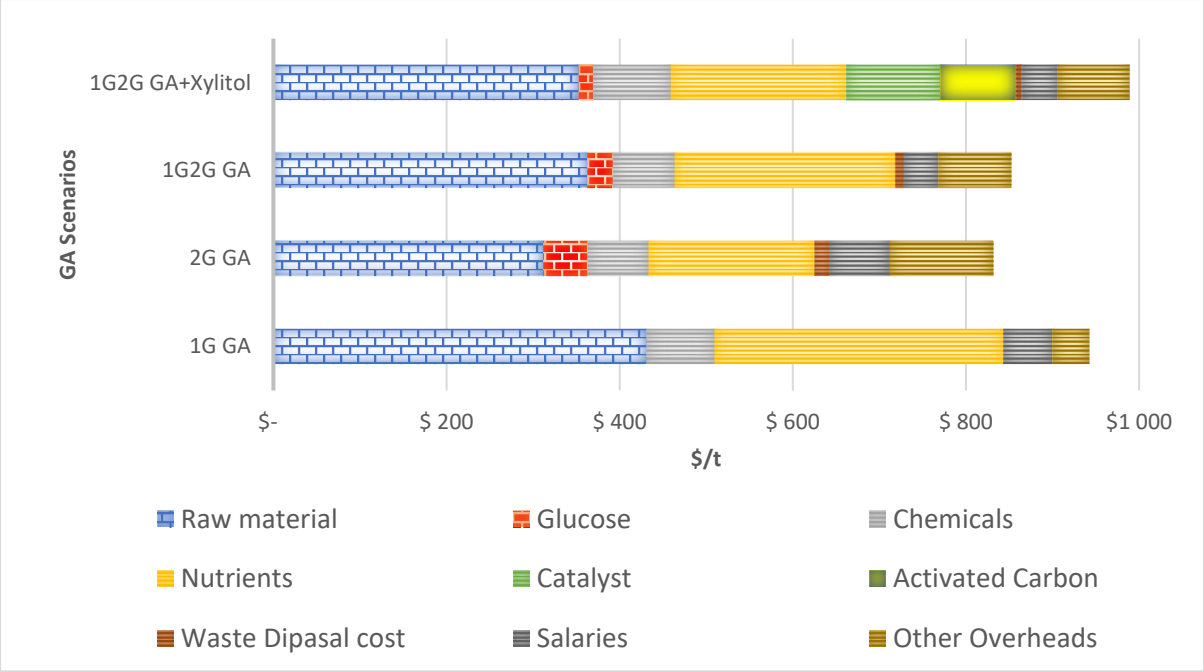

Figure 29: Total operation cost per tonne product/s breakdown for GA scenarios

4.1.2.2 Comparison of the key economic indicators

The comparisons of major profitability assessment parameters for the GA scenarios are shown in Table 35. In particular, the determined economic parameters of the 2G GA scenario reported in literature(Özüdoğru, 2018), and the new and updated GA scenarios under the new assumptions fully explained in detail below are presented. Overall, the scenarios have proved to be profitable, with the IRR ranging from 25.3% to 59.8% and the MSP's below market price of $3600/t (Özüdoğru et al., 2019).

Table 35: Comparisons of key economic indicators for GA scenarios

Indicators	**GA scenarios**				
	2G GA*	**Updated 2G GA**	**New 1G GA**	**New 1G2G GA**	**New 1G2G GA + Xylitol**
TCI (M$)	218.60	606.64	144.48	715.17	711.62
TCOP (M$)	24.90	64.30	54.60	115.30	137.53
TCI per product ($/t) [a]	203.86	313.59	103.39	203.31	204.62
TCOP ($/t)[b]	1317.92	831.88	976.28	819.68	988.87
Total sales (M$/yr)	302.70	280.50	202.62	510.06	513.14
NPV (M$)	866.50	66.64	318.02	518.41	461.64
IRR (%)	31.2%	25.3%	59.8%	36.4%	35.1%
GA MSP ($/t)	nd	2969	1687	2205	1926

[a] Determined considering product produced over a plant lifetime of 25years; [b] determined based on the total cost of production and annual product produced assuming full capacity operation; Nd. Not determined; * Özüdoğru et al. (2019)

As can be noticed in the table above, the 2G GA scenario reported by Özüdoğru et al. (2019) has higher TCOP of $1318/t compared to $832/t in the updated 2G GA scenario. This is because, 2G GA scenario considered offsite enzymes, which resulted in high TCOP, whereas the updated scenarios consider onsite enzyme production which subsequently increased the TCI from $204/t to $278/t. Although, the updated 2G GA scenario has higher production rate (15 t/h) than 2G GA scenario (12.3 t/h) reported by Özüdoğru et al. (2019). It has lower IRR (25.3%) than the existing scenario (30.1%). This can be explained by the extra revenue that was brough by the sale of electricity and 6480-hour annual plant operation by the latter. Under the new consideration the plant operates for 5000 hours and the sale of electricity in no longer considered, because it is no longer incentivized. Generally, an annual operation of 5000 hours is more realistic to account for the uncertainty in time efficiency of the sugar mill that currently operates for 9 months (6480 hours).

Through the integration of 1G and 2G feedstock, there is a clear economy of scale benefit. This is resulted by three main factors: 72% increase in production rate due to incorporation of 1G feedstock in the process; 100% 2G biomass available for utilisation due to 0 bypass requirement; and smaller CHP plant capacity for 1G2G GA process in comparison to 2G GA process (165 t/h vs 177 t/h), which makes the 1G2G GA scenario to have better economic results in comparison to 2G GA configuration. As can be seen in Table 35, 1G2G GA scenario achieved lower MSP at $2205/t and higher IRR of 36.4% than 2G GA scenario with MSP of $2969/t and IRR of 25.3%. These results are consistent with the same configurations that have been reported in literature for bioethanol (Daystar et al., 2015).

Despite only 52% of lignocelluloses (33.8 t/h DM) fed for conversion into a multiproduct scenario (1G2G GA+Xylitol) compared to 100% in 1G2G GA scenario, 1G2G GA+Xylitol achieved lower MSP for GA ($1926/t vs $2205/t) in comparison. This can be explained by the co-production of GA and xylitol contributing 75% and 25% respectively to the total sales ($510.5 million per annum). Furthermore, the high market price of xylitol co-product results in a large reduction in MSP of GA (Santos et al., 2018).

The 1G GA scenario is the least capital intensive ($103.4/t) compared to 2G and 1G2G scenarios. This is expected, because the cost intensive areas, such as CHP, and pretreatment have been eliminated due to processing clean 1G feedstock in a less energy intensive process. Furthermore, 1G GA is the most profitable scenario with the highest IRR of 59.8% and lowest MSP of $1687/t.

It is therefore clear that the option to diversify sugar mills' products by penetrating GA markets is an attractive investment as shown by the economic performances of the investigated scenarios. Moreover, 1G GA is the most attractive investment with the lowest TCI and MSP. However, for a more diversified product range, the multi-production of GA with xylitol can be considered. To fully exploit the presented value of the raw material and to cater for market volatility (Farzad et al., 2017b).

4.1.3 Sensitivity analysis

The economic sensitivity analyses results for the GA scenarios are presented in Figure 31, showing the effects of ±30% changes on TCI, VOC, FOC, income tax and operating hours for: (1)1G GA, (2)2G GA (3) 1G2G GA, (4) 1G2G GA+ xylitol. Less sensitive parameter such as assumptions for working capital and maintenance (Nieder-Heitmann et al., 2019) were excluded, instead they were taken as implanted factors in TCI and VOC respectively. To simplify the analyses raw materials costs uncertainty quantification were evaluated at total variable cost, instead of individual raw materials. The fact that workers' salaries were estimated based on US standards, while for South African context salaries will be considerably lower, this may result in overestimated MSP. The uncertainty of this are quantified through variable VOC.

As can been seen in Figure 31, all the scenarios have shown the greatest sensitivity to TCI and operating hours. The (a)1G GA and (c)1G2G xylitol scenarios are still profitable with MSPs lower than the market price $3600/t even after the introduction of unfavourable conditions in the parameters. However, in (b)2G GA and (d)1G2G GA scenarios, decreasing annual operating hours to 3500 results in MSPs above the market prices at $3966/t and $2850/t respectively. Reduced operation time is possible due to time inefficiencies in the sugar mill. However, operating at an optimistic efficient time of 6500 hours per year could further improve the economics by 10% on MSP.

As demonstrated in Figure 31 (a), scenario 1G GA, showed differing results compared to other scenarios, in terms of sensitivity between TCI and VOC. The parameters showed to be more or less the same with a 15% decrease and increase to the MSP. This is because the yearly operational cost for 1G GA scenarios is high and the required capital investment is low. The TCI is only 2.2-fold of the TCOP, whereas, in other scenarios TCI exceeds TCOP 6-folds. Similar, results have been obtained in literature for low capital investment project (Dogbe et al., 2020).

As can be seen for (d) 1G2G GA+Xylitol, TCI is a major sensitive parameter. With this scenario, a 30% reduction in capital investment could result in this scenario being the best with the lowest MSP of $1328/t for GA corresponding to 31% reduction from current base MSP ($1926/t) , in comparison to 1G GA, 2G GA and 1G2G GA that only experience less than 20% reduction in the base MSP's.

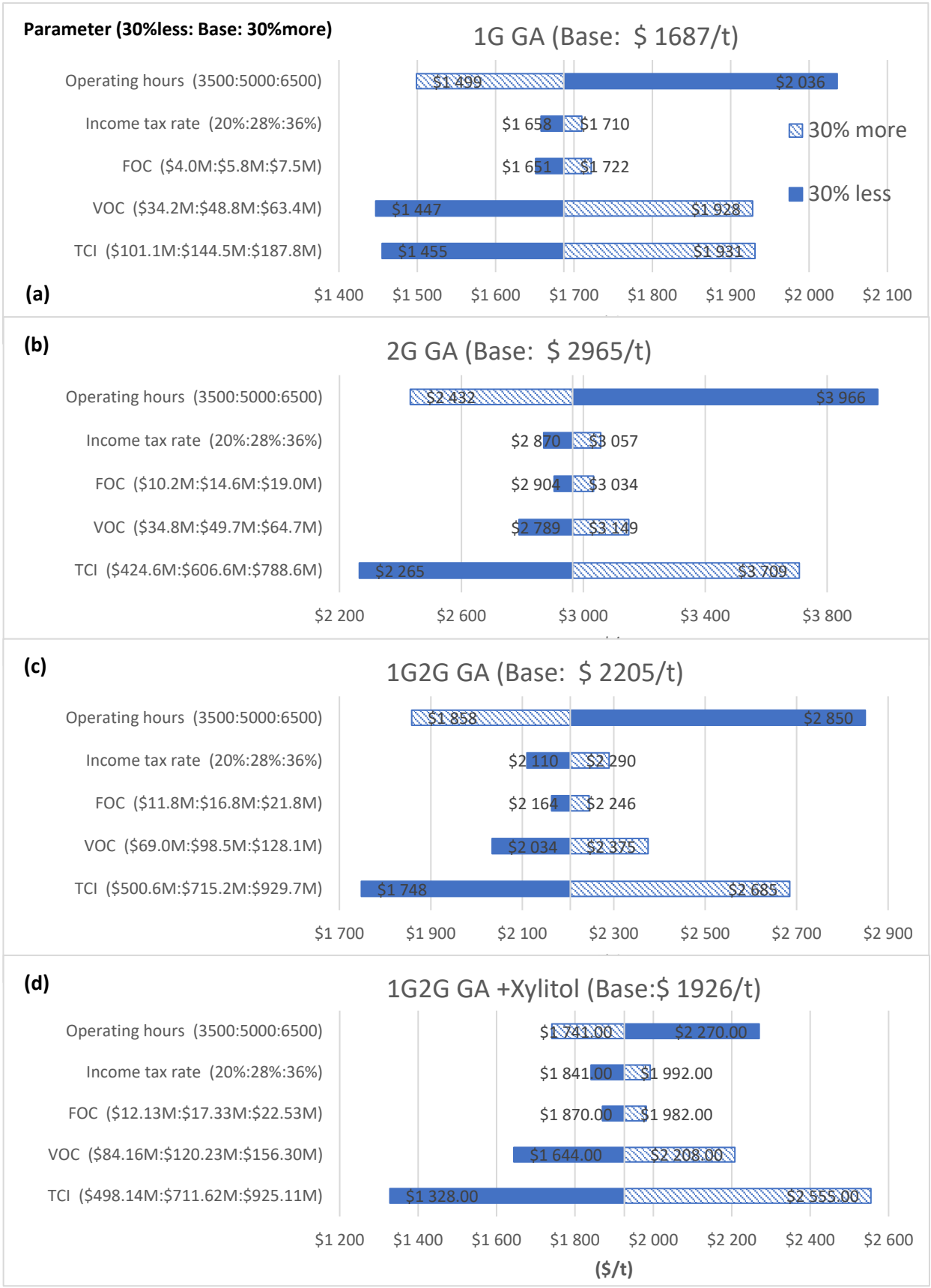

Figure 30: The GA scenarios MSP sensitivity analyses to ±30% changes to the economic parameters; (a)1G GA, (b)2G GA (c) 1G2G GA, (d) 1G2G GA+ xylitol

4.2 Levulinic acid

4.2.1 Mass and energy balance

Presented in Table 36, are the overall mass, and energy balances results showing bypass ratio, amount of feedstock utilised, products produced, CHP feeds and energy demands (cooling, heating, and power) for the developed LA biorefinery scenarios in this study (1G LA, update 2G LA,1G2G LA and 1G2G LA+Xylitol) and the 2G LA scenario developed by Kapanji et al. (2019).

Table 36: Overall mass and energy balances for the LA biorefinery scenarios

Parameters		**LA scenarios**				
		2G LA[#]	**Updated 2G LA**	**1G LA[+]**	**1G2G LA**	**1G2G LA+ Xylitol**
Bypass ratio		44%	-	-	-	-
1G feed (t/h)		-	-	25.4	25.4	25.4
2G feed (t/h DM)		36.4	65.0	-	65.0	65.0
Product (t/h)		7.2[c]	11.7	7.2	18.5	7.2 [a]
		3.4[d]	-	-	-	11.1 [b]
Product recovery	1	98.9%	94.9%	96.0%	94.4%	96.0%
	2	-	-	-	-	99.5%
Heating (MW)		70.1	82.0	25.5	107.0	95.7
Cooling (MW)		76.1	99.1	17.9	127.6	110.4
Power (MW)		1.6	6.9	1.3	5.7	10.2
Steam Demand (t/h)		73.6	140.0	45.2	181.2	118.0
CHP feed (t/h DM)	Bypass	28.6	-	-	-	-
	Lignin/Biochar	-	44.30	1.30[+]	45.4	68.1
	Biogas	2	12.4	5.2[+]	15.2	5.2
Power produced (MW)		13.7	29.4	-	26.4	37.4
Residue remains (t/h DM)		-	4.0	-	7.3	10.1
Surplus power (MW)		12.2*	13.9	-	12.2	18.6

[a] Levulinic acid production rate; [b] Xylitol production rate; Levulinic acid production rate; [d] Furfural production rate, [+]CHP feeds are fed to an additional low-pressure boiler; * Sold to the grid; # by Kapanji et al., (2019)

Point to highlight, the current configurations considered sole production of LA and have employed LLE extraction followed by fractionation in the DSP in order to reduce the energy demands of the process. Unlike the configuration reported by Kapanji et al. (2019) that considered the co-production of furfural and LA through direct fractionation of acid hydrolysis crude mixture of LA. Although the Biofine process is widely known to produce LA and furfural, their recovery and purification to the required market purity are very energy intensive (Girisuta et al., 2013). Hence, in this study, instead of purifying furfural further in the more

energy-intensive process, the produced furfural was considered as waste. Therefore, it was digested in the WWT along with the produced formic acid for biogas production. This is similar to the configuration developed by (Sadhukhan et al., 2016), which proved to be self-energy sufficient by just considering filtered lignin residues and biogas produced from WWT for producing steam of the process.

Moreover, in these scenarios, the production of biochar (humins) is considered. Humins is an unavoidable product produced during the degradation of pentose and hexose sugars during the acid hydrolysis at server conditions (Kang et al., 2018a). However, the benefit of this product, is that it can be utilized to provide the heating in the process due to its high heating value of 20 MJ/kg that is comparable to that bagasse (Sadhukhan et al., 2016). Furthermore, it is worth noting that, the newly developed configurations (updated 2G, 1G2G and 1G2G multi-product), considered the reduction in energy demands of the process to liberate more bagasse for utilization in the process.

As can be seen in Table 36, the 1G LA scenario producing 7.2 t/h LA, is the lowest steam user (45.2 t/h) compared to other scenarios. This is attributed to the scale of the plant. The raw material processed in 1G LA scenario (25 t/h) is lower compared to other 2G scenarios (113.5 t/h). Furthermore, pre-treatment of 2G feedstock represented by the first reactor in a Biofine configuration, is energy intensive which does not exist in 1G plant.

It is important to realise that, the 1G LA scenario requires 45.2 t/h of steam to supply the heating of the process. However, this steam demand is more than extra capacity of existing boiler (30.5 t/h). Therefore, the deficit of 14.7 t/h is supplied using a low-pressure boiler that burns 5.2 t/h biogas produced from WWT, as well as 32.3 t/h of bagasse that is left in the existing boiler (Dogbe et al., 2020).

On the other hand, the updated 2G LA scenario requires more steam (140 t/h) compared to the 2G LA scenario (73 t/h) reported by (Kapanji et al., 2019). This is due to changes in process configuration and the heat-integration network of the process and the reduced bypass ratio in the 2G LA scenario. Consequently, the newly developed LA process (updated 2G LA) produced 11.7 t/h LA, which is higher than 7.2 t/h LA that has been reported in literature (Kapanji et al., 2019).

Incorporation of hot return condensate as described in section 3.1.4 and considering the produced furfural and formic acid as waste for biogas production has resulted in all developed LA scenarios requiring no bypass of lignocellulose to be energy self-sufficient. Mainly because

of the return condensate is HHPS that returns at 260°C and forms over 30% of the total return condensate. Furthermore, a high flow of solid residue containing lignin and biochar (44.1-45.2 t/h DM for scenarios processing 2G feedstock) and biogas is the major contributor for a no bypass requirement.

Ideally, up to 98% of LA can recover from the crude acid hydrolysis mixture. However, slightly lower recoveries ranging from 94.6% to 96% of LA are obtained in this study. This is attributed to losses during evaporation of furfural and inefficiency in the extraction column caused by solvent recycling. It is worth mentioning the optimization of such columns in AspenPlus® is very challenging.

As presented in Table 36, the 1G2G LA scenario has the highest production rate (18.5 t/h), as a result of processing both 1G and 2G feedstocks for LA synthesis. While the integrated 1G2G LA+ xylitol reported a lower production rate (7.2 t/h) even though it had zero bypass ratio. This was due to different configurations for 1G2G LA and 1G2G LA+Xylitol. In order to obtain xylose for utilization for xylitol production, bagasse acid hydrolysis (pretreatment) was incorporated. Then the produced liquid hydrolysate containing xylose was taken for xylitol production, and the solid hydrolysate was sent to the CHP. The reason for sending the latter to CHP, was to avoid incorporation of further enzymatic hydrolysis that will result in further incorporation of enzyme production in the process. However, such configuration to utilize solid hydrolysate can be investigated in the future.

Considering that LA is still an emerging biochemical, serving a niche market estimated at 6 ktpa (Gerardy et al., 2020). To avoid flooding the market, it would mean that its production would have to be small thereby resulting in high selling prices. Even so a study by Kapanji et al., (2019), has shown that the production of LA for niche market results in an unprofitable scenario. Therefore, only overproduction of LA has the potential to result in reduced selling prices. Therefore, the current scenarios aimed at reducing the selling prices of LA in order to target a wide range of markets.

With the LA market expected to boom in the coming years, the market value is expected to go over $618 million in 2026 (Stratistics Market Research, 2019) due to biofuels that can be derived from LA. So, using statistics provided by Stratistics Market Research, (2019) that shows that in 2017, LA market segment accounted for $270 million. Using a maximum selling price of $3000/t for a niche market (Gerardy et al., 2020), the global market can be estimated

at 90 ktpa. Considering this estimated global market, the developed scenarios constitute 65% (2G LA), 44% (1G LA and 1G2G LA+Xylitol), and 103% (1G2G LA).

The processes' energy demands per product produced for LA are presented in Figure 31. The specific energy demands presented exclude the needs of the sugar mill, only biorefinery complexes are considered. In terms of heating, it can be seen that the 2G LA scenarios reported by Kapanji et. at. (2019) (presented as "existing 2G") demands more heating energy per product (9.7 MW/t) in comparison to the scenarios developed in this study (1G LA, 2G LA, 1G2G LA and 1G2G LA+Xylitol at 3.6, 7.0, 5.8 and 5.2 MW/t product/s respectively). Owing to the energy intensive fractionation trains for furfural recovery and LA purification (Isoni et al., 2018). While the 1G LA showed to be the least energy-demanding process. This can be explained by the less complicated process configuration for both reaction and purification systems. Moreover, the reaction for the 1G LA process happens at less severe conditions compared to 2G GA processes to produce a concentrated LA slurry that further simplifies the subsequent purification process Kang et al. (2018).

It can be noticed that unlike in the 1G2G GA vs 1G2G GA+ Xylitol scenarios, with the latter being the most energy intensive. The 1G2G LA was more energy intensive compared to 1G2G LA+ Xylitol, because in the multiproduct scenario for LA and xylitol production (1G2G LA+Xylitol), 1G feedstock is used for LA production while 2G feedstock is used for xylitol production instead of having LA produced from both 1G and 2G feedstocks. The updated 2G LA scenario showed the highest cooling demand, due to the need to condense a huge amount of MIBK from solvent stripper for recycling into the extraction column. The high electricity demand in the 1G2G LA xylitol scenario can be attributed to the pumping of 2G slurry and blowers that processes the voluminous amount of air required to dry the xylitol product to its specifications of 98% purity.

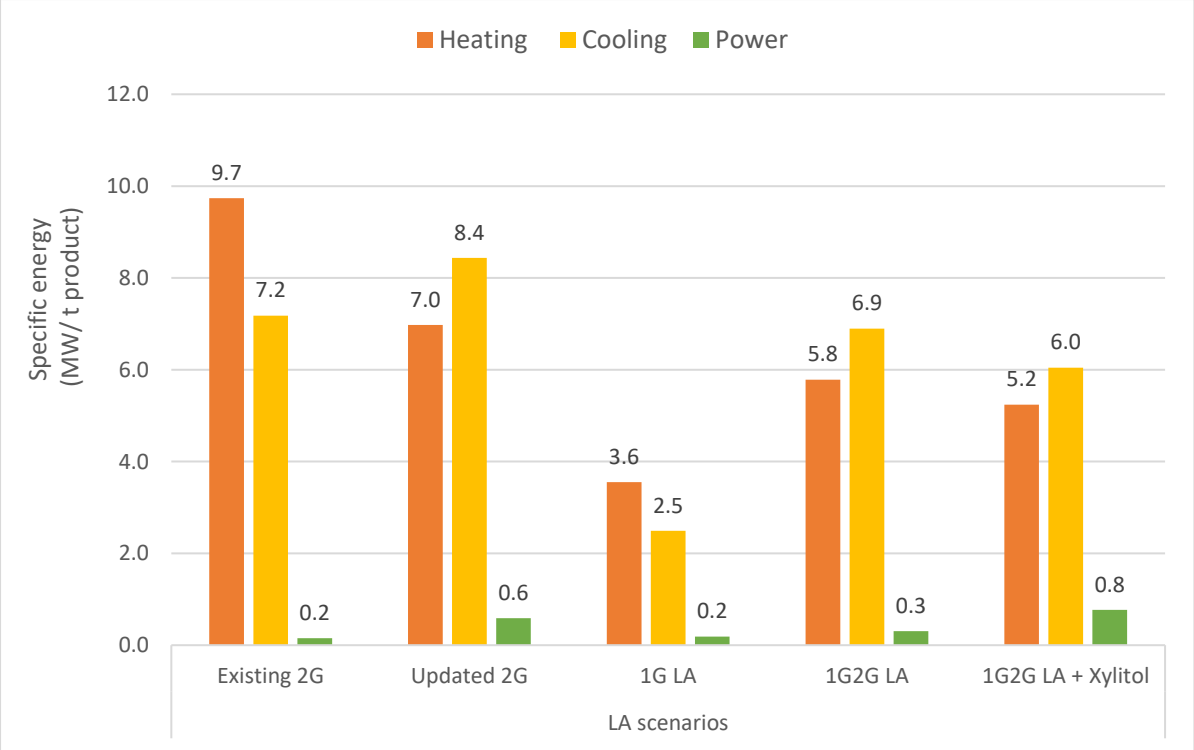

Figure 31: Specific energy demand for the LA scenarios

4.2.2 Economic performances

4.2.2.1 Capital and Operating cost

From the generated mass and energy balances, Capex and Opex estimations were determined for LA biorefineries considering all the marginal costs as a result of annexing new biorefineries into an existing sugar mill. Table 37, shows the summary of the TCI cost breakdown including TEC, TDC and TIDC of the developed scenarios in this study.

Employment of the Biofine process, results in the elimination of pretreatment (A-100), enzymatic hydrolysis (A-200) and enzyme production (A-300) areas for processes utilising 2G feedstock. Due to direct processing of solid feedstock in two stage reactor system. However, when xylitol is co-produced, A-100 and A-200 are re-introduced to obtained pure xylose for xylitol production. In A-100, lignocelluloses biomass is hydrolysed using dilute acid at less severe operating conditions (9 bar and 150°C) in comparison to the first Biofine process reactor (25 bar and 225°C) to yield 90% xylose. Subsequently in Area 200 toxic substances are removed and xylose is isolated. The installed cost in the for the downstream processing (A-600) includes cost of LA and xylitol purification.

Table 37: Capital cost breakdown for the LA scenarios

Area	Installed cost ($ million)			
	1G LA	2G LA	1G2G LA	1G2G LA +Xylitol
Area 100: Pre-treatment	-	-	-	45.64
Area 200: Enzymatic hydrolysis +detoxification	-	-	-	11.36
Area 300: Seed train+ Enzymes production	-	-	-	-
Area 400: Fermentation	-	-	-	-
Area 500: Reaction	10.22	46.99	56.76	23.59
Area 600: Downstream processing	16.66	47.74	57.93	25.06
Area 700: WWT	22.89	48.42	56.23	54.95
Area 800: CHP	13.11	83.45	89.90	90.88
Area 900: Storage (5% of ISBL)	1.34	4.74	5.73	5.28
Area 110: Utilities (6.5 % of ISBL)	1.75	6.16	7.45	6.87
ISBL Total	**26.87**	**94.73**	**114.69**	**105.64**
Total Equipment Cost	**65.97**	**237.49**	**274.00**	**263.62**
Warehouse (4% ISBL)	1.07	3.79	4.59	4.23
Site development (9% ISBL)	2.42	8.53	10.32	9.51
Additional piping (4.5% ISBL)	1.21	4.26	5.16	4.75
Total Direct Costs (TDC)	**70.67**	**254.07**	**294.07**	**282.11**
Proratable Expenses (10% TDC)	7.07	25.41	29.41	28.21
Field Expenses (10% TDC)	7.07	25.41	29.41	28.21
Home Office and Construction (20% TDC)	14.13	50.81	58.81	56.42
Project Contingency (10% TDC)	7.07	25.41	29.41	28.21
Other Costs incl. start-up, permits etc. (10% TDC)	7.07	25.41	29.41	28.21
Total Indirect Costs (TIDC)	**42.40**	**152.44**	**176.44**	**169.26**
Fixed Capital Investment (FCI = TDC + TIDC)	113.07	406.51	470.51	451.37
Working Capital (5% FCI)	0.00	0.00	0.00	0.00
Total Capital Investment (TCI = FCI + WC)	**113.07**	**406.51**	**470.51**	**451.37**

As can be seen in Table 37, the 1G scenario benefited from a low-cost low-pressure boiler at $13.11 million that supply a steam deficit of 14.7 t/h. Whereas in scenarios processing 2G feedstock, the installation of a new efficient high-pressure boiler was required to avail high portion of bagasse for utilisation in the biorefinery complex.

The integrated 1G2G LA scenario requires higher TCI ($ 470.51 M) compared to a multi-product facility ($451.37M). This is primarily due to plant capacities; in 1G2G LA scenario, both 1G and 2G feedstocks are processed for LA production in a parallel reaction system for the respective feedstock with integrated downstream processing units. Unlike in the 1G2G LA+Xylitol scenario where 1G and 2G feedstocks are used for LA and xylitol productions respectively.

The total operating cost per product for LA scenarios are presented in Figure 32. This is calculated based on the annual operating cost incurred per annual total products produced on

full capacity operation. As can be observed, the raw material, extraction solvent (MIBK) are the major contributors to TCOP per product. Furthermore, the Raney Ni catalyst used for hydrogenation of xylose to produce xylitol and activated carbon used for separating inhibitors results in the multi-product scenario to have the highest TCOP ($/t). It can be noted that Raw material cost contribute the same in 1G2G LA and 1G2GLA+ Xylitol scenarios, this is due to the same cost for raw material (cost of 1G and 2G) and almost similar biorefinery outputs (18.5 t/h LA vs. 18.2t/h LA+Xylitol). The MIBK has the highest contribution to TCOP in 1G2G LA scenario due high amount required to extract LA as a result of mixing LA crude mixture from 1G site and 2Gsite. Although, extraction with MIBK bring the energy savings benefits into the process, it however results in a significant increase the cost of production. The more detailed Opex calculations are presented in Appendix E.B,

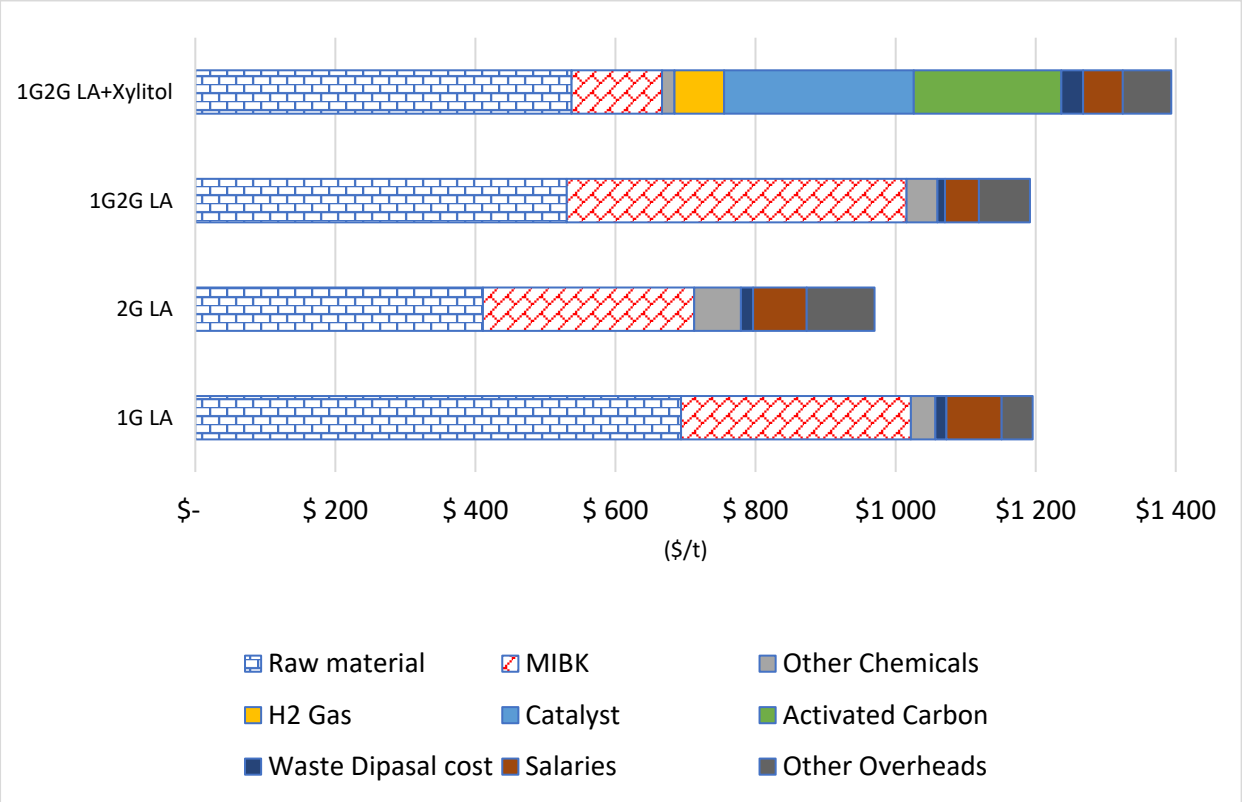

Figure 32 Total operation cost per tonne product/s ($/t) for the LA scenarios

4.2.2.1 Comparisons of key economic indicators

The calculated TCI per product over produced 25 years, TCOP per product, total sales NVP, IRR, and LA MSP for existing LA scenarios and scenarios considered in this study are presented in Table 38. The new scenarios' profitability considered in this study were assessed using an average market price of $2750/t (Gerardy et al., 2020). Whereas, the 2G LA scenario reported in literature was assessed at a commodity market price of $905/t (Kapanji et al., 2019). However, for the scenario (existing 2G LA) to be deemed profitable (20% IRR), LA needed to sell at $1080/t.

Table 38: Comparisons of key economic indicators for LA scenarios

Indicators	**LA scenarios**				
	2G LA*	**Updated 2G LA**	**New 1G LA**	**New 1G2G LA**	**New 1G2G Multi-product**
TCI (M$)	218.9	406.5	113.1	470.5	451.4
TCOP (M$)	24.9	57.0	43.0	110.2	127.3
TCI ($/product) [a]	133.8	290.7	132.1	213.4	207.8
TCOP ($/t)[b]	532.1	970	1 196	1 190	1 395
Total sales (M$)	n.r	161.5	98.9	254.6	314.6
NPV (M$)	139	-38.1	73.7	31.4	184.2
IRR (%)	17.1%	18.1%	31.8%	21.3%	27.6%
LA/Xylitol MSP ($/t)	1080	2950	2 102	2600	1133/2851

[a] Determined considering product produced over a plant lifetime 25years; [b] determined based on the total cost of production and annual product produced assuming full capacity operation; n.r. Not reported, * by Kapanji et al. (2019)

Moreover, the scenario benefited from the lowest cost of production ($532/t) compared to the new scenarios developed in this study. This can be explained by the feedstock cost ($10.79/t) that was considered by Kapanji, (2016) which is significantly lower compared to the lignocellulos's feedstock prices considered in this study of $34.34/t and $74.05/t DM for wet bagasse and trash respectively. In addition, the high cost of MIBK that is needed for solvent extraction can also be taken as the reason for contributing to differing total cost of production. Previously, separation was conducted through fractionation of crude acid hydrolysis mixture containing LA (Kapanji et al., 2019). Thereby resulting in a more energy intensive process and more fractionation steps. In this study, crude acid hydrolysis mixture containing LA, is firstly taken into an extraction column to strip of the acid and reduce the water content, and subsequently reducing number of fractional steps and energy of the process (Sadhukhan et al., 2016).

An attempt to configure an energy self-sufficient biorefinery (2G LA) by considering the free separate furfural as waste stream to produced biogas, resulting in more bagasse available for utilisation to produce more LA did not result in an improved economic outcome in comparison to what was previously done by Kapanji et al. (2019). The current 2G LA configuration resulted in a much higher MSP of $29502/t compared to the attained MSP of $1080/t by Kapanji et al. (2019). However, the economics improved when 1G2G was considered under the same design basis. The scenario was profitable with MSP and IRR of $2600/t and 23% respectively.

Despite the low product yield achieved through the novel design for 1G LA. It is the most profitable scenario with IRR of 31.8% attaining the lowest MSP of $2102/t, agreeing with other 1G biorefinery configurations that shows better economic viability compared to 2G biorefinery configuration (Dogbe et al., 2020), primarily benefiting from a shared CHP facility and installation low cost low pressure boiler that supplies only 15.7 t/h steam deficit.

On the other hand, the multi-product complex (1G2G LA+Xylitol) achieved the lowest MSP for LA at $1133/t. However, through this scenario xylitol is the main product since it is produced in large quantities compared to LA (11t/h vs 7.2t/h) and it is sold at market price of $3900/t. Xylitol contributes more to totals sales than LA accounting for 68.6% and 31.4% of the total revenues respectively. Therefore, the xylitol MSP of $2851/t is attainable which is lower than then market price of $3900/t when LA is sold at market price of $2750/t. Thus, the option to co-produce LA with xylitol in a configuration that considers 1G for the LA and 2G for the xylitol production, is a potential pathway to provide LA at the lowest MSP ($1133/t).

4.2.3 Sensitivity analysis

The economic sensitivity analysis results for the LA scenarios are presented in Figure 34 showing the effects of ±30% changes to the economic parameters: (a)1G LA, (b)2GLA, (c)1G2G LA, (d-e) 1G2G SA+ xylitol. Also, the economically unattractive 2G LA scenario's sensitivity analyses results are present to determine cases that could result in the scenario to be viable. Overall, the greatest sensitivity is on the TCI, VOC, and operational hours. While, income tax and FOC show the least sensitivity on MSP. Usually, similar trends are observed in these parameters (Humbird et al., 2011; Nieder-Heitmann et al., 2019).

The sensitivity of TCI and VOC on MSP for 1G LA (a) scenario are more or less the same with 15% decrease and increase to the MSP. Similar, results have been obtained in literature for low capital investment project (Dogbe et al., 2020). Unlike 1G LA scenario, scenarios processing 2G feedstock showed to be more sensitive to TCI compared to VOC. This is due to large capital

investments. Nonetheless, the scenarios still attained MSP below market price of $2750/t after the in after the introduction of unfavourable conditions in all the parameters. The 1G2G LA and 1G2G LA+Xylitol scenarios are also showing profitable results under the given economic assumption after the introduction of unfavourable conditions (+30%) in all the parameters. With an exception for unfavourable condition for an annual operation of 3500 hour. An inefficient annual operating time of 3500 hours result in result in MSP above the market price at $3320/t and $2810/t for 1G2G LA and 1G2G LA+Xylitol respectively.

On the other hand, the unprofitable (b)2G LA scenario could become profitable when TCI reduces, and annual operating hour is increased to 6500. Increased operating hours are possible due to improved efficiently the current operation of the sugar mill, while sourcing equipment from low cost supplier could warrant a decrease in TCI thereby improving profitability of the scenario.

Scenario 1G2G LA+Xylitol, showed deferring results compared to other scenarios. The most sensitive parameters (operational time, TCI, and VOC) resulted in the lowest MSP ranging from -$52/t to $228/t for favourable conditions. These are caused by a higher production rate of xylitol (11 t/h) than the production rate of LA (7.2 t/h) in the multi-product complex. Moreover, the selling price of xylitol used for this evaluation ($3900/t) is higher than of LA ($2750/t). Meaning that, xylitol contributes more to the cash flow of the process than LA.

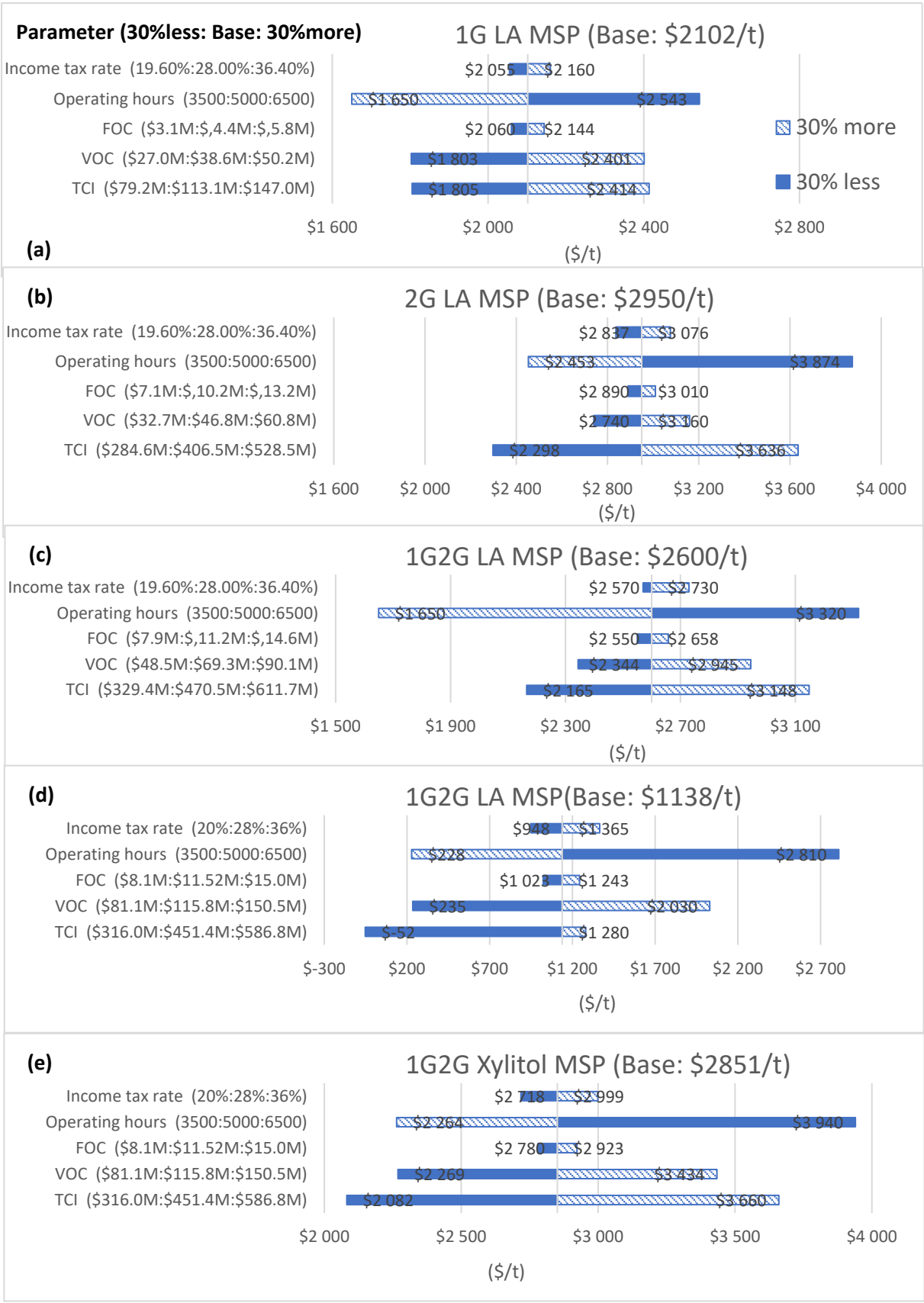

Figure 33: The LA scenarios MSP sensitivity analyses to ±30% changes to the economic parameters; (a)1G LA, (b) 2G LA, (c)1G2G LA, (d-e) 1G2G LA+ xylitol

4.3 Succinic acid

4.3.1 Mass and energy balance

The overall performance of different SA scenarios in terms of mass and energy balances are presented in Table 39. The existing 1G SA scenario developed by Dogbe et al., (2020) was updated to consider a new 1G flow rate of 25.4 t/h from 23.2 t/h that was last considered and incorporation of WWT for water recycling in the process. While the existing 2G SA scenario was updated to consider the new pretreatment reaction conditions by Humbird et al., (2011) that yields 90 wt% xylose in comparison to 83 wt% that was previously used (Nieder-Heitmann et al., 2019) and the new configuration at new operating condition that is further explained below. In the newly considered scenarios, obtaining high yields for xylose is important because of the subsequent conversion into xylitol in the multi-product complex (1G2G SA+ Xylitol).

Table 39: Overall mass and energy balances for the SA biorefinery scenarios

Parameters		**SA scenarios**					
		1G SA*	**2G SA#**	**Updated 1G SA**	**Updated 2G SA**	**1G2G SA**	**1G2G SA +Xylitol**
Bypass ratio		-	28%	-	10%	22%	50%
1G feed (t/h)		21.2	-	25.4		25.4	25.4
2G feed (t/h DM)			46.8	-	58.5	50.7	32.8
Product (t/h)		11.6	13.5	15.3	20.2	34.1	18.5[a]
							5.6[b]
Product recovery	1	98.2%	98.3%	97.8%	98.1%	97.7%	98.1%[c]
	2	-	-	-		-	99.5%[d]
Heating (MW)		27.3	72.1	24.7	58.0	75.1	89.0
Cooling (MW)		36.1	46.6	42.6	55.3	90.8	111.4
Power (MW)		1.3	3.5	3.0	8.6	10.8	13.7
Steam Demand (t/h)		-	129.2	45.2	96.6	126.4	152.1
CHP feed (t/h DM)	Bypass	-	18.2	-	6.5	14.3	32.2
	Lignin	-	30.60	-	22.20	20.9	12.5
	Biogas	-	5.9	2.3[e]	12.3	15.1	6.1
Power produced (MW)		-	7.8	-	29.8	33.5	36.2
Residue remains (t/h DM)		-		-	0.8	0.9	1.1
Surplus power (MW)		-	4.6	-	12.4	14.1	13.9

[a] Succinic acid production rate; [b] Xylitol production rate; [c] succinic acid recovery after fermentation; [d] Xylitol recovery after reaction, [e]biogas fed to an additional low-pressure boiler, * Dogbe et al. (2020), # Nieder-Heitmann et al. (2019)

As can be seen in Table 39, there is a reduction of 32.6 t/h in steam demand for the 2G SA process. The simulation model developed by Nieder-Heitmann et al. (2019) conducted acid hydrolysis at a much higher temperature of 180°C, whereas the current pretreatment design,

acid hydrolysis is conducted at 158°C. Furthermore, the solid loading water in the design by Nieder-Heitmann et al. (2019), was directly extracted from the CHP system using a let-down station configuration at 176°C and 9 bar. Although this configuration resulted in a less high-pressure steam demand of 0.19 t_{HPS}/t_{DM} compared current configuration at 0.43 t_{HPS}/t_{DM} required to be injected in the pretreatment reactor. It resulted in a boiler throughput much higher compared to the current design (4523 t_{steam}/t_{DM} vs 3706 t_{steam}/t_{DM} ;t_{steam}/t_{DM} denote the amount of steam produced by the boiler for both sugar mill and biorefinery complex per amount of feedstock processed in the biorefinery complex for product production).

The bypass ratio was reduced from 28% to 10% in 2G SA scenarios. This was possible due to the reduction in steam demand of the process from 129.2 t/h (in a simulation developed by Nieder-Heitmann et al.(2019)) to 90.1 t/h (updated 2G SA), as well as higher biogas fed into the CHP (12.6 t/h) for updated 2G SA compared to (4.9 t/h) in the existing 2G scenario. However, comparing all scenarios, the multiproduct complex (1G2G SA+Xylitol) required the highest bypass ratio of 50%. Similar to other multiproduct facilities studied in this research, this is attributed to the energy-intensive nature of the xylitol production process (Mountraki et al., 2017). The xylose concentration step prior to hydrogenation and xylitol concentration step prior to crystallization, in addition to the already energy-intensive SA due to pretreatment and downstream processing, results in a very energy-intensive process. Furthermore, despite only processing half of the bagasse (32.5 t/h DM), the process requires 152.1 t/h of steam, which is the highest compared to the other SA scenarios.

The updated 1G SA scenario produced 15.3 t/h product which is higher compared to the existing 1G SA scenario that produced 11.6 t/h. However, considering the scales of the two processes, the production rate is 10% extra in the updated scenario. This might be due to the assumptions made in iterating the conversion ratios to obtain 0.95g/g yield SA from 150 g/l sugar substrate fed into the fermenter whilst ensuring that there is about 20g/l of fructose remaining in the fermentation broth (Chan et al., 2012). Furthermore, 45.2 t/h of steam is required to supply the heating in an updated 1G SA scenario which is more than, 30.5t/h that can be supplied using the existing boiler (Dogbe et al., 2020). Therefore, the deficit of 14.7 t/h is supplied using a low-pressure boiler that burns 2.5 t/h biogas produced from WWT, as well as 32.3 t/h of bagasse that is left in the existing boiler.

As can be seen in Table 39 the updated 2G SA scenario produces 20.5 t/h of product from processing 58.5 t/h DM of lignocellulose, which is significantly higher than 13.5 t/h product in the existing 2G SA scenario that processes 46.8 t/h DM of lignocellulose. Different

pretreatment conditions adopted for the updates in this study and reduction in bypass ratio can be the main reasons for obtaining better production rate compared to previous study (Nieder-Heitmann et al., 2019). With this process, more sugars were therefore available for fermentation thereby resulting in a significantly higher production rate.

The integrated 1G2G SA scenario attained the highest SA production of 36.7 t/h compared to 1G2G SA+Xylitol because of the low bypass ratio of 22% for 1G2G SA which is lower compared to 50% in the 1G2G SA+ Xylitol complex. Other than the scale of process 2G feedstocks; 50.7 vs 32.8t/h DM for 1G2G SA and 1G2G SA+ Xylitol, respectively. The fermentation process in the 1G2G SA configuration was conducted by separate fermentation of 1G feedstock and co-fermentation of pentose and hexose sugars from both the cellulose and hemicelluloses hydrolysates of 2G in order to ensure maximum substrate utilisation. Whereas in the 1G2G SA+Xylitol scenario, the hemicellulose hydrolysate was utilised for xylitol production, and cellulose hydrolysate was mixed with 1G feedstock co-fermentation. Hence there is a lower production rate if SA in the latter compared to the former (18.5 t/h vs 34.1 t/h).

Ideally, the *E. coli KJ122* strain has been engineered for molasses which contains sucrose predominantly at a fraction greater than 70 wt% on a dry basis (Chan et al., 2012). Since, combining 1G substrate with 2G glucose results in sugar proportion changes, resulting in glucose denominating production medium. Therefore, future experimental work is recommended to investigate whether changes to the sugar proportion still hold for the results obtained by Chan et al. (2012). It is widely known that the changes to the fermentation conditions might significantly impact on yield and product concentration. The product yield being directly related to the production rate, this might have a significant impact on the process's economics.

The current biobased SA global production is estimated at 49 ktpa, with a market price of approximately $2860/t (Rosales-Calderon and Arantes, 2019). Including its fossil-based counterpart, the total production is estimated at 201 ktpa globally. With scenario 1G SA, 2G SA, 12G2 SA, and 1G2G SA+Xylitol producing 76.5 ktpa, 183.5 ktpa, and 92.5 ktpa respectively. This means that the scenarios produce more than 40% of the global market which may flood the market. Fortunately, SA selling at lower prices than the current market prices may cause other markets to open resulting in an increased demand for SA. Therefore, overproduction of SA can be justified if the scenarios obtain lower selling prices than the current market price.

The processes' energy demands per product produced for SA scenarios are presented in Figure 34. The specific energy demands presented exclude the needs of the sugar mill, only biorefinery complexes are considered. Overall, the multi-product complex is the most energy-demanding process in comparisons to the newly developed configurations (2.8 MW/t, 3.5 MW/t and 0.4 MW/t for heating, colling and electricity respectively). Due to energy-intensive processes such as pretreatment, xylitol production, and SA purification process. While the 1G SA scenarios showed to be the least energy-demanding process as a result of the elimination of the pretreatment section and lower feedstock processed (1.6 MW/t, 2.8 MW/t and 0.2 MW/t for heating , colling and electricity respectively). It can be seen from Figure 34, that there is an improvement in the update scenarios (1G SA and 2G SA). In terms of heating demands, 1G SA scenario reduced from 2.4 MW/t to 1.6 MW/t while 2G SA reduced from 5.3 MW/t to 2.9 MW/t. This can be explained by the new process configuration that was integrated into the processes. Similarly, the cooling demand was higher in existing scenarios compared, to the newly developed scenarios.

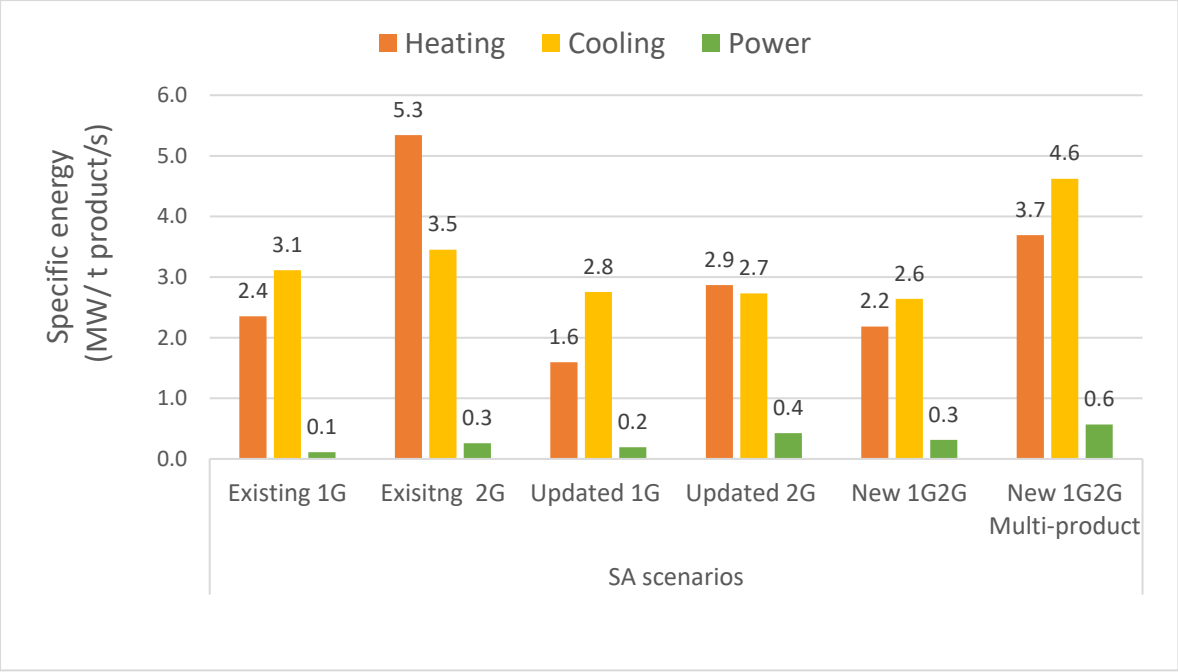

Figure 34 Specific energy demands for the SA scenarios

4.3.2 Economic performances

4.3.2.1 Capital and Operating cost

After the mass and energy balances had been conducted, the results were used for economic assessment of different scenarios. This involved Capex and Opex estimations to determine the production cost of biorefineries considering all the marginal costs as a result of annexing new

biorefineries into an existing sugar mill. Table 40, shows the summary of the TCI cost breakdown including Total equipment cost (TEC), Total direct cost (TDC) and total indirect cost (TIDC) of the new scenarios that have been developed through this study. The installed cost for A-100 and A-200 are comparable to previous studies (Dogbe et al., 2020; Nieder-Heitmann et al., 2019). However, the cost for WWT (A-700) is high due to a different WWT process adopted for treating waste streams. The WWT technology for treating waste effluent and biogas production adapted in this study is similar to that developed by Humbird et al., (2011). The installed cost for this technology in 2011 was $44 million for a plant that treats 411t/h of waste effluent.

Table 40: Capital cost breakdown for the SA scenarios

Area	Installed cost ($ Million)			
	1G SA	2G SA	1G2G SA	1G2G SA + Xylitol
Area 100: Pre-treatment	-	51.41	50.28	39.462
Area 200: Enzymatic hydrolysis +detoxification	-	33.96	27.81	36
Area 300: Seed train+ Enzymes production	0.81	19.04	17.66	13.252
Area 400: Fermentation	21.74	38.92	58.29	39.852
Area 500: Reaction	-	-	-	8.6208
Area 600: Downstream processing	11.66	20.15	22.63	24.474
Area 700: WWT	24.40	48.93	60.62	50.424
Area 800: CHP	13.11	65.08	69.19	73.007
Area 900: Storage (5% of ISBL)	1.71	8.17	8.83	8.0831
Area 110: Utilities (6.5 % of ISBL)	2.22	10.63	11.48	10.508
ISBL Total	**34.21**	**163.47**	**176.67**	**161.66**
Total Equipment Cost	**75.65**	**296.29**	**326.80**	**303.68**
Warehouse (4% ISBL)	1.37	6.54	7.07	6.4665
Site development (9% ISBL)	3.08	14.71	15.90	14.55
Additional piping (4.5% ISBL)	1.54	7.36	7.95	7.2748
Total Direct Costs (TDC)	**81.64**	**324.89**	**357.71**	**331.97**
Proratable Expenses (10% TDC)	8.16	32.49	35.77	33.197
Field Expenses (10% TDC)	8.16	32.49	35.77	33.197
Home Office and Construction (20% TDC)	16.33	64.98	71.54	66.395
Project Contingency (10% TDC)	8.16	32.49	35.77	33.197
Other Costs incl. start-up, permits etc. (10% TDC)	8.16	32.49	35.77	33.197
Total Indirect Costs (TIDC)	**48.98**	**194.94**	**214.63**	**199.18**
Fixed Capital Investment (FCI = TDC + TIDC)	**130.62**	**519.83**	**572.34**	**531.16**
Working Capital (5% FCI)	6.53	25.99	28.62	26.558
Total Capital Investment (TCI = FCI + WC)	**137.16**	**545.82**	**600.96**	**557.72**

As presented in Table 40, the installed cost for the fermentation area (A-400) for the 1G2G SA scenario is more or less the summation of 1G SA and 2G SA scenarios, mainly because the fermentation processes were conducted separately for the 1G and 2G feedstocks in the 1G2G scenario. However, there is a 29% reduction in the installed cost for the downstream processing due to 1G broth and 2G broth mixing.

Furthermore, the installed cost for the fermentation area (A-400) in 2G is lower ($38.93 million) than that of the 1G2G SA+Xylitol scenario ($39.85 million) despite the former having higher capacities than the latter (20.2t/h vs 18.5 t/h SA for 2G SA and 1G2G SA + Xylitol respectively). There exists an economic trade-off between the residence time and initial

substrate concentration. Although an *E. coli KJ122* strain used in the G2G SA + Xylitol scenario can yield 0.96 g/g SA from an initial 150g/l. The long residence time of 72 hours hinders its ability to become cost-competitive with *A. succininogenes* used in the 2G SA scenario that requires a shorter residence time (36 hours) to yield 0.88g/g of SA from an initial 100g/l substrate.

The total cost of production for SA scenarios are presented in Figure 35. Overall, raw material, nutrient and extraction solvent are the major contributors to TCOP per product. However, the cost for nutrients in the 2G SA scenario does not contribute much as compared to scenarios processing 1G feedstock. This is due to the use of expensive ($4200/t) AM1 salt medium in 1G scenarios required for seeding *E. coli* strain and supplementing nutrients for SA for fermentation (Chan et al., 2016). Although expensive, this salt medium reduced the complexities of dealing with the separation on nutrient in the downstream. The multi-product scenario has the highest TCOP per product. This is ascribed to the use of expensive Raney Ni catalyst used for hydrogenation of xylose to produce xylitol. The more detailed Opex calculations are presented in Appendix E.C.

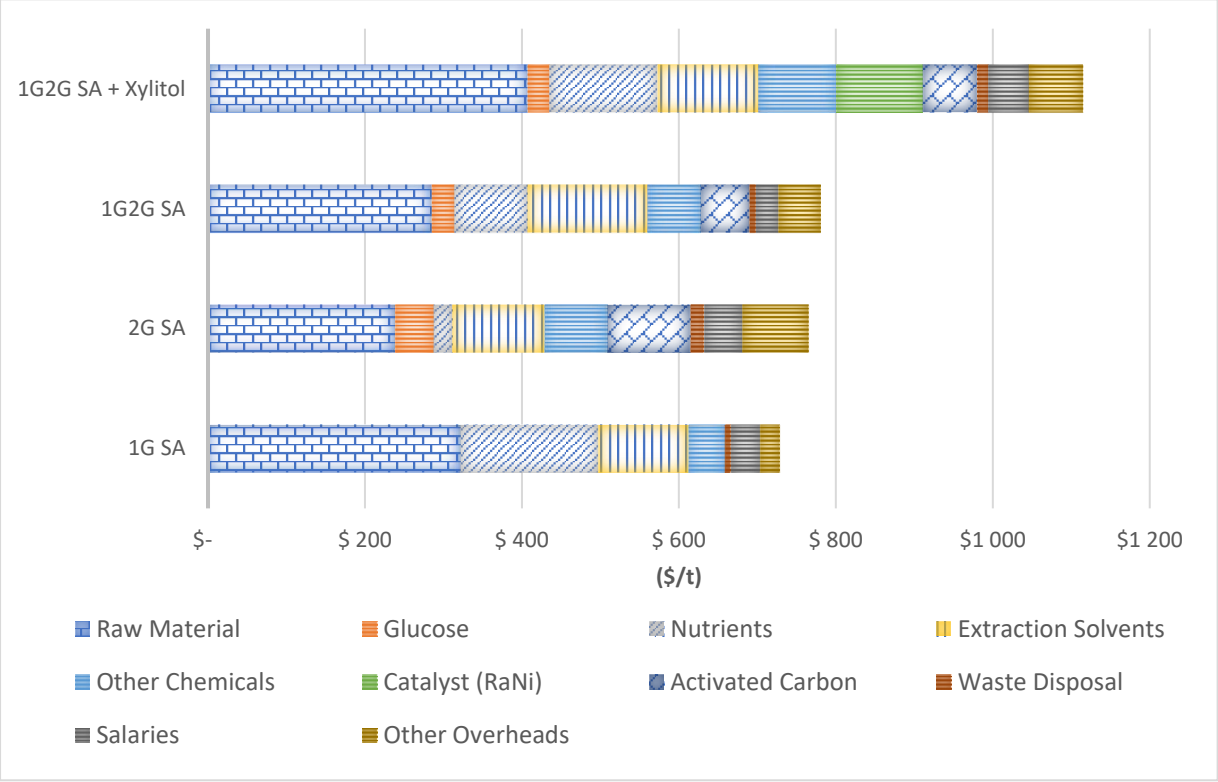

Figure 35: Total operation cost breakdown for the SA scenarios per product produced

4.3.2.2 Comparisons of key economic indicators

The calculated TCI per product over produced 25 years, TCOP per product, total sales NVP, IRR, and SA MSP for existing SA scenarios and scenarios considered in this study are presented in Table 41. Overall, all the scenarios have proved to be profitable, with the IRR ranging from 25.9% to 58.3% and the MSP's below the market price of $2 500/t SA.

Table 41: Comparison key economic indicators for SA scenarios

Parameters	SA scenarios					
	Existing 1G SA	Existing 2G SA	Updated 1G SA	Updated 2G SA	New 1G2G SA	New 1G2G Multi-product
TCI (M$)	80.70	344.50	137.16	600.96	600.96	557.2
TCOP (M$)	40.30	32.71	56.39	77.44	134.34	134.40
TCI ($/t product) [a]	55.66	204.15	70.90	237.65	139.76	241.17
TCOP ($/t)[b]	694.83	373.91	728.74	765.60	781.06	1029.86
Total sales (M$)	125.67	n.r	192.50	252.88	426.99	250.50
NPV (M$)	422.00	900.66	309.70	85.00	406.95	179.88
IRR (%)	57.1%	36.4%	58.3%	23.1%	32.8%	26.4%
SA MSP ($/t)	1348	n.d	1220	2237	1745	1888

[a] Determined considering product produced over a plant lifetime 25years; [b] determined based on the total cost of production and annual product produced assuming full capacity operation; Nd. Not determined & n.r Not reported

It can be noted that the existing 1G SA and 2G SA have lower TCI per product of $56/t and $204/t compared to the updated 1G SA and 2G SA at $71/t and $234/t respectively. This can be explained by the high cost of integrated WWT in the new processes. Likewise, TCOP's per product in existing 1G SA and 2G SA are lower than in the updated 1G SA and 2G SA at $695/t vs $737/t and $374/t vs $690/t respectively due to the high cost of extraction solvent in the developed scenarios. In the present designs, a portion of recycled TMA solvent was purged while the result was recycled back into the process. This configuration was simulated as a closed recycled loop in AspenPlus® model to realistically predict the performance of the process. Whereas, the previously developed models, this challenge of TMA recycle was solved by breaking the recycle loop and integrating a pseudo recycle stream depicting the output of a recycle stream. However, the pseudo stream didn't consider the impurities contained in the recycle stream. As a result, the new scenarios required comparably higher TMA solvent make-up than the reported in previous models (Nieder-Heitmann et al., 2019).

Contrarily, the updated 2G SA scenario that produced 20.5 t/h SA product is comparably higher than the existing 2G SA at 13.5t/h attained lower IRR 25.9% compared to 36.4% of the existing scenario. This can be explained by the cost credit that was considered for selling electricity to

the national grid by the latter. However, the present cases do not consider electricity production, because it is no longer incentivized. Moreover, the cost bagasse ($42.50/t vs $10.6/t average price of both bagasse and trash) is higher and operating hours are less (5000 vs 6480 hours) in the present case compared to the existing scenarios.

Although, the 1G2G SA+Xylitol scenario reported the highest TCOP per product of $1310/t. It obtained lower MPS ($1 933/t) compared to the 2G SA scenario ($1220/t). Due to the co-production of xylitol that sells at a higher market price of $3900/t consequently resulting in the multiproduct complex to have the highest revenue annually($443M). Although relatively a high MSP on the updated 2G SA scenario is observed, the economies of scale benefits are shown in the 1G2G SA when SA MSP lowers to $1672/t.

4.3.3 Sensitivity analysis

The economic sensitivity analysis results for the SA scenarios are presented in Figure 37, showing the effects of ±30% changes to the economic parameters: (a)1G SA, (b)2G SA, (c) 1G2G SA, (d) 1G2G SA+ xylitol. Overall, the greatest sensitivity is on the TCI, VOC, and operational hours. However, the scenarios still show profitable results under the given economic assumption when after the introduction of unfavourable conditions (+30%). with an exception of 1G2G SA+Xylitol scenario that sees MSP rising above the market prices ($2712/t) when a yearly operation 3500 hours. on the other hand, income tax and FOC show the least sensitivity on MSP.

As demonstrated in Figure 37, (a) 1G SA scenario, showed deferring results compared to other scenarios, in terms of sensitivity between TCI and VOC. The VOC showed to be the most sensitive with an approximately 19% increase and decrease on the MSP for 30% unfavourable condition in comparison to a 12.2% increase and decrease for TCI. This is because the yearly operational cost for 1G GA scenario is significantly higher and the required capital investment is considerably lower compared to the other scenario. The TCI is only 2.1-fold of the TCOP, whereas, in other scenarios, TCI exceeds 3.3 folds of TCOP. Usually, such a trend on sensitivity is found for 1G biorefineries due to the lower capital investment required (Dogbe et al., 2020).

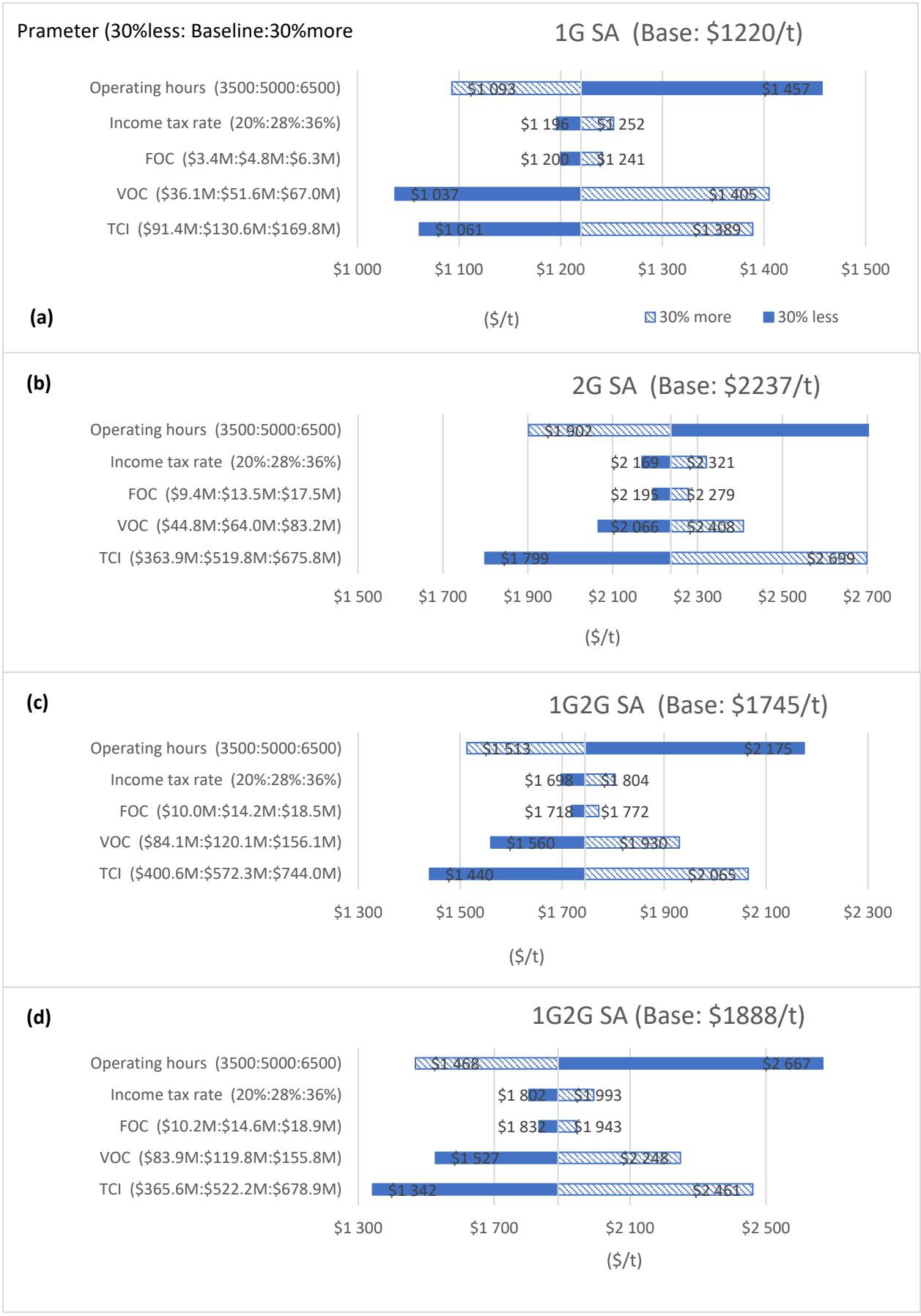

Figure 36: The SA scenarios MSP sensitivity analyses to ±30% changes to the economic parameters; (a)1G SA, (b)2G SA (c) 1G2G SA, (d) 1G2G SA+ xylitol

4.4 Overall analysis and comparisons of biorefineries

4.4.1 Technical and economic comparisons of 2G biorefineries

Overall, the significant changes in the updated 2G scenarios' energy systems were mainly due to changes in the bio digestion assumptions, changes in the pre-treatment configurations, new heat integration network, and elimination of energy-intensive units. The current developed 2G scenarios attained lower or rather some required no bypass at all for the biorefinery complex's self-sufficiency. The 2G GA reduced from 35% to 0, 2G SA from 28% to 10% and 2G LA from 44% to 0%.

As shown in the mass and energy balances in section 4.1.1, 4.2.1 and 4.3.1 there was a substantial increase in biogas production from the 2G scenarios reported in the literature (Kapanji et al., 2019; Nieder-Heitmann et al., 2019; Özüdoğru et al., 2019) to the current 2G simulations developed for this study. The updated 2G scenarios had high biogas production rate at 18.5 t/h, 12.4 t/h and 13.3 t/h than the literature counterpart at 5.1 t/h, 2 t/h and 13.3 t/h for GA, LA and SA respectively.

According to the simulation by Özüdoğru, (2018) and Nieder-Heitmann et al. (2019), the assumptions made for the set of anaerobic digestion (AD) stochiometric reaction were based on the work done by Rajendran et al. (2014) and Tchobanoglous et al., (2003). Based on these stoichiometric assumptions, comparably lower biogas was produced in the AD at 163 g per kg COD digested than the NREL WWT technology used for this study at 228 g / kg COD digested (Humbird et al., 2011). Although the AD design Kapanji et al. (2019) was similar to the one used for this study. A significant increase biogas production was due to consideration of furfural as waste.

The reported ideal amount of CH_4 that can be produced ranges from 220-255 g/kg COD removed (Filer et al., 2019; Inayat et al., 2019). Even though all the AD configurations used in this study followed the well-established WWT technology by (Humbird et al. (2011) that falls within the reported range for CH_4 yield, it was assumed that CH_4 yield does not change irrespective of the wastewater effluent COD level, and there was no biodegradation. Since the amount of biogas produced in the AD has an impact on the amount of on the overall energy supply, a detailed design around the AD systems taking into account the impacts of biodegradable and unbridgeable COD’s in the wastewater effluent could improve the prediction of the overall energy supply of a specific biorefinery.

Although the current changes in the pretreatment configuration resulted in an increased steam (0.43 $t_{HPS}/t_{DM)}$ to operate the acid hydrolysis reactor at 158°C and 9 bar, from the previous configuration that obtained 0.19 t_{HPS}/t_{DM} (Nieder-Heitmann et al., 2019), 0.26 t_{LPS}/t_{DM} (Özüdoğru, 2018). The CHP system configuration to recycle hot condensate as per Table 9, along with energy cuts through new heat integration (discussed through sections 4.1.1, 4.2.1 and 4.3.1 t), reduced the overall heating of the processes.

Despite the efforts to reduce the overall energy of the systems and to improve the production rate. From an economic standpoint, the updated 2G scenarios did not improve compared to those reported in literature (Kapanji et al., 2019; Nieder-Heitmann et al., 2019; Özüdoğru et al., 2019). This shows that the new economic assumptions to reduce the yearly operation hours from 6840 hours to 5000 hours and increase in feedstock prices from $10.6/t to $42.50/t had a negative impact on the overall economic performance of the 2G scenarios. Furthermore, the decision not to sell the electricity to the national grid, since it is no longer incentivised, is one factor that contributed to the negative impact on the overall economic performance.

4.4.2 Comparisons to multiproduct facilities

The multiproduct facilities evaluated the opportunity to diversify the sugar mills product ranges, not only to fully exploit the presented value of the raw material but also to present scenarios that can cater to market volatility (Farzad et al., 2017b). Xylose, the sugar that accounts for nearly 30% of sugars derived from lignocellulose, cannot be fully utilised in the GA and SA fermentation process. Although in the 2G SA fermentation process, xylose can be co-fermented with hexose sugar where only 57% of it is consumed for product yield. Its co-fermentation and other hexose sugars remain a challenge for the 2G GA fermentation process. In the chemical process for LA production, 40% of xylose is converted to furfural, which is considered waste in all LA cases. Practically, for all these cases, xylose's significant fractions end up in the WWT, where it is digested for CH_4 production. However, by integration xylitol producing facilities with LA and GA there is a substantial improvement in the economic performance from 1G2G sole product facilities to 1G2G multiproduct facilities.

Using xylose for xylitol production instead of being directed to AD for biogas production has had a huge impact on the systems' energy supply. All the fermentative (GA and SA) 1G2G sole product facilities increased bypass ratio when their 1G2G multiproduct facilities were considered. GA scenarios increased from 0% s to 48%bypas ratio, while SA increased from 22% to 50% bypass ratio. On the other hand, LA production's chemical process remained at a

0% bypass ratio even after reconfiguration for xylitol production. The reason for 0% was mainly due to the process route followed as described fully in section 4.2.1. The resultant high bypass ratio were not only due to the diversion of xylose for xylitol production that resulted in a decrease in biogas production but also the energy-intensive nature of the xylitol production process route. The xylitol process includes an evaporation unit that concentrates xylose stream to 20wt%, an energy-intensive hydrogenation reactor operated at 130°C and an evaporation unit that concentrates xylitol before crystallisation. Overall, these units constitute to the energy intensiveness of the process.

Although there was a substantial increase in bypass ratio from sole product complex to multiproduct complex for the fermentation processes of GA that resulted in a decrease of product production rate from 26 t/h to 21 t/h, the economic performance of multiproduct facilities (MSP of $1926/t) was better compared to the sole product counterpart ($2205/t). However, for the SA fermentation process. A substantial decrease in product production rate from 34.1 t/h to 18.2 t/h in 1G2G sole product complex and 1G2G multiproduct complex, respectively. Resulted in worse economic performance for multiproduct facilities (MSP of %1888/t) than the sole product counterpart ($1745/t). This can be accounted for by the reduction in sale for SA from $427million to $250.50 million when 1G2G sole product scenario was upgraded to 1G2G multiproduct scenario. Whereas for GA there was an increase in sales from $510.06 million to $513.14 million. Similarly, the 1G2G LA scenario's MSP improved from $2600/t to $1133/t due to improvements on total sales ($254.6-314.6/t). from these results it can be deduced that for a 1G2G multi-product complex to have better economic performance compared to a sole product 1G2G facility counterpart, the total sale should always be higher.

Table 42, Compares the profitability of multi-product biorefineries. The GA multiproduct complex shows the best economic viability with an IRR of 35.1% and NPV of $461.4 million. Although profitable, the LA and SA complexes are, however, hindered by factors such as overproduction.

Table 42: Profitability of multiproduct biorefinery complexes

Parameters	Multiproduct complexes		
	1G2G GA + Xylitol	1G2G LA+ Xylitol	1G2G SA+ Xylitol
Bypass	48%	-	50%
TCI ($/t product)	204.6	207.8	138.4
TCOP ($/t)	988.87	1 395	1 029.86
NPV (M$)	461.64	184.2	179.88
IRR (%)	35.1%	27.6%	26.4%
MSP ($/t)	1926	1133/2851	1888

4.4.3 Price fluctuations on Profitability

Different market reports have shown that there have been fluctuations in the market prices of the products of interest over the last decade (Gerardy et al., 2020; Rosales-Calderon and Arantes, 2019; Stratistics Market Research, 2019). In Figure 37 it was investigated how such fluctuations in market price will impact the viability of certain scenarios. The average market prices used were varied with a ±30% margin to evaluate the impacts of IRR. As can be seen in Figure 37, 1G scenarios were the most sensitive to their respective market price changes. However, the scenarios remained profitable. If the market prices for GA, LA were to drop to $2538/t, $1925/t and $1750/t respectively. There will be about 35% reduction on the current IRR.

The 2G and 1G2G LA scenarios show that if the market price were to drop by more than 30%, these scenarios would be in a risk of not being profitable. Nonetheless the, the devolvement of LA processes that produces LA at a more cost competitive price remains a challenge worldwide. As result, the market price remains high ($2500-3000/t).

In multi-product facilities, the market price fluctuations for xylitol are less sensitive for the co-production of GA and SA scenarios. This can be explained by the higher production rate of GA and SA compared to xylitol (1G2G GA+Xylitol: 21.4 t/h vs 6.4 t/h; 1G2G SA: 18.5 t/h vs 5.6 t/h). On the other hand, the 1G2G LA+ Xylitol scenario is most sensitive to xylitol price. Dropping the market price of xylitol by 30% result in an IRR of 15%.

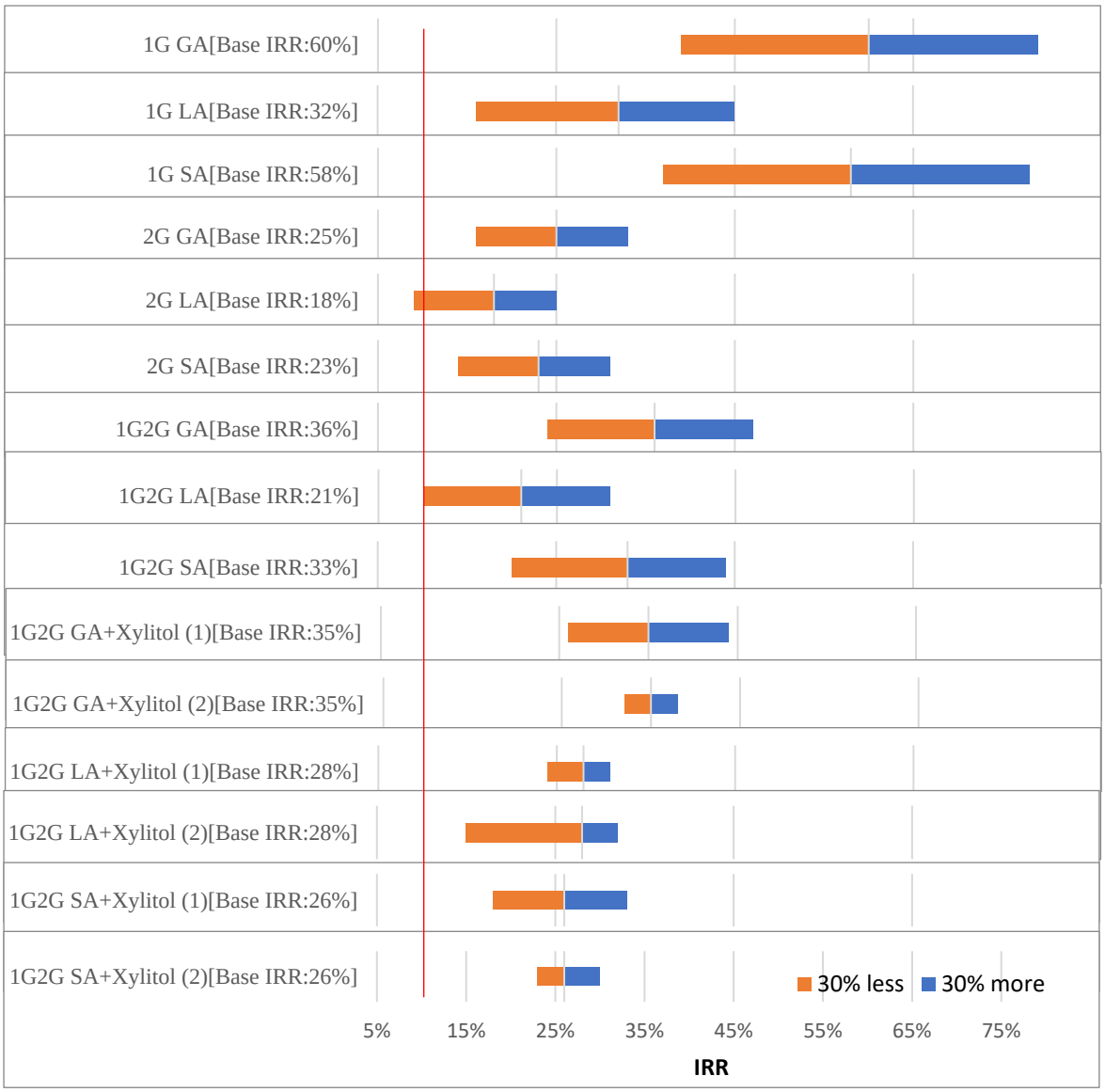

Figure 37: The effect of product price fluctuations on process viability of the developed scenarios. On multiproduct facilities (1) denotes the changes market price of the first product and (2) represent changes of xylitol market price. The red line shows the minimum acceptable discount rate of 9.5%

5 Conclusions and recommendations

An overall aim of this study was to determine if the profitability of sugarcane biorefineries producing glutamic acid, levulinic acid could be further improved from the previously attained profitable scenarios that utilised the second-generation (2G) feedstock (lignocelluloses), by further considering first-generation (1G) feedstock (A-molasses). A cleaner raw material that results in the elimination of the costly pretreatment and enzymatic hydrolysis processes. Furthermore, the integration of feedstocks (1G and 2G) was investigated to evaluate the economies of scale benefits through sole production of glutamic acid (GA), levulinic acid (LA), and succinic acid (SA). Thereafter, the multi-production of the aforementioned with xylitol was also considered.

5.1 Objectives of the study

The objectives of the study were to develop processes and different configurations that have not been considered for the revitalisation of the South African sugar industry before and compared their economic viability with other studied configurations and feedstocks.

1. **To design and evaluate the profitability of 1G biorefinery scenarios producing LA and GA as well as updating the 1G biorefinery for SA.**

An additional two 1G biorefineries configuration for GA and LA to build on the existing work have been developed. Literature experimental data formed the basis of these developments. According to these configurations, the GA process using a novel integrated reactor-membrane system produces 0.56 tonne product per 1 tonne carbon source fed with no by-products. In comparison, the LA process produces 0.36 tonne product and 0.34 tonne humins per 1 tonne carbon source. Equally important, formic acid is also produced in equimolar with LA. However, by-production of formic acid is considered as waste. Therefore, it is digested for biogas production that is subsequently used for the steam generation process. Considering energy self-sufficiency in the processes, the steam consumption of 1G glutamic scenario was met by the existing facility's boiler. However, due to the energy-intensive nature of the 1G LA scenarios, an additional low-pressure boiler was required to supply the deficit in steam demand of 14.7 t/h and. Lastly, the 1G biorefineries proved to be less capital intensive compared to 2G biorefineries which makes them attractive for low capital investment projects.

Although the production of these biochemicals has been commercialised from hexose sugars, their direct production from molasses has not been commercialised. Through this study, the

literature gap for a detailed techno-economic assessment for the first-generation production of GA and LA has been covered.

The major changes made in the 1G SA scenario includes an update for 1G feedstock from 21.1 t/h to 25.4 t/h as well as improving the overall heat energy demands of the processing.

2. **To update existing 2G biorefineries producing LA, GA, and SA.**

The 2G biorefineries simulations that we previously developed were updated to the current technical data and economic assumptions, for better comparisons. The improvements included, closing mass and energy balances loops by directing COD waste to the digester for biogas generation, and improving the heat demand of the process to make more bagasse available for utilisation in the biorefinery complex as well as assessing their economic performance for 5000 hours annual operations instead of 6480 hours. Furthermore, the new costs of feedstock (2G) considering the marginal cost of sugar mill as a result of integration was updated to a higher price of $42.50/t from $10.6/t (average price of both bagasse and trash).

For the updated 2G GA scenario, evaporative crystallisation was replaced with cooling crystallisation thereby improving the overall heat energy of the process and bypass ratio was reduced from 35% to 0%. Consideration for hemicelluloses fractions for digestion using Humbird et al., (2011) anaerobic configuration resulted in a comparably higher biogas production rate than the one that was previously used for GA configuration based on Tchobanoglous et al., (2003). Although, the current study by Jin et al., (2020) has a possible use of pentose and hexose sugars for GA fermentation, fermentation of pentose sugars is not considered for the fermentative production of GA. This can be evaluated in future studies.

Previously the 2G LA scenario considered co-production for LA and furfural in an energy-intensive configuration. In this study, only sole production of LA was considered, and furfural along with other Biofine process by-products was digested for biogas production. As a result, the bypass ratio was reduced from 44% to 0%. Moreover, the incorporating solvent extraction resulted in lower heat demand in comparison to the former, using direct fractionation of crude acid hydrolysate. However, the use of MIBK as extraction had a considerable impact on the economics of the process. It is therefore recommended that future studies investigate other cheaper extractions solvents.

A key highlight on the updated 2G SA scenario is a consideration for TMA solvent recycling that was simulated in a closed-loop arrangement incorporated with purge to predict the performance of the downstream processing best. However, this had a drawback on the

economical production of SA compared to the existing scenario. Furthermore, through improved heat integration network, bypass ratio was reduced from 28% to 10%.

Regardless of the efforts to reduce the overall energy of the systems and to improve the production rate in 2G scenarios. From an economic standpoint, the updated 2G scenarios did not improve compared to those reported in literature (Kapanji et al., 2019; Nieder-Heitmann et al., 2019; Özüdoğru et al., 2019). This shows that the new economic assumptions to reduce the yearly operation hours from 6840 hours to 5000 hours and increase in feedstock prices from $10.6/t to $42.50/t had a negative impact on the overall economic performance of the 2G scenarios. Furthermore, the decision not to sell the electricity to the national grid, since it is no longer incentivised, is one factor that contributed to the negative impact on the overall economic performance

3. **To develop integrated 1G2G biorefinery configurations to produce GA, LA and SA, as well as multi-product biorefinery configurations for production of GA, LA and SA with xylitol**

The designs for integrated 1G2G biorefineries followed parallel reaction or fermentation systems due to limited literature data. Although there was a possible downstream integration for LA and SA scenarios, the GA scenarios followed parallel downstream processing due to the need to recycle unconverted sugars and to ensure maximum product recovery for GA. On the other hand, for a multiproduct for LA and xylitol used 1G and 2G respectively for their production.

Since there is no phase change that requires heating in the downstream processing to recover the GA product. Due to membranes separation and cooling crystallisation. Integrating 1G2G feedstock does not influence the overall heating demand of the process.

Although the 1G2G LA complex is steam demanding at 181.2 t/h, the energy self-sufficiency of the scenario can be maintained using 15.2 t/h of biogas and 45.4 t/h filtered lignin residues with no bypass required. The high amount of biogas produced is due to high amount of furfural, formic acid and acetic acid that is considered as waste then after its directed to the anaerobic digester for CH_4 production. On the other hand, the 1G2G SA complex required 22% which increased from10% for the 2G scenario signifying that integration of 1G and 2G for SA has an impact on the bagasse supply.

There is an evident economy of scale benefit through the integration of 1G and 2G feedstock. Which yield better economic performance results in comparison to 2G only scenarios. However, other factors such as smaller CHP plant capacity for 1G2G GA process in

comparison to 2G GA process (165 t/h vs 177 t/h) in GA scenarios, sharing of the downstream processing technologies in 1G2G LA and 1G2G SA scenarios contribute to the overall effect on the improved economic performances.

Diverting xylose for xylitol production instead of; being directed to anaerobic digestion for biogas production in 2G GA scenario and utilised for fermentation in 2G SA scenario resulted in a significant increase in bypass ratio for both scenarios. GA scenarios increased from 0% s to 48%bypas ratio, while SA increased from 22% to 50% bypass ratio. Not only because there was a significant reduction in the amount of biogas sent to the CHP, but also integrated xylitol production unit is energy intensive. In comparison, LA production's chemical process remained at a 0% bypass ratio even after reconfiguration for xylitol production. This is due to the configuration followed to produce LA from 1G and xylitol from 2G, thereby resulting in large amount of solid resides available for utilisation in CHP (68.1 t/h).

4. **To compare the economic viability of different for configurations of newly built 1G scenarios, updated 1G, and 2G, 1G2G and 1G2G multi-product facilities**

The major profitability indicators that were looked at, in this study for comparisons of different scenarios are internal rate of return (IRR), net present value (NPV), and minimum selling price (MSP). Overall, the 1G biorefineries showed better economic viability compared to their other configurations' counterparts. Unlike configurations processing 2G feedstock, in 1G biorefineries benefits from the elimination of cost-intensive processing units such as high-pressure boiler, pretreatment, and enzymatic hydrolysis.

On the other hand, there is an evident economy of scale benefits through the integration of 1G and 2G feedstocks. This is demonstrated by an increase in IRR and a decrease in MSP. The biochemicals; SA and LA are both platform chemicals for BDO, obtaining lower selling prices compared to commodity chemical, which would justify overproduction as it would force the new market to open. However, overproduction scenarios for SA and LA did not obtain MPS below $1500/t for the potential replacement of maleic anhydride, which serves as raw material for 1,4-butanediol (BDO) production.

Comparatively, the economic performance of multiproduct facility of 1G2G GA (MSP of $1926/t) was better than the sole product counterpart ($2205/t). In contrast, the economic performance of a multiproduct facility for SA was worse (MSP of %1888/t) than the sole product counterpart ($1745/t). Despite both scenarios having a substantial increase in bypass ratio from the sole product 1G2G complex to multiproduct 1G2G complex. Similarly, the 1G2G LA scenario’s MSP improved from $2600/t to $1133/t.

. Table 43 summarises the profitability indicators of different configurations.

Table 43: Summary of profitability indicator

Scenarios		Indicators		
		IRR (%)	MSP ($/t)	NPV (M$)
1G	GA	59.8	1687	318.0
	LA	31.8	2102	73.7
	SA	58.3	1220	309.7
2G	GA	25.3	2969	66.6
	LA	18.1	2950	-38.1
	SA	23.1	2237	85.0
1G2G	GA	36.4	2205	548.4
	LA	21.3	2600	31.4
	SA	32.8	1745	407.0
MP	GA	35.1	1926	461.6
	LA	27.6	2851*	184.2
	SA	26.4	1888	179.9

*Xylitol MSP

In summary, it is therefore clear that the option to diversify sugar mills' products by penetrating markets offered by products interest is an attractive investment as shown by the economic performances. Nonetheless, the scenario with the best economic performances is 1G GA, with IRR of 59.8% and MSP of $1687/t that is nearly 50% lower than the market price ($3600/t). Followed by 1G SA at IRR of 58.3% and MSP of $1220/t. Similar priority can also be observed in 2G and 1G2G configuration. Also, for a more diversified product range, the multi-production of GA with xylitol can be considered because there are no issues with market size penetration.

5.2 Recommendations for future work

This study provided insight on the economic viability standpoint of different biorefinery configurations producing different biochemicals of considerably good market opportunities. Some of the developed designs were based on novel technologies and experimental literature data. Although, most scenarios were economically viable. It is worth noting that the process is only as good as its assumptions. Therefore, further sensitivity analyses studies on processes' major operation units such as reaction systems and fermentations specifically for the newly developed 1G configurations could provide insight in quantifying the certainty associated with assumptions around these units because sugar substrate utilisation, is considered as one of the major influencers on the profitability of scenarios.

The techno-economic evaluation alone does not fully justify the sustainability and competitiveness of the proposed biorefineries in the eyes of investors or decision-makers. A

study on the Life cycle assessment considering the environmental and social impact of biorefineries could be further investigated.

With integrated 1G2G scenario showing a slight increase in steam demands by 7.2 t/h. This scenario could be investigated using a low-pressure boiler installation and determining the economic outcome of such. Furthermore, a study by Jin et al. (2020). has paved the way for utilising xylose and glucose as co-fermentation substrates for glutamic acid production. Such a configuration could be further investigated using a low-pressure boiler.

There are several novel configurations reported in literature for the production of LA. This includes an alcoholysis of hexose sugar to form alcohol-ester that can be subsequently hydrolysed to form LA reaction pathway and different downstream processing configurations. However, the economic viability of these configurations has not been assessed in a greater detail in literature. Future studies could assess these configurations to establish the most economical one for implementation with relevance to the South African sugar industry.

Through this study, it was evident that the employment of MIBK as an extraction solvent in LA biorefineries is also a significant contributor to the operating costs of the processes. Therefore, it is recommended that configurations using low-cost extraction solvent such as furfural should be investigated. Eventually, decreasing the cost of production will improve the economics of such biorefineries.

Since in this study, flowsheet design aimed at reducing process complexities by employing less processing steps while ensuring maximum substrate utilisation. Future studies could look at the possibility of combining hexose sugars from hydrolysed molasses and bagasse for LA production. Because LA production from pure hexose (glucose) sugars has comparable yield with Biofine process. Furthermore, experiments could be done to evaluate the effects of yield for direct combination of bagasse and molasses for LA production.

The design for the combination of sugar streams in the 1G2G SA+xylitol configuration for co-fermentation of 1G and 2G substrates was purely based on the assumption that changes on the sugar proportion as a result of combining glucose stream with molasses for fermentation using *E.coli* strain still holds as to those of using molasses. Therefore, future experimental work is recommended to verify the impact of sugar proportion changes (ratio of sucrose, glucose and fructose) on *E.coli KJ122* engineered for sucrose utilisation.

The economic production of obtaining pure, rich xylose hydrolysate and hydrogenation processes are the major bottlenecks for chemical routes production of xylitol. The current

research has been focused on the fermentative production of xylitol with improved yields. Further studies could investigate the techno-economic assessment of sugarcane valorisation into xylitol using fermentative pathways since the chemical route has an associated high cost of production. Ultimately, the goal is to have better viability to ensure sustainable xylitol production to fulfil the ever-growing sugar alcohol market demands.

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7 Appendices

Appendix A : Components

Table 44: Components

Component	Chemical formula	Properties used
Water	H_2O	Aspen databank
Sucrose	$C_{12}H_{22}O_{11}$	Aspen databank
Glucose	$C_6H_{12}O_6$	Aspen databank
Fructose	$C_6H_{12}O_6$	Aspen databank
Glutamic acid	$C_5H_9NO_4$	Aspen databank
Levulinic acid	$C_5H_8O_3$	Aspen databank
Succinic acid	$C_4H_6O_4$	Aspen databank
Xylitol	$C_5H_{12}O_5$	Aspen databank
Cellobiose	$C_{12}H_{22}O_{11}$	Aspen databank
Arabinose	$C_5H_{10}O_5$	NREL databank
Xylose	$C_5H_{10}O_5$	NREL databank
Glucolig	$C_6H_{12}O_6$	NREL databank
Solubilised lignin	$C_8H_8O_3$	NREL databank
Arabolig	$C_5H_{10}O_5$	NREL databank
Xylolig	$C_5H_{10}O_5$	NREL databank
HMF	$C_6H_6O_3$	Aspen databank
Furfural	$C_5H_4O_2$	Aspen databank
Acetic acid	$C_2H_4O_2$	Aspen databank
Formic acid	CH_2O_2	Aspen databank
Arabitol	$C_5H_{12}O_5$	Aspen databank with specified SV
Ammonia	NH_3	Aspen databank
Sulfuric acid	H_2SO_4	Aspen databank
Urea	CH_4N_2O	Aspen databank
DAP	$(NH_4)_2SO_4$	Aspen databank
Sodium hydroxide	NAOH	Aspen databank
Oxygen	O_2	Aspen databank
Nitrogen	N_2	Aspen databank
Carbon dioxide	CO_2	Aspen databank
Methane	CH_4	Aspen databank
Hydrogen	H_2	Aspen databank
MIBK	$C_6H_{12}O$	Aspen databank
Octanol	$C_8H_{18}O$	Aspen databank
TOA	$C_{24}H_{51}N$	Aspen databank
TMA	C_3H_9N	Aspen databank
Sodium-bicarbonate	$NAHCO_3$	Aspen databank
Magnesium sulphate	$MgSO_4$	Aspen databank
Cellulose	$C_6H_{10}O_5$	NREL databank
Glucan	$C_6H_{10}O_5$	Estimated as dilactic acid
Xylan	$C_5H_8O_4$	NREL databank
Arabinan	$C_5H_8O_4$	NREL databank
Lignin	$C_8H_8O_3$	NREL databank
Acetate	$C_2H_4O_2$	NREL databank
Ash	CaO	NREL databank
Enzyme		NREL databank
Biomass (also used as a C.glutamicum strain)	$C_5H_7O_2N$	Properties estimated as glutaric acid
E-coli	$CH_{1.77}O_{0.49}N_{0.24}$	NREL databank
Tar/ humins	$C_{18}H_{20}O_{10}$	Properties estimated as xylose [a]
Lime	$CA(OH)_2$	NREL databank

Component	Chemical formula	Properties used
Calcium Sulphate	$CASO_4$	NREL databank
Carbon	C	NREL databank

Appendix B : Aspen Screen shots

Through this section the screen shots of the main areas are provided. The considered mains areas are production areas (fermentation and reaction) and product recovery and purification (downstream processing).

- 1G GA (Figure 37)
- 2G GA (Figure 38)
- 1G2G (Figure 37+Figure 38 = figure X)
- 1G2G GA multiproduct (figure X +Figure 39)
- 1G LA (Figure 41)
- 2G LA (Figure 41)
- 1G2G LA (Figure 41+Figure 41)
- 1G2G GA multiproduct (Figure 41+Figure 39)
- 1G SA (Figure 42+Figure 43)
- 2G SA (same as 1G SA=figure Y)
- 1G2G SA (Figure 42+ figure Y +Figure 43)
- 1G2G SA multiproduct (Figure 42+ figure Y +Figure 43+Figure 39)

Appendix B.A. : Glutamic acid process flow diagrams

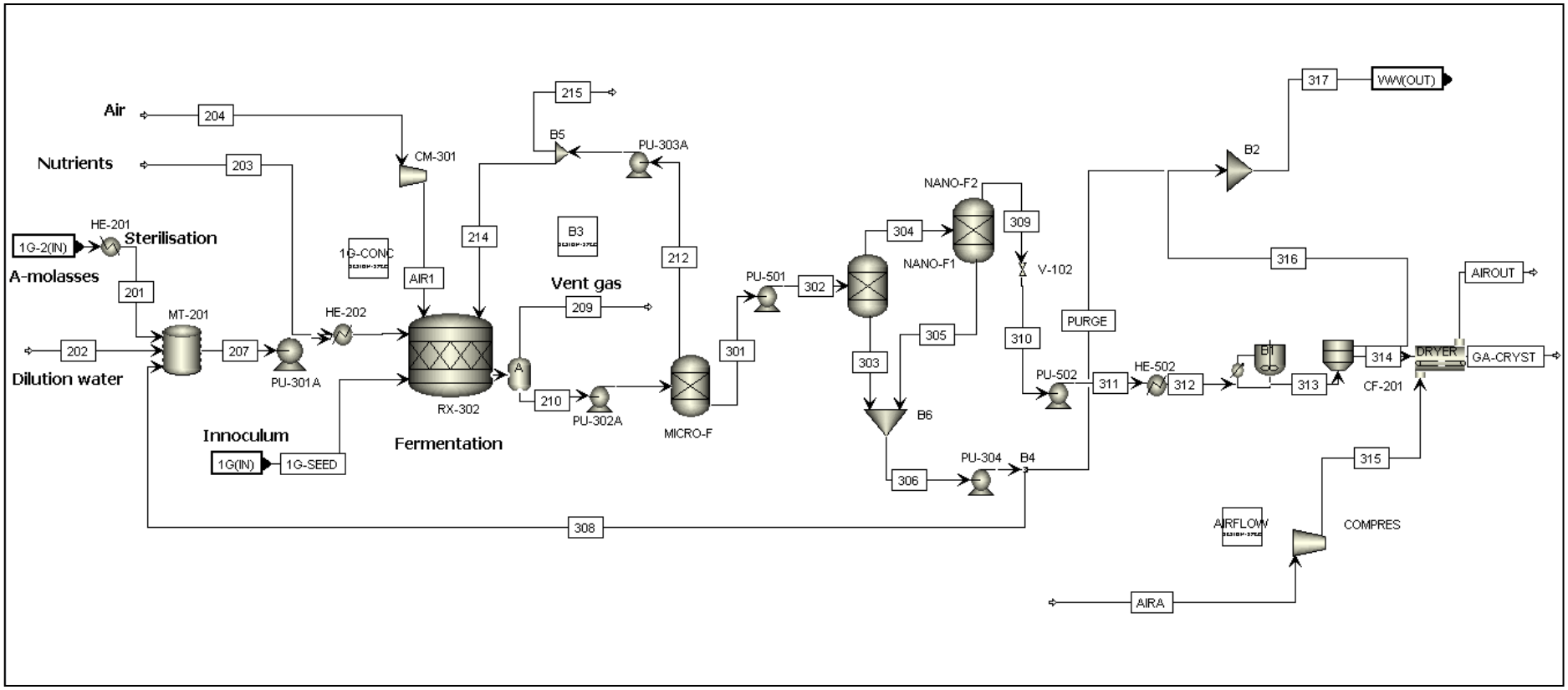


Figure 38: 1G GA fermentation +Product recovery Aspen screenshot

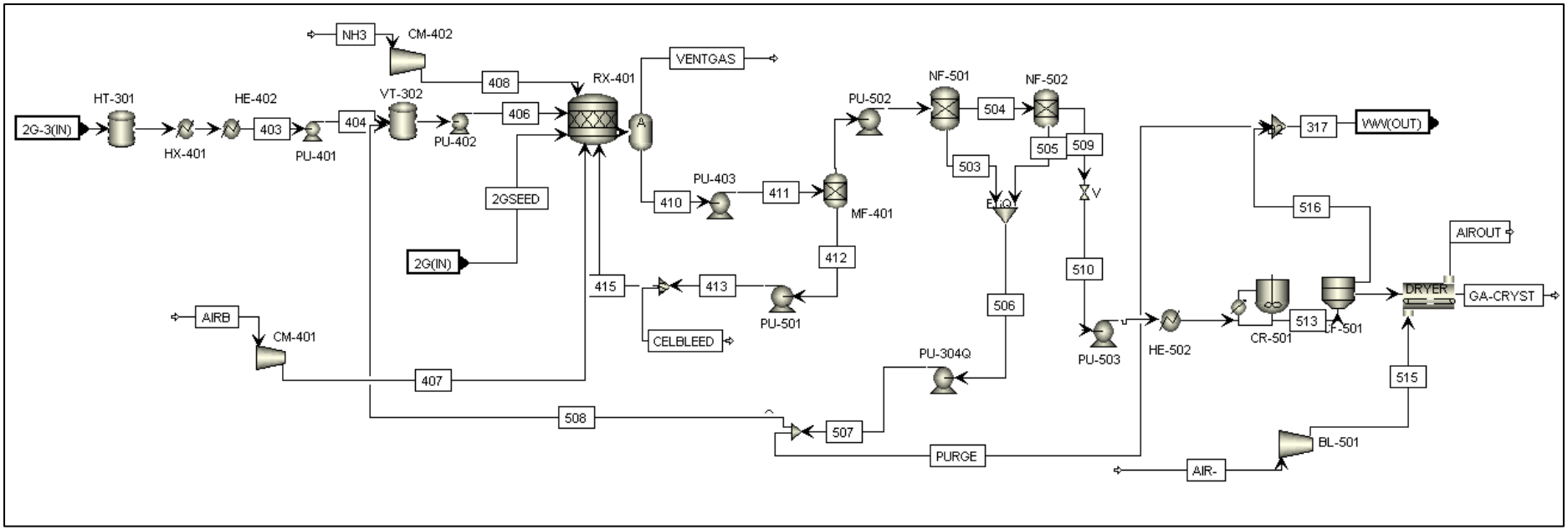


Figure 39: 2G GA fermentation +Product recovery Aspen screenshot

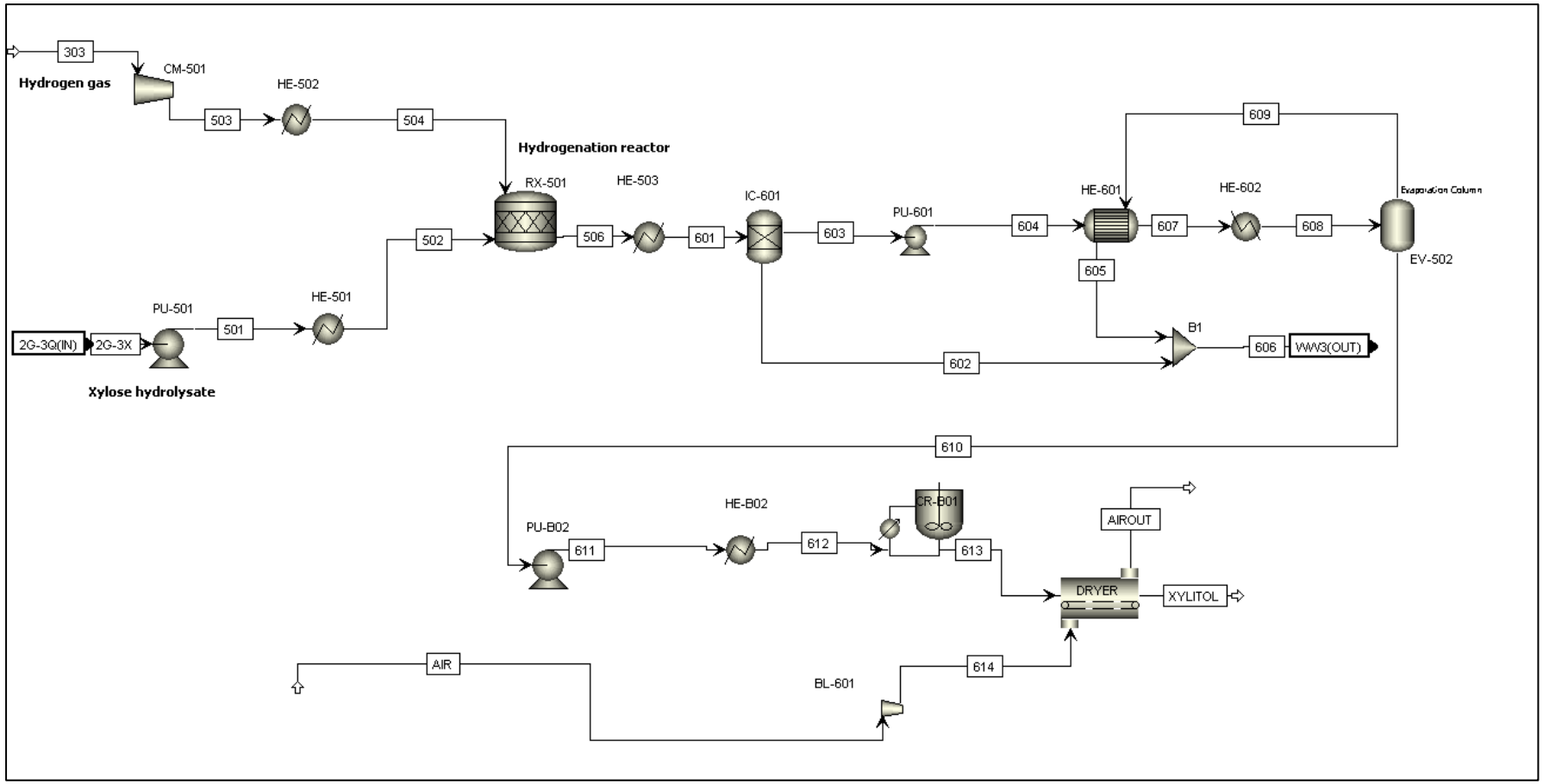


Figure 40: 1G2G Xylitol production + Recovery Aspen screenshot

Appendix B.B. : Levulinic acid process flow diagrams

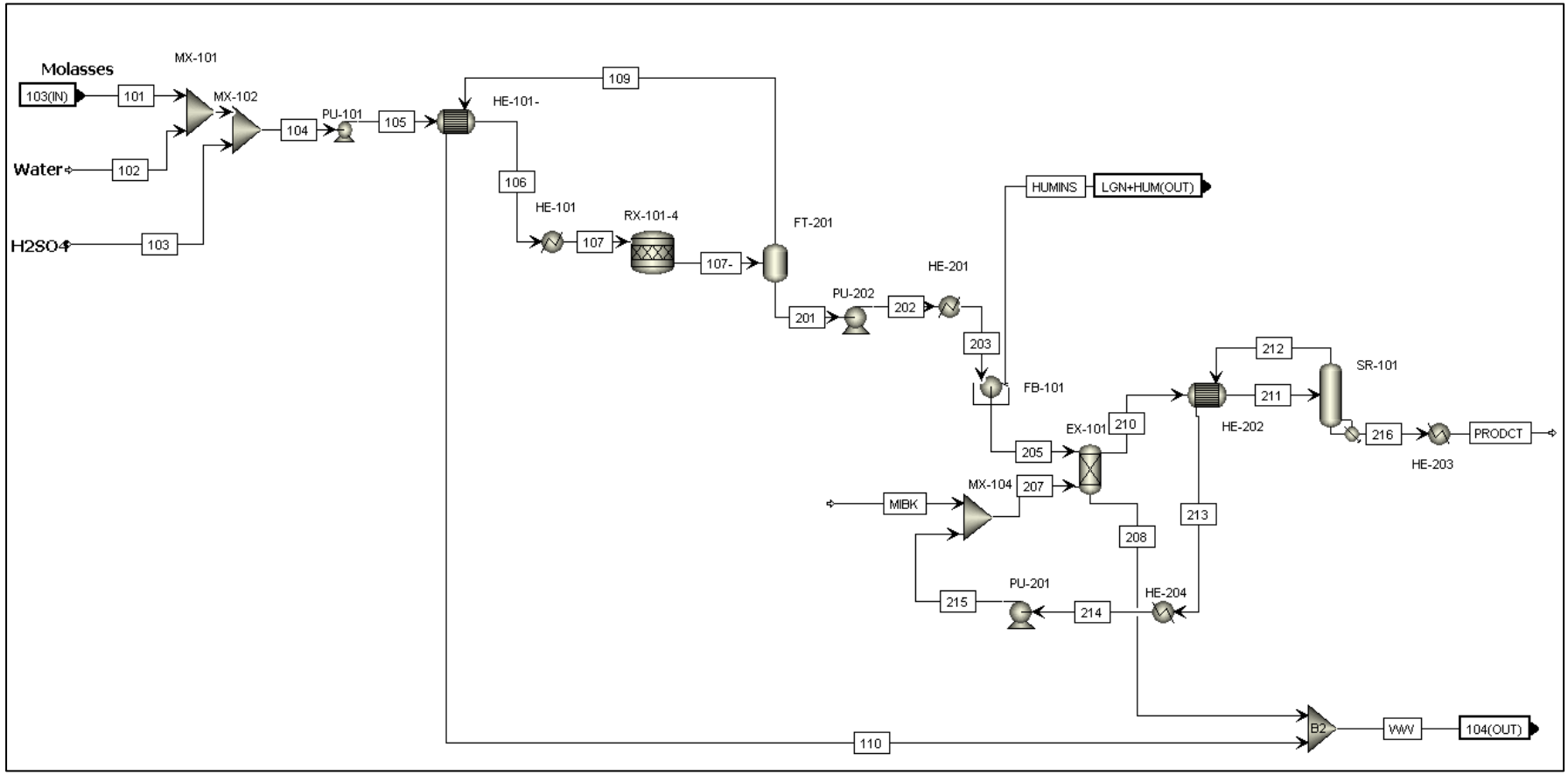


Figure 41: 1G LA Reaction +Product recovery Aspen screenshot

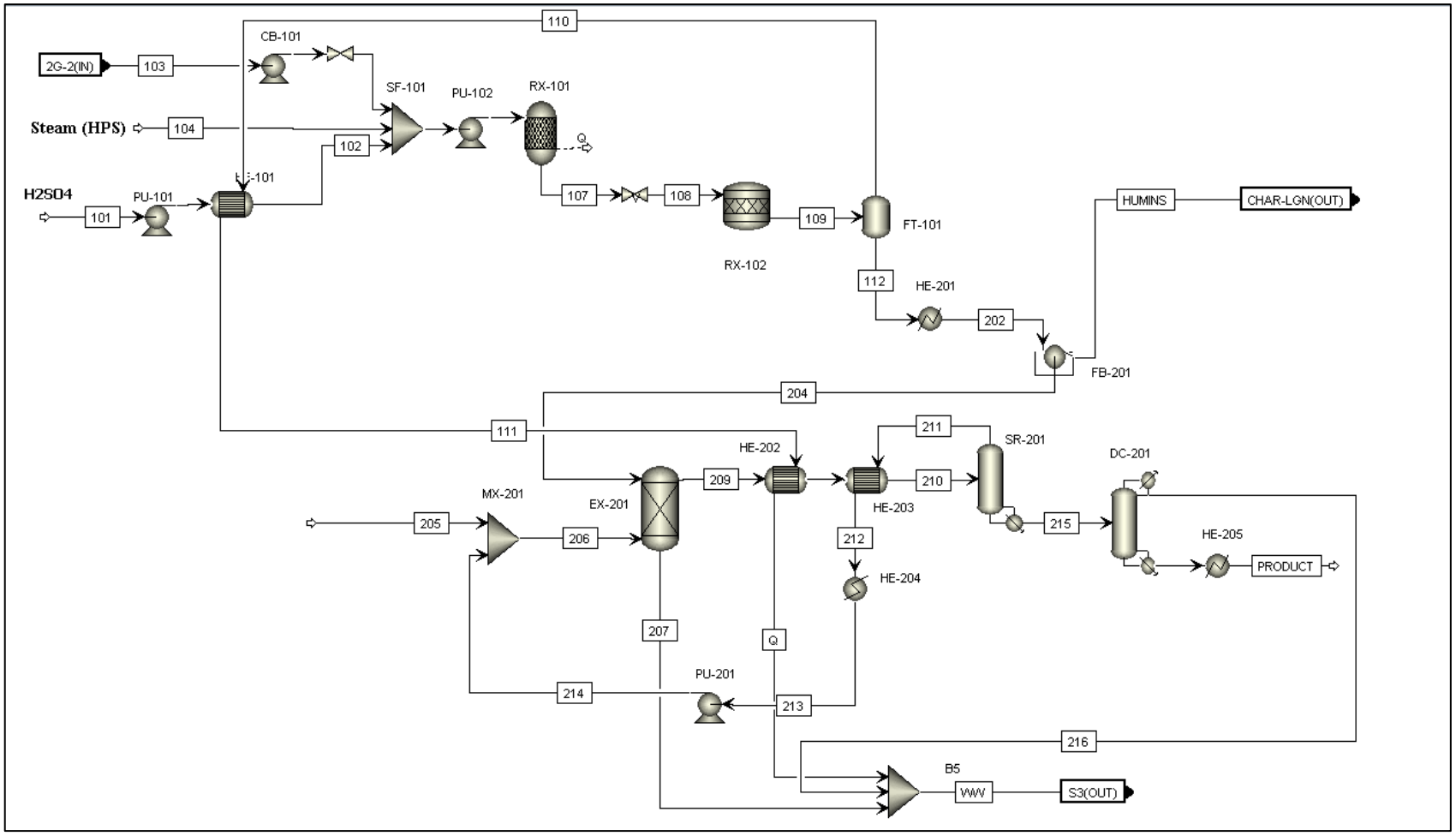


Figure 42: 2G LA Reaction +Product recovery Aspen screenshot

Appendix B.C. : Succinic acid process flow diagrams

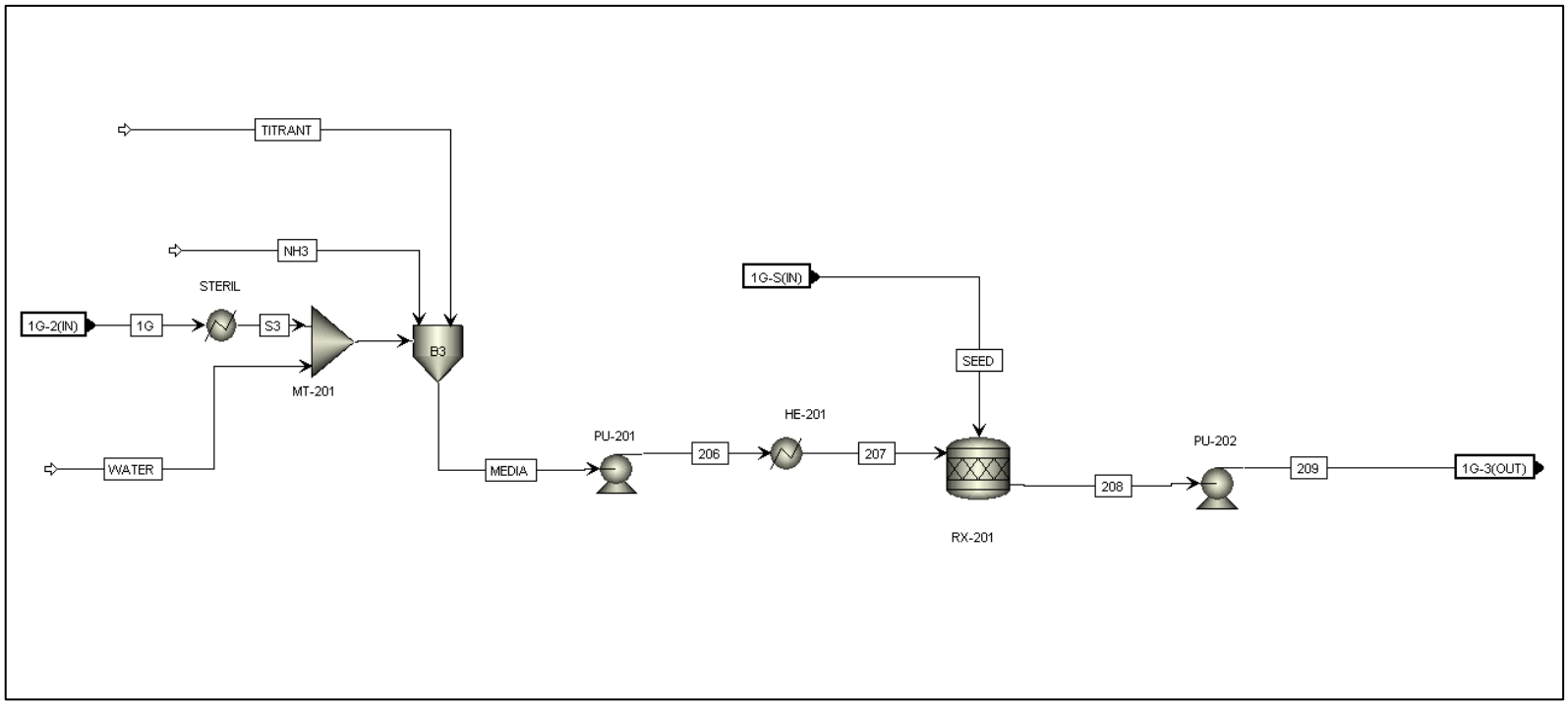


Figure 43: 1G SA fermentation

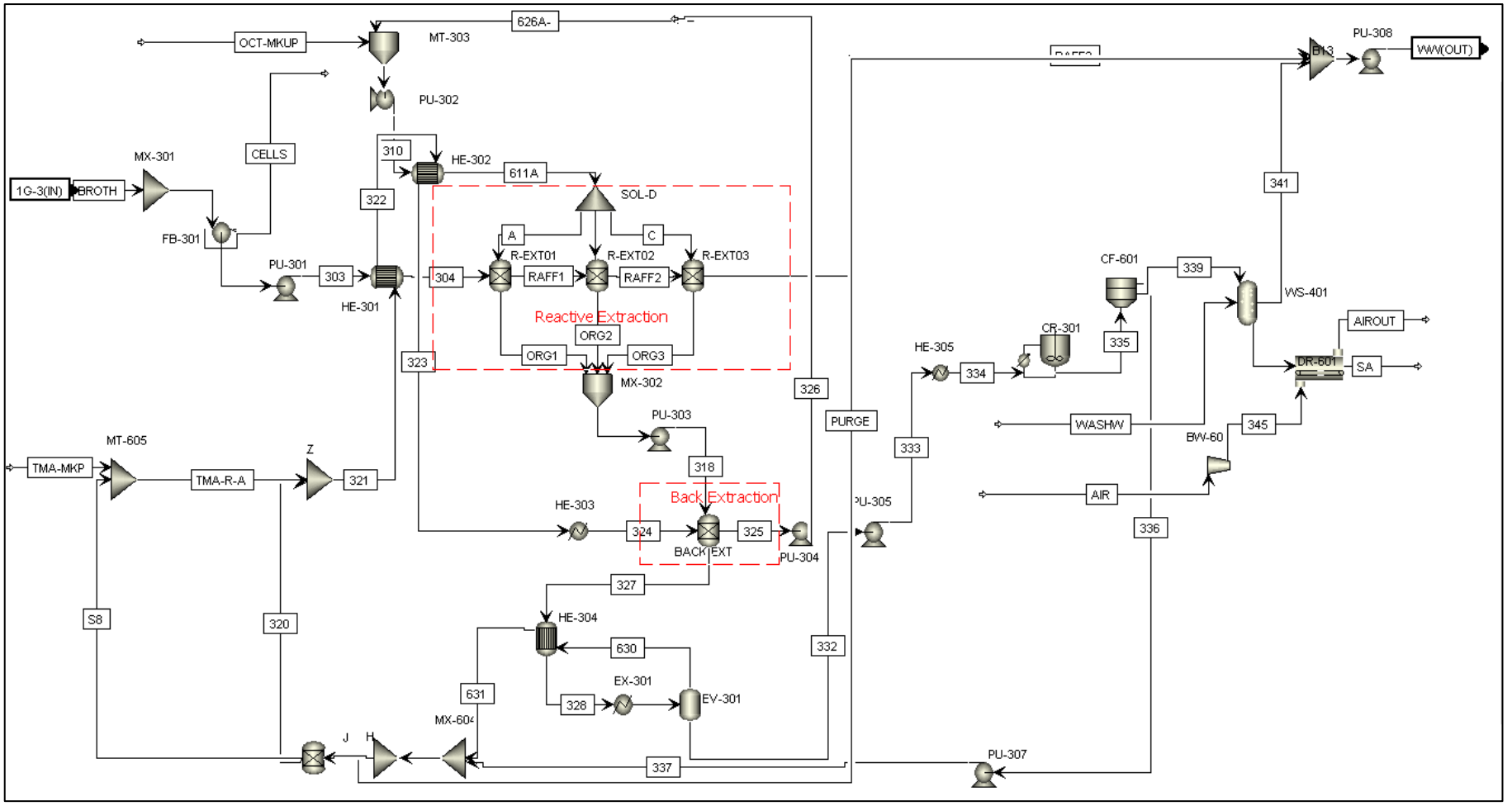
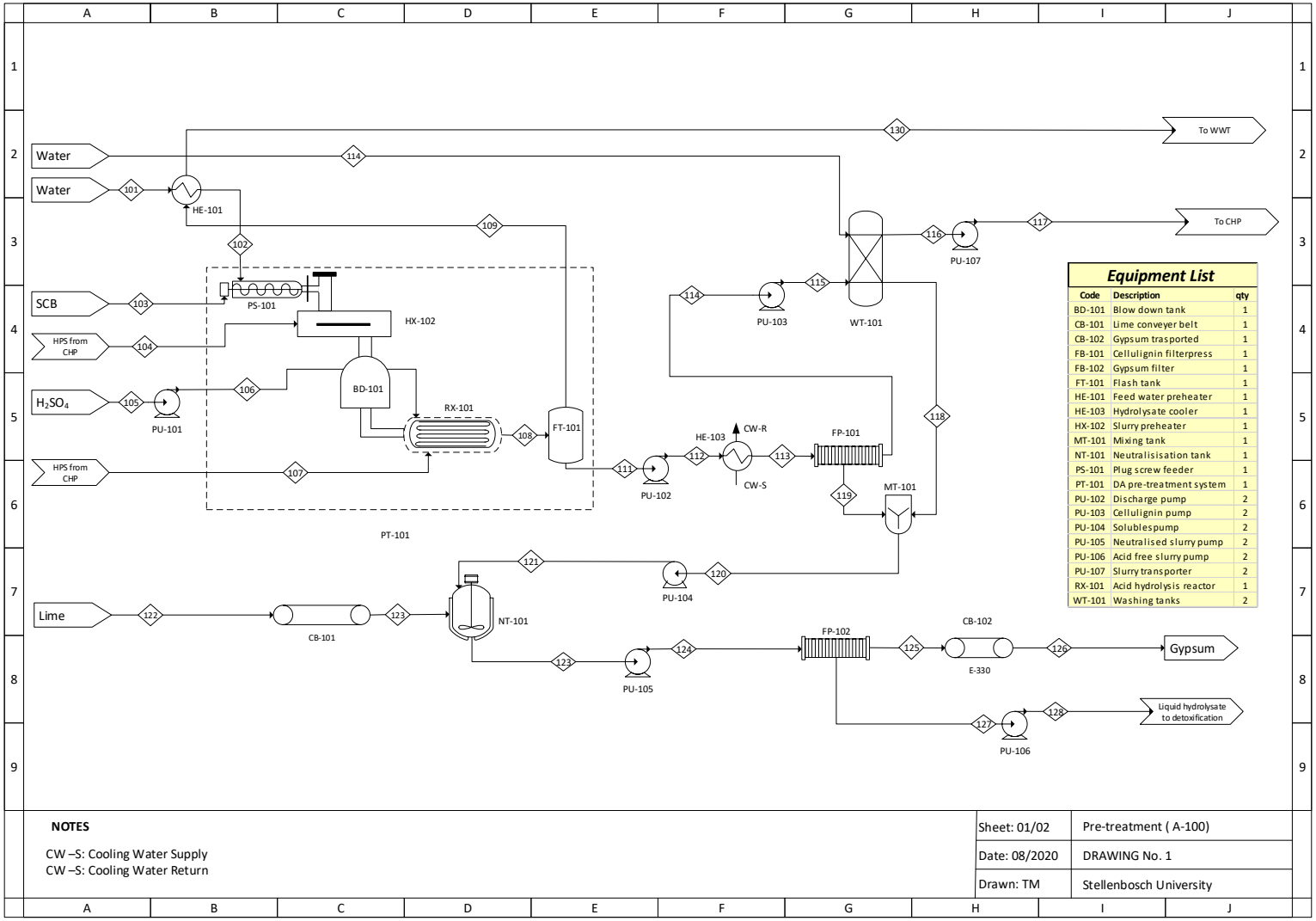


Figure 44: Downstream processing for succinic acid

Appendix C : Process flow diagrams



Equipment List

Code	Description	qty
BD-101	Blow down tank	1
CB-101	Lime conveyer belt	1
CB-102	Gypsum trasported	1
FB-101	Cellulignin filterpress	1
FB-102	Gypsum filter	1
FT-101	Flash tank	1
HE-101	Feed water preheater	1
HE-103	Hydrolysate cooler	1
HX-102	Slurry preheater	1
MT-101	Mixing tank	1
NT-101	Neutralisisation tank	1
PS-101	Plug screw feeder	1
PT-101	DA pre-treatment system	1
PU-102	Discharge pump	2
PU-103	Cellulignin pump	2
PU-104	Solublespump	2
PU-105	Neutralised slurry pump	2
PU-106	Acid free slurry pump	2
PU-107	Slurry transporter	2
RX-101	Acid hydrolysis reactor	1
WT-101	Washing tanks	2

Figure 45: Detailed Pretreatment PFD

Appendix D Economic analysis information

Appendix D.A. : US Gulf Coast basis exponents for cost estimations

Table 45: CEPCI Purchased Equipment Cost (Ce) Constants, Ce = a + bSn (US Gulf Coast basis, Jan 2007, CEPCI = 509.7) (Sinnott et al., 2005)

Equipment	Units for Size, S	S_{lower}	S_{upper}	a	b	n
Agitators and Mixers						
Propellor	driver power, kW	5	75	15000	990	1.05
Spiral ribbon mixer	driver power, kW	5	35	27000	110	2
Static Mixer	Litres/s	1	50	500	1030	0.4
Compressors						
Blower	m3/h	200	5000	3800	49	0.8
Centrifugal	driver power, kW	75	30000	490000	16800	0.6
Reciprocating	driver power, kW	93	16800	220000	2300	0.75
Conveyers						
Belt, 0.5 m wide	length, m	10	500	36000	640	1
Belt, 1.0 m wide	length, m	10	500	40000	1160	1
Crystallizers						
Scraped surface crystallizer	length, m	7	280	8400	11300	0.8
Dryers						
Direct contact rotary	area, m2	11	180	13000	9100	0.9
Spray dryer	evap rate kg/h	400	4000	350000	1900	0.7
Evaporators						
Vertical tube	area, m2	11	640	280	30500	0.55
Agitated falling film	area, m2	0.5	12	75000	56000	0.75
Exchangers						
U-tube shell and tube	area, m2	10	1000	24000	46	1.2
Double pipe	area, m2	1	80	1600	2100	1
Thermosyphon reboiler	area, m2	10	500	26000	104	1.1
U-tube kettle reboiler	area, m2	10	500	25000	340	0.9
Plate and frame	area, m2	1	500	1350	180	0.95
Filters						
Plate and frame	capacity, m3	0.4	1.4	110000	77000	0.5
Vacuum drum	area, m2	10	180	-63000	80000	0.3
Pressure vessels						
Vertical, 304 ss	shell mass, kg	120	250000	15000	68	0.85
Horizontal, 304 ss	shell mass, kg	120	50000	11000	63	0.85
Pumps and drivers						
Single-stage centrifugal	flow, L/s	0.2	126	6900	206	0.9
Explosion proof motor	power, kW	1	2500	-950	1770	0.6
Condensing steam turbine	power, kW	100	20000	-12000	1630	0.75
Reactors						
Jacketed, agitated	volume, m3	0.5	1000	53000	28000	0.8
Jacketed, agitated, glass lined	volume, m3	0.5	25	11000	76000	0.4
Tanks						

Equipment	Units for Size, S	S_{lower}	S_{upper}	a	b	n
Floating roof	capacity, m3	100	10000	97000	2800	0.65
Cone roof	capacity, m3	10	4000	5000	1400	0.7

Appendix D.B. : Scaling Exponents

Table 46: Scaling factors(Gorgens et al., 2016)

Equipment	*n* Exponents
Agitators	0.5
Compressors	0.6
Distillation columns	0.6
Heat exchangers	0.7
mixers	0.5
Pressure vessels	0.7
Pumps	0.8
Tanks	0.7
Solids handling equipment	0.8

Appendix D.C. : Installation factors

Table 47: Installation factors (Gorgens et al., 2016)

Equipment	Multiplier
Agitators, carbon steel	1.6
Agitators, stainless steel	1.5
Boiler	1.8
Compressors, motor driven	1.6
Cooling Tower	1.5
Distillation columns, stainless steel	2.4
Heat exchangers, shell & tube, SS	2.2
Heat exchangers, plate & frame, SS	1.8
Heat exchangers, plate & frame, air cooled	2.8
Inline mixers	1
Skidded equipment	1.8
Solids handling equipment (incl. filters)	1.7
Pressure vessels, carbon steel	3.1
Pressure vessels, SS	2
Pretreatment reactor system	1.5
Pumps, SS	2.3
Pumps, carbon steel	3.1
Tanks, field-erected, carbon steel	1.7
Tanks, field-erected, SS	1.5
Tanks, storage, plastic	3
Tanks, storage, carbon steel	2.6
Tanks, storage, SS	1.8
Turbogenerator	1.8

Appendix D.D. : Other Capital cost estimation data

Table 48: Major equipment cost estimation

Equipment	**Sizing and costing comment**	**Installation factor**	**References**
Fermenters (biological reactors)	Sized based on 950m^3 Assumed 12 hours cleaning times Costed based on 950m^3 tanks as per hum bird	1.8	Humbird et al., 2011
Membranes	Sized with the permeate flow rate and average flux, Costing based on the resultant	1.7	Woods, 2007
Distillation columns	Costing based on distillation column design and heuristics	2.5	Sinnott et al., 2005
Extraction Columns	Costing based on distillation column design and heuristics and costs provided	3.1	Korchinsky et al., 1982 & Rocha et al., 1989
Crystallisers	Costing based on US gulf coast basis (2014) cost corelations	2.5	McNulty et al., 2014
Reactors	Sized for volume (m^3) and costing based on the US Gulf Coast basis (2007) Jacketed, agitated reactor	2	Turton et al., 2012
Chromatography columns	Sized for shell mass and costed as a vessel based on the US Gulf Coast basis (2007)	2	Turton et al., 2012
Flash tanks	Sized for shell mass and costed as a pressure vessel based on the US Gulf Coast basis (2007)	2	Turton et al., 2012

Table 49: Other Capital cost estimations

EQ. no	Equipment Description	Base scale	Units	Year of Quote	Bare cost	Scaling factor	Installation factor	References
A-100: Pretreatment								
FH-101	Feed hooper	94697	kg/hr	2009	$ 251 000	0.6	1.7	[1]
LH-101	Lime hooper	94697	kg/hr	2009	$ 251 000	0.6	1.7	[1]
DD-101	Dust collector	94697	kg/hr DM	2009	$ 46 650	0.6	1.7	[1]
RX-101	DA reactor System	83333	kg/hr DM	2009	$ 19 812 400	0.6	1.5	[1]
FT-101	Filter press	31815	kg/hr	2010	$ 1 647 350	0.8	1.7	[1]
NT-101	Naturalisation tank	31815	kg/hr	1997	$ 71 000	0.7	1.4	[2]
A-300: Seed train+ Enzyme production								
AG-301	4th Seed Vessel Agitator	5.5	kW	2009	$ 26 000	0.5	1.5	[1]
AG-302	5th Seed Vessel Agitator	7.3	kW	2009	$ 43 000	0.5	1.5	[1]
AG-303	Seed Hold Tank Agitator	11	kW	2009	$ 31 800	0.5	1.5	[1]
ST-101A	Seed tank 1	0.075	m^3	2009	$ 37 700	0.7	1.8	[1]
ST-101B	Seed tank 2	0.75	m^3	2009	$ 58 300	0.7	1.8	[1]
ST-101C	Seed tank 3	7.5	m^3	2009	$ 78 800	0.7	1.8	[1]
ST-101D	Seed tank 4	75	m^3	2009	$ 176 000	0.7	1.8	[1]
ST-101D	Seed tank 5	750	m^3	2009	$ 590 000	0.7	1.8	[1]
EN-300e	Enzyme production plant	620	kg/hr	2009	$ 10 889 085	0.6	1.7	[1]
A-700: Wastewater Treatment								
EV-701	Evaporation system	382170	kg/hr	2009	$ 3 726 657	0.6	1	[1]
RO-701	Reverse Osmosis system	382170	kg/hr	2009	$ 2 167 681	0.6	1	[1]
MR-701	Membrane reactor	382170	kg/hr	2009	$ 5 145 962	0.6	1	[1]
RX-701	Anaerobic aeration	382170	kg/hr	2009	$ 2 647 125	0.6	1	[1]

EQ. no	Equipment Description	Base scale	Units	Year of Quote	Bare cost	Scaling factor	Installation factor	References
RX-702	Anaerobic basin	382170	kg/hr	2009	$ 21 471 250	0.6	1	[1]
HE-701	Aerobic digester blower	382170	kg/hr	2009	$ 1 895 881	0.6	1	[1]
PU-701	Aerobic sludge screwer	382170	kg/hr	2009	$ 24 510	0.6	1	[1]
PU-702	Feed cooler Anaerobic	382170	kg/hr	2009	$ 82 221	0.6	1	[1]
BF-701	Biogas flare	382170	kg/hr	2009	$ 32 310	0.6	1	[1]
CF-701	WW feed pump Anaerobic	382170	kg/hr	2009	$ 226 955	0.6	1	[1]
CF-702	Waster Anaerobic pump	382170	kg/hr	2009	$ 91 473	0.6	1	[1]
PU-703	Aeration basin pump	382170	kg/hr	2009	$ 82 355	0.6	1	[1]
PU-704	Return act. sludge pump	382170	kg/hr	2009	$ 173 828	0.6	1	[1]
PU-705	Centrifuge feed pump	382170	kg/hr	2009	$ 60 001	0.6	1	[1]
PU-706	Centrate pump	382170	kg/hr	2009	$ 69 413	0.6	1	[1]
CF-701	Centrifuge	382170	kg/hr	2009	$ 6 366 336	0.6	1	[1]
A-700: CHP								
CHP	Boiler (High pressure)	234813	kg/hr	2009	$ 26 967 416	0.6	1.8	[1]
CHP	Boiler (Low pressure)	45000	kg/hr	2018	$ 4 906 376	0.6	1.8	[3]
CHP	Turbines	41334	kW	2009	$ 8 949 886	0.6	1.8	[1]
CHP	Deaerator	234812	kg/hr	2009	$ 290 201	0.6	1.8	[1]
CHP	Hot water Softener	234813	kg/hr	2009	$ 74 215	0.6	1.8	[1]
MAJOR EQUIPMENT								
Rx-xxx	Biological reactors (fermenters)	3500	m^3	2009	$ 844 000	0.6	2	[1]
NF/MF-xxx	Ultra-filters		m^2					
List of common equipment whose cost was estimated based on heuristics and literature corelations								
CV-X01	Conveyer belt		m^2	2007			1.7	[4]

EQ. no	Equipment Description	Base scale	Units	Year of Quote	Bare cost	Scaling factor	Installation factor	References
PU-xxx	Pump		m^3/h	2007			2.2	[4]
BL-xxx	Blower		m^3/h	2007			2.3	[4]
CM-xxx	Compressor		m3 /h	2007			2.3	[4]
HE-xxx	Heat exchangers		m2	2007			2.2	[4]
CF-xxx	Belt filter		kg/hr	2007			1.5	[4]
DR-xxx	Dryers		kg/hr	2007			1.5	[4]

[1] Humbird et al., 2011

[2] Aden et al., 2002

[3] Quote from Dogbe et al., 2018

[4] Sinnott et al., 2005

Appendix D.E. : Consumables prices

Table 50: Consumables prices

Components	Price ($/ton)	Scenarios								References
		1G GA	1G LA	1G2G GA	1G2G LA	1G2G SA	1G2G GA+ Xylitol	1G2G SA+ Xylitol	1G2G LA + Xylitol	
A Molasses	$138	✓	✓	✓	✓	✓	✓	✓	✓	Dogbe et al., 2020
Bagasse	$74				✓	✓	✓	✓	✓	Dogbe et al., 2020
Activated carbon	$600					✓	✓	✓	✓	Özüdoğru et al., 2019
Agar Slant	$6 500	✓				✓	✓	✓		Alibaba
AM1	$4200					✓		✓		Chan et al., 2016
Ammonia	$335	✓	✓	✓	✓	✓	✓	✓	✓	Özüdoğru et al., 2019
Biotin	$400 000	✓		✓			✓			Özüdoğru et al., 2019
Chromatography resin SAC	$0.10						✓	✓	✓	Özüdoğru et al., 2019
Chromatography resin WBA	$0.10						✓	✓	✓	Özüdoğru et al., 2019
$FeSO_4*7H_2O$	$95	✓		✓		✓	✓	✓		Özüdoğru et al., 2019
Glucose	$400			✓		✓	✓	✓		Alibaba
H_2 gas	$ 6 500						✓	✓	✓	Özüdoğru et al., 2019
H_2SO_4	$ 112		✓	✓	✓	✓	✓	✓	✓	Özüdoğru et al., 2019
K_2HPO_4	$ 185	✓		✓			✓			Nieder-Heitmann et al., 2019
KH_3CO_3	$ 95					✓		✓		Özüdoğru et al., 2019
Lime	$75			✓		✓	✓	✓		Özüdoğru et al., 2019
$MgSO_4*H_2O$	$ 95									Özüdoğru et al., 2019
MIBK	$2 085		✓		✓				✓	Alibaba
$MnSO_4*H_2O$	$ 450			✓			✓			Özüdoğru et al., 2019
$NaHCO_3$	$ 200					✓		✓		Nieder-Heitmann et al., 2019
Octanol	$ 1 015					✓		✓		Nieder-Heitmann et al., 2019
Oleic acid	$ 2 000	✓		✓			✓			Özüdoğru et al., 2019
Raney Nickel	$18 500						✓	✓	✓	Özüdoğru et al., 2019
TMA	$3 000					✓		✓		Nieder-Heitmann et al., 2019
Tween	$1 800	✓		✓			✓			Özüdoğru et al., 2019
Urea	$242	✓		✓						Özüdoğru et al., 2019
Water	$ 0.00									Humbird et al., 2011
Yeast extract	$31 500	✓		✓			✓			Pal et al., 2015

Appendix E : Cost of Production

Appendix E.A. : Total cost of production GA scenarios

Table 51: Variable cost calculations for GA scenarios ($)

AREA	Consumables	GA scenarios ($)			
		1G GA	2G GA	1G2G GA	1G2G GA + Xylitol
Raw Materials	Sugar cost	16856597	-	16856597	16856597
	Bagasse and trash	-	24119612	24119612	24119612
	C-molasses	8093215	-	8093215	8093215
	Make-water	-	-	-	-
A-100&A-200	H2SO4	-	864080	864080	501760
	Lime	-	429750	429750	249000
	Chromatography resin SBA	-	-	-	76893
	Activated carbon	-			12084150
1G	Agar	10627500	-	10627500	10627500
A300	Urea	131890	-	131890	131890
	K2HPO4	0	-	-	-
	*MgSO4*H2O*	20710	-	20710	20710
	*FeSO4*7H2O*	10355	-	10355	10355
	*MnSO4*H2O*	245250	-	245250	245250
	Yeast extract	6771298	-	6771298	6771298
2G	Glucose	-	704665	704665	405517
	Ammonia	-	25125	25125	25125
	Urea	-	-	-	-
	K2HPO4	-	9865	9865	5677
	Yeast extract	-	13679756	13679756	7872357
A-300		-	3968000	3968000	2300400
A-400	Urea	4226712	-	4226712	4226712
	Biotin	2	-	2	2
	Tween 80	207972	-	207972	207972
	K2HPO4	1553250	-	1553250	1553250
	*MgSO4*H2O*	51775	-	51775	51775
	*FeSO4*7H2O*	2071	-	2071	2071
	*MnSO4*H2O*	4905	-	4905	4905
	thiamine HCl	3	-	3	3
	Amonia	-	4187500	4187500	4187500
	Biotin	-	3	2	2
	Tween 60	-	260550	256950	149940
	Oleic acid	-	2	2	4
	*MgSO4*H2O*	-	137513	135613	79135
	*FeSO4*7H2O*	-	825	814	475
	*MnSO4*H2O*	-	3908	3854	2249
A-500-700	Raney Nickel	-	-	-	15164339
	Chromatography resin WBA	-	-	-	36568
	H2 gas	-	-	-	3250000
Subtotals		48803504	48391157	97189093	119317007
	Ash and Gypsum Wastes Disposal				
	Ash	-	428353	428353	428353
	Waste Streams	-	927590	927590	484330
Subtotals		0	1355943	1355943	912683
Totals Variable Cost		48803504	49747101	98545036	120229690

Table 52: Fixed cost calculations for GA scenarios

Position	GA scenarios			
	1G GA	2G GA	1G2G GA	1G2G GA+ Xylitol
Plant Manager	168458	168458	168458	168458
Plant Engineer	160436	160436	160436	160436
Maintenance Supervisor	65320	65320	65320	65320
Maintenance Technician	275033	366711	366711	366711
Lab Manager	64174	64174	64174	64174
Lab Technician	91678	91678	91678	91678
Lab Tech-Enzyme	-	275033	275033	275033
Shift Supervisor	220027	220027	220027	220027
Shift Operators	458389	916777	916777	1145972
Shift Oper-Enzyme	-	275033	275033	275033
Yard Employees	96262	96262	96262	96262
Clerks & Secretaries	123765	123765	123765	123765
Total Staff Salaries	**1723541**	**2823674**	**2823674**	**3052868**
Labour burden (90%)	1551187	2541307	2541307	2747581
Total Labour cost	**3274728**	**5364980**	**5364980**	**5800450**
Maintenance	1527742	5214459	6655182	6787956
Property Insur. & Tax	963180	4044254	4767805	4744154
TOTAL FOC	**5765651**	**14623693**	**16787968**	**17332559**

Appendix E.B. : Total cost of production LA scenarios

Table 53: Variable cost calculations for LA scenarios ($)

AREA	Consumables	LA scenarios			
		1G LA	2G LA	1G2G LA	1G2G LA+Xylitol
Raw Materials	Sugar cost	16856597	-	16856597	16856597
	Baggase abd trash	-	24119612	24119612	24119612
	C-molasses	8093215		8093215	8093215
	Make-water	-	-	-	-
A-100&A-200	H2SO4		-	-	-
	Lime	-	-	-	128331
	Chromatography resin				
	SBA	-	-	-	19249575
	Activated carbon	-	-		142375
A300	H2SO4	459760	3120880	3295040	864080
	MIBK	11801100	17722500	44869200	11801100
	NH3	795387	795387	795387	142375
A-500-700	Raney Nickel	-	-	-	24736991
	Chromatography resin				
	WBA	-	-	-	86341
	H2 gas	-	-	-	6467500
Subtotals		**38006059**	**45758379**	**98029051**	**112953716**
Ash and Gypsum Wastes Disposal					
	Ash	83925	445977	428353	428353
	Waste Streams	487290	580900	557590	2407590
Subtotals		571215	1026877	985943	2835943
	Totals Variable Cost	**38577274**	**46785257**	**99014995**	**115789660**

Table 54 Fixed cost calculations for LA scenarios

Position	LA scenarios ($)			
	1G LA	2G LA	1G2G LA	1G2G LA+Xylitol
Plant Manager	168458	168458	168458	168458
Plant Engineer	160436	160436	160436	160436
Maintenance Supervisor	65320	65320	65320	65320
Maintenance Technician	275033	366711	366711	366711
Lab Manager	64174	64174	64174	64174
Lab Technician	91678	183355	183355	91678
Lab Tech-Enzyme	-	-	-	-
Shift Supervisor	110013	220027	220027	220027
Shift Operators	458389	916777	916777	1375166
Shift Oper-Enzyme	-	-	-	-
Yard Employees	96262	96262	96262	96262
Clerks & Secretaries	-	123765	123765	123765
Total Staff Salaries	**1489763**	**2365285**	**2365285.3**	**2731996.2**
Labour burden (90%)	1340787	2128757	2128757	2458797
Total Labour cost	**2830549.8**	**4494042**	**4494042.1**	**5190792.8**
Maintenance	806215	2841880	3440603	3169221
Property Insur. & Tax	791516	2845571	3293587	3159588
TOTAL FOC	**4428281**	**10181494**	**11228232**	**11519602**

Appendix E.C. : Total cost of production SA scenarios

Table 55: Variable cost calculations for SA scenarios ($)

AREA	Consumables	SA scenarios ($)			
		1G SA	2G SA	1G2G SA	1G2G SA+Xylitol
Raw Materials	Sugar cost	16856597	-	16854609	16856597
	Bagasse and trash	-	24119612	24119612	24119612
	C-molasses	8093215	-	8093215	8093215
	Make-water	-	-	-	-
A-100&A-200	H2SO4	-	710640	710640	436800
	Lime	-	352500	352500	217500
	Chromatography resin SBA	-	0	-	69750
	Activated carbon	-	10694865	10693607	8294865
1G	AM1	1230600	-	1230600	1292130
	Ammonia		-	125036	125036
2G	NaHCO3	-	-	-	-
A-300	Ammonia	-	164150	164150	-
	MgSO4*H2O	-	2375	2375	-
	K2HPO4	-	403750	403750	-
	Glucose	-	4992000	4992000	3360000
A-400	*AM1*	12306000	-	12306000	18 177 600
	KH3CO3	3125500	-	3125500	3125500
	Ammonia	484075	-	484075	484075
	thiamine HCl	3	-	3	0
	Amonia	-	1182550	1182550	-
	NaHCO3	-	5695500	5695500	-
	K2HPO4	-	1876416	1876416	-
	*MgSO4*H2O*	-	187642	187642	-
A-600	Octanol	659750	685125	735875	609000
	TMA	8250000	11332500	35332500	14902500
A-500-700	Raney Nickel	-	-	-	13204375
	Chromatography resin WBA	-	-	-	25000
	H2 gas	-	-	-	3087500
Subtotals		**51005737**	**62399625**	**128628374**	**118065999**
	Ash and Gypsum Wastes Disposal				
	Ash	-	428353	428353	461084
	Waste Streams	566100	1297590	927590	1297590
Subtotals		566100	1725943	1355943	1758674
Totals Variable Cost		**51571837**	**64125569**	**129984317**	**119824673**

Table 56: Fixed cost calculations for SA scenarios

Position	SA scenarios ($)			
	1G SA	2G SA	1G2G SA	1G2G SA+Xylitol
Plant Manager	168458	168458	168458	168458
Plant Engineer	160436	160436	160436	160436
Maintenance Supervisor	65320	65320	65320	65320
Maintenance Technician	229194	366711	366711	366711
Lab Manager	64174	64174	64174	64174
Lab Technician	91678	91678	91678	91678
Lab Tech-Enzyme	0	275033	275033	275033
Shift Supervisor	55007	220027	220027	220027
Shift Operators	458389	687583	687583	1375166
Shift Oper-Enzyme	0	275033	275033	275033
Yard Employees	96262	96262	96262	96262
Clerks & Secretaries	123765	123765	123765	123765
Total Staff Salaries	**1512682**	**2594480**	**2594480**	**3282063**
Labour burden (90%)	1361414	2335032	2335032	2953856
Total Labour cost	**2874097**	**4929511**	**4929511**	**6235919**
Maintenance	1026151	4955111	6083473	4866394
Property Insur. & Tax	914368	3663325	4383744	3745309
TOTAL FOC	**4814616**	**13547948**	**15396729**	**14847621**