# Value chain diversification in the sugar industry using quantitative economic forecasting models

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*In loving memory of my father, Ghafeer Ahmed, who is the bravest, most loving and kindest man I will ever know.*

*1958-2019*

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# Abstract

The South African sugar industry is facing increasing pressure from global sugar markets where the price of sugar is significantly lower than in domestic markets, as well as from the implementation of the health levy which has resulted in beverage manufacturers replacing sugar with non-taxable sweeteners. To maintain the industry infrastructure and to increase the demand for sugar, a diversification route for sucrose is needed.

Most of the studies focused on identifying a diversification solution for bioproducts are survey or experienced based and so, one of the main aims of this study was to use mathematical modelling of industrial manufacturing data to identify one single industry to explore sucrose-based chemicals. Datasets published by Statistics South Africa, The World Bank, Trading Economics and by the Organization for Economic Cooperation and Development were considered, from which the monthly manufacturing industries' sales data published by Statistics South Africa was selected for model building.

Seven different types of models were considered, including the Naïve method, simple and weighted moving averages, simple exponential smoothing, Holt's method, Holt-Winters' method and Auto-Regressive Integrated Moving Average (ARIMA) models. Each type of model was analysed in the context of the eight industries' data, from which ARIMA models were identified as those which were broad enough to cater for the varying degrees of trends and seasonality in the data without oversimplifying the data's behaviour. The other seven were not suitable either because their narrow applicability was not suitable to most of the datasets at hand or because they would provide an oversimplified model which would not be robust for future datapoints. The models were then built using training and test data splits with the auto.arima function in R Studio.

From these, selection matrices were constructed to evaluate the industries' forecasts on sales growth and revenue generating potential, the results of which identified the beverages' industry to the best option for investment. One of the objectives of the study was to identify a sucrose-based chemical for investment that is not highly commercialized in order to widen the range of investment options available. To this end, only four of the less commercialized chemicals explored showed significant advancement based on published research and patents, namely caprolactam, dodecanedioic acid, adipic acid and muconic acid. However, all four chemicals would feature mainly in the textiles industry, which the model identifies as not being a high growth industry and thus would limit the revenue generating potential.

The main beverage constituents of common drinks were then explored, from which non-nutritive sweeteners were chosen based on their wide applicability. From the six sweeteners considered, sucralose is the most widely used sweetener with the least number of reported serious health risks; this is thought to compensate for sucralose being a mid-price range product. Sucralose would also allow the sugar industry to leverage beverage manufacturers' replacement of sugar with sweeteners to comply with the Health Protection Levy.

The techno-economic analysis performed for the selected synthetic sucralose production process proved profitable in the first year of operation, as did a refined configuration using a lower ethyl acetate flow rate. This is largely due to the retail price of sucralose being close to 8 times the purchase cost of the most expensive raw material used.

Although this profitability analysis is promising, further investigation into the fixed capital costs involved should be done prior to the sugar industry investing in sucralose. Recommendations for further work to improve the profitability of this scenario include the consideration of forming a strategic partnership with key players in the beverages' industry, exploring alternative production routes, and using other time series models to validate the results achieved here.

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# Glossary of Terms

| | |
|---|---|
| Additive decomposition model | A variation of a decomposition model used when the seasonal variation is relatively constant in a time series |
| Auto-Regressive Integrated Moving Average | A forecasting technique that uses a linear combination of past values of the variable. |
| Bagasse | Dry sugarcane residue left after juice extraction in the manufacture of sugar |
| Biochemical | A chemical which originates from a biological raw material |
| Bioprocess | The process which converts raw biomaterial into a product |
| Bioproducts | Products that are made from a bio-source |
| Biorefinery | A refinery that primarily deals with biomass conversion into products |
| Box-Jenkins models | Alternatively known as ARIMA models |
| Decomposition model | A technique used to decompose a time series into its individual trend and seasonal components |
| Detrended | A dataset which has had its trend component removed from the original data |
| Fly ash | Powder like by-product of burning bagasse |
| Forecast | The output value of a model fitted to a dataset, typically used to predict data's behaviour beyond the dataset |
| Holt's Method | An extension of SES to allow forecasting of data with a trend |
| Holt-Winter's Method | An extension of Holt's method to capture seasonality using a forecast equation and three smoothing equations |
| Lignocellulosic | A mixture of lignin, cellulose and hemicellulose |
| Mean Absolute Percentage Error | A measure of prediction accuracy of a forecast |
| Molasses | Dark, thick syrup which remains after sugar has been extracted from cane juice |
| Multiplicative decomposition model | A variation of a decomposition model used when the seasonal variation increases over time |
| Naïve model | A forecasting technique which sets all forecasts to the value of the last observation in the source dataset |
| Platform chemical | Chemicals which can be converted into more end products |
| Residual | The value that describes the numerical difference between a forecasted/fitted value and the original data point |
| Seasonality | A characteristic of a time series which describes predictable changes in the data that recur over a period |
| Simple Exponential Smoothing (SES) | A forecasting technique that calculates the next point outside of a dataset using an exponentially decreasing weight for past observations |
| Simple Moving Averages | A forecasting technique that calculates the next point outside of a dataset using the rolling average |
| Stationarity | A characteristic of a time series which describes the statistical properties of the data not changing with time |
| Sucrose | Table sugar. A disaccharide comprising of one molecule each of glucose and fructose |

| | |
|---|---|
| Technoeconomic analysis | An analysis of a product or process based on process modelling, engineering design and economic evaluation |
| Technology Readiness Level | A scale to measure the maturity of a technology or product |
| Test data | The part of the original dataset set aside for testing models |
| Time series | A data series recorded in a sequence of time points |
| Time series analysis | The evaluation of a time series, often accompanied by fitting a model |

# Acronyms and Abbreviations

| | |
|---|---|
| ACS | American Chemical Society |
| ARIMA | Auto-Regressive Integrated Moving Average model |
| ARMA | Auto-Regressive Moving Average model |
| MAPE | Mean Absolute Percentage Error |
| OECD-FAO | Organization for Economic Cooperation and Development - Food and Agriculture Organization |
| SACU | Southern African Customs Union |
| SADC | Southern African Development Committee |
| SASA | South African Sugar Association |
| SMRI | Sugar Milling Research Institute |
| SSBs | Sugar Sweetened Beverages |
| Stats SA | Statistics South Africa |
| TRL | Technology Readiness Level |
| US DOE | United States' Department of Energy |

# 1 Introduction

## 1.1 The South African sugar industry in context

The sugar industry in South Africa has been a prominent feature of the economic landscape since the mid-nineteenth century, when immigrants from Mauritius introduced sugar planting and processing technology to the Natal province. Since then, the industry has evolved from an integrated system combining cane production and milling to a competitive setup with ‘planters’ and ‘millers’ operating as rivals for profit, and for influence over legislation (Dubb et al., 2017).

Growth of the domestic sugar industry has largely been in parallel with increased production across the Southern African region, with political developments heavily influencing export opportunities into overseas territories and expansion of South African companies within the region. The end of apartheid shaped investment policy and subsequently led to Illovo and Tongaat Hulett acquiring several sugar production facilities in Malawi, Tanzania, Eswatini (formerly Swaziland), Mozambique and Zimbabwe. Of the three most influential sugar companies in the region, Transvaal Sugar Limited (TSB Sugar; now owned by RCL Foods) chose not to expand its territories northward, and established itself instead within South Africa as the largest domestic producer (Dubb et al., 2017).

Moreover, since South Africa’s integration within the Southern African Development Community (SADC) in 1994, the entire regional production of sugar is largely controlled by Illovo, Tongaat Hulett and TSB, who collectively account for nearly 90% of the entire regional sugar output (Dubb et al., 2017). In addition to belonging to SADC, Botswana, Lesotho, Namibia, South Africa and Eswatini are in a trade agreement known as the Southern African Customs Union (SACU) which encourages interchange of goods between member countries at a single tariff and no customs duties between them.

In the face of growing international competition with cheaper sugar from mainly Brazil and India, SACU members have become unified in their lobbying efforts to protect regional markets where sugar can be traded at higher prices than the global market. The regional sugar industry is also protected by a dollar-based reference price tariff system that is based on the long-term average world price of sugar, which comes into place when the global trading price drops below the reference price.

Besides trading in sugar regionally, South Africa has an international presence as one of the top 15 sugar producing countries worldwide. Bulk raw sugar is sold to refineries in the Middle East, United States and Eastern countries such as Korea and Japan.

Figure 1 presents the trend in South Africa's crushed cane production between the 2005/2006 and 2018/2019 seasons.

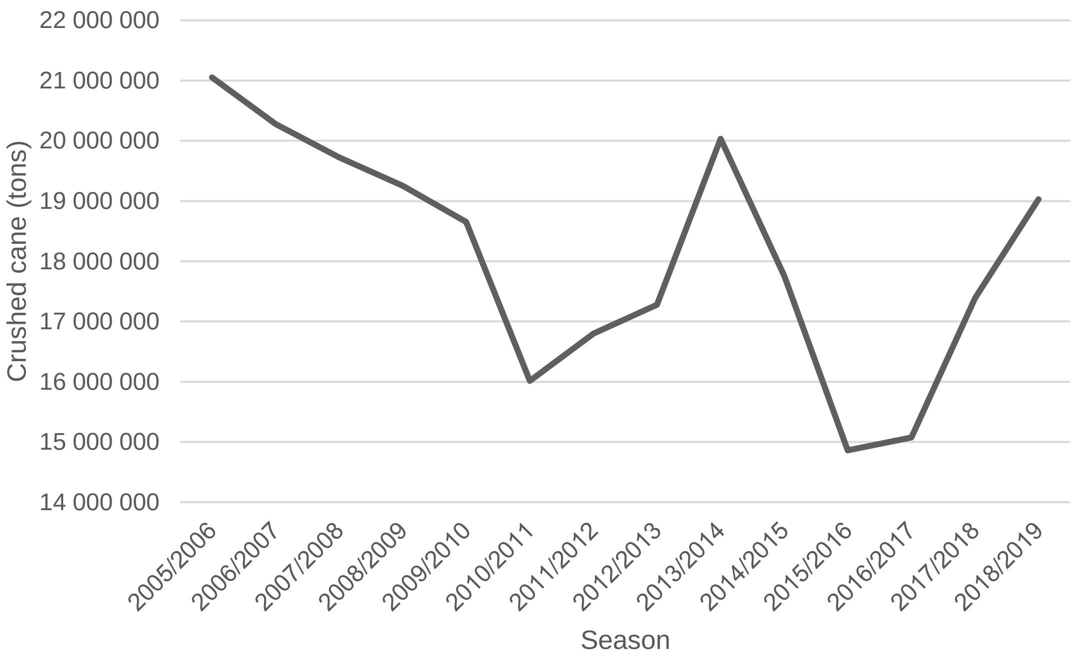


Figure 1: Crushed cane production trend in South Africa from 2005 till 2019 (adapted from SASA, no date)

The trend seen in Figure 1 shows that the most cane crushed in a single season was in 2005/2006, after which production declined steadily at a rate of about 2.5% annually till the 2009/2010 season but then dropped by 14.1% in the 2010/2011 season, followed by an increase and then a dip again of 26% from 2013/2014 to 2015/2016. Both dips are attributed to severe droughts in South Africa Baudoin *et al.* (2017).

The trend seen in Figure 1 shows that the industry starts to increase crushed cane production within at most two seasons following a severe drought. Figure 2 overleaf presents the trends in total saleable sugar obtained from the crushed cane, as well as trends in the sugar consumed in the national market and exported sugar into international markets.

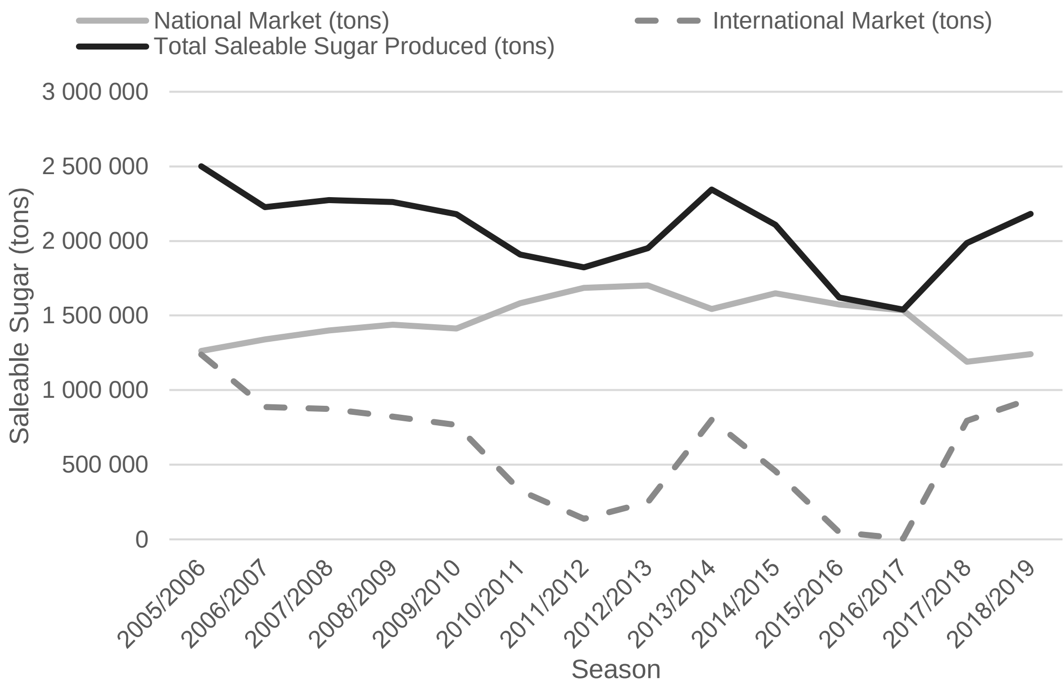


Figure 2: Trends in South Africa's total saleable sugar; sugar consumed in the national market; and sugar exported into international markets (adapted from SASA, no date)

The trend observed in total saleable sugar in Figure 2 corresponds to the severe droughts that impacted crushed cane production in 2010/2011 and 2015/2016, although the total saleable sugar started recovering only in the 2012/2013 season once the crushed cane had been converted into saleable product. Likewise, total saleable sugar production increased again only in 2017/2018 after the drought experienced in 2015/2016.

If observed closely, the trend in saleable sugar exported to international markets is almost the exact opposite to the observed year on year trend of saleable sugar consumed in the national market. Evidently the sugar industry delivers product where possible to the national market first and then to the international markets; in the 2015/2016 season, the national consumption dropped only by 4.6% whereas exports dropped by a massive 89%, which was then repeated in the 2016/2017 season.

Yet despite the damaging effects of droughts on the sugar industry, it remains a hub of job creation. The South African Sugar Association (SASA) values the industry at USD 939 million and reports there to be 85 000 direct and 350 000 indirect jobs, as well as 22 949 registered cane growers. SASA further estimates the industry to support the livelihoods of approximately 1 million people nationally, which is more than 2% of South Africa’s population ((SASA), no date), making it a critical source of employment and revenue generation in South Africa.

The number of jobs invested in the industry is an indication of the extensiveness of the sugar value chain; which ranges from manufacturing bulk raw sugar; refined sugar in both white and brown forms, and sugar syrups. Molasses, a by-product of sugar processing, is an extremely valuable animal feed within the agricultural industry as well as having other uses such as in the production of bioethanol. The revenue streams from sugar are therefore diverse, but the majority of sugar sales came from the sale of white and brown sugar and direct sugarcane sales up to 2014, and thereafter shifted to industrial sugar comprising the larger portion of national sales ((SASA), no date).

## 1.2 Background to the project

Interest in diversifying the sugar value chain has been sparked by several factors, including climate change, low global sugar prices and rising oil prices. Developments in climate change-related mandates in the European Union (EU) and the United States of America (USA) over the past decade have targeted use of renewable raw materials such as sugarcane and have spearheaded other countries to follow suit and include bioethanol produced from sugar blended into gasoline fuels for vehicles.

The South African government has been working on the implementation of its biofuel strategy, originally drafted in 2006 with a five-year pilot plan; the strategy proposed to achieve a 2% bioethanol content in petrol. In December 2019, the South African Cabinet approved the Biofuels Regulatory Framework, which will enable implementation of the Biofuel Industrial Strategy. The framework stipulates five key areas to be regulated: a protocol to mitigate the risk of the biofuels program on food security; mandatory blending regulations to create a demand for biofuels; the cost recovery mechanism for the proposed blending; subsidy programs to support biofuel farmers and manufacturers; and selection criteria for biofuel projects requiring a subsidy (South African Cabinet, 2019).

The USA and the EU have also invested heavily into research and development into the transformation of sugar into one of its many derivatives via platform chemicals, which function as base chemical building blocks. These platform chemicals can either be exported directly or can be converted further into value-added products such as fibres, textiles, polymer or paints. Using bio-based chemicals in this manner further adds to mitigation efforts against global petrochemical dependence and climate change.

Research into diversification of sugar products comes at a crucial time when intense global competition is leading companies to optimize costs by any means necessary, often retrenching staff and discontinuing jobs to replace them with mechanised processes. Between 2009 and

2014, Illovo is reported to have reduced its permanent and part-time workforce by 25% despite increases in production (EngineeringNews, 2019).

Although climate change and automation-related job losses are valid reasons for diversifying South Africa's sugar value chain, the most pertinent driver of research into alternate uses of sugar is undoubtedly the Health Protection Levy, also known as the sugar tax. The tax was implemented in April 2018, aiming to prevent and control non-communicable diseases and to control rising obesity rates. Originally stipulated as 2.1 cents per gram of the sugar content in beverages that exceeds 4 grams per 100 ml, the levy has been revised to 2.21 cents per gram of sugar above the allowed limit (Pilane and Green, 2019).

While this initiative has proven lucrative for government, generating over USD 153 million between April and December 2018 and may deliver health benefits, it has had a serious negative impact on the sugar industry. Beverage manufacturers have been quick to strategize a way around the policy by reformulating their products to use artificial sweeteners and reduce the amount of actual sugar used. As a result, the sugar industry has been left with a surplus of raw sugar which is currently exported at prices below cost of production. As of February 2019, SASA has estimated that more than 200 000 tons of sugar has been exported at a loss (Mchunu, 2019).

In light of South Africa's precarious financial position, diminished foreign investments and an obesity rate of 70% in women and 31% in men (BusinessTech, 2019), the sugar tax is likely to continue playing an important role in domestic revenue generation and policies around health. As such, the sugar industry and people of South Africa stand to gain tremendously by re-routing sugar into alternate avenues, with increased value generation and the continued support of the livelihood of 1 million people.

The Sugar Milling Research Institute (SMRI) is at the forefront of driving research for the industry and has so far worked with universities around the country to generate viable ideas for value generation from sugarcane and sugar for implementation in the short and long term. The Universities of Stellenbosch, KwaZulu-Natal and Cape Town are each working on projects investigating the diversification of the sugar value chain using all parts of sugarcane, including raw sugar in the form of sucrose and by-products.

## 1.3 Focus of this project

This project is focused on identifying and evaluating the medium to long-term opportunities for South Africa's sugar industry to invest in. It is focused on identifying which manufacturing industries will continue to grow in the next 20 years based on historical performance.

While based on South Africa's sugar industry, the study investigated the diversification of industries in general using economic data and quantitative forecasting methods. In so doing, the project adds to the research being conducted by the SMRI and creates a framework which can potentially be used to investigate alternate avenues for resources in other industries and in other countries.

The use of the economic data and forecasting is included to create a quantitative, rather than qualitative, basis for assessing investment opportunities within a country's economy. The framework is intended to remain relevant over time by using data which is likely to be readily available in the future.

The aim of the project was therefore to develop a quantitative approach to evaluate opportunities in the South African economy for the sugar industry to diversify its value chain.

## 1.4 Scope and constraints

The project extends only to investigating the opportunities for sucrose derived from sugarcane to be used as a platform chemical or a further derivative within the South African economy. While multiple chemicals may be identified for future research and investment, only one chemical that is suggested as an opportunity for investment is assessed in detail.

The predictive models explored are Naïve, Simple Moving Averages, Weighted Moving Averages, Simple Exponential Smoothing, Holt's Method, Holt-Winter's method and Auto-Regressive Integrated Moving Average (ARIMA) models but only ARIMA models are used for the actual forecasting. SuperPro Designer is the only simulation tool used.

The limitations of the project include:

- Materials from the wider sugar value chain are not considered
- Forecasts are limited to within 20 years of the last date in the dataset used
- Of the available techniques to construct ARIMA models, only the auto.arima function in R is used here.

## 1.5 Structure of dissertation

Section 2 presents the literature review; which focuses on the production process of sugar, global trends in sugar production, key drivers of diversification in the sugar value chain, alternative products and industries which sugar is being diverted into, and types of models commonly used by decision makers in product portfolio selections.

Following on from the literature review, Sections 3 to 7 each focus on a part of the project's findings and are structured to present the reasoning behind the decisions made in the study and the results of that section.

Section 3 therefore presents the first part of the project, in which the dataset used to analyse manufacturing activity in South Africa is selected. The section defines the attributes needed in the desired dataset and discusses why not all the datasets investigated are deemed suitable for further analysis.

Section 4 discusses the modelling techniques tested on the selected dataset and ultimately discusses the utilisation of the selected dataset in building Auto-Regressive Integrated Moving Average (ARIMA) models to model and forecast South Africa's manufacturing industries' performance. The remainder of the section is then divided into first discussing the methods by which the models were constructed and how the best performing industry would be identified using selection matrices, followed by the results of the models built and their validation against a test set. The final two subsections discuss the forecasts taken from the selected models, and the outcome of the selection matrices, determining which industry would be the premise for chemical selection in Section 6.

Section 5 then focuses on the viability of sucrose-based platform chemicals as diversification options. This section deals especially with those platform chemicals previously considered to be only at pilot level phase or below on a Technology Readiness Level (TRL).

Section 6 focuses on the selection of the chemical which will form the basis of the subsequent technoeconomic analysis. The section provides context of the main categories of beverages and their constituents. An assessment is presented on the three aspects on which the candidate chemicals were evaluated, namely selling price, applicability and safety.

Next, Section 7 presents the techno-economic analysis done for sucralose. First, the chemical process by which sucralose is produced is presented, followed by an analysis of the processes and technologies available for each step of its production, from which the best configuration is selected. The results of simulating production using the selected configuration and an analysis of the plant's profitability over 12 years are discussed last.

Finally, the entire study's conclusions are then presented in Section 8, and recommendations given on ways to further improve the results and possible next steps.

All assumptions made in the simulation and profitability analysis, purchase and selling prices used in costing, graphs of historic sales and forecasts, as well as selection matrices for all eight industries are included in the appendices.

# 2 Literature Review

In Section 2.1, a high-level overview of the evolution of sugar and its production is provided. This is followed by a review of the trends in the global sugar market in Section 2.2. Challenges facing existing sugar value chains are also examined. Section 2.3 reviews ongoing research into sugar valorisation and innovation mandates of note around the globe.

The resulting spectrum of methodologies developed by policy makers to screen sugar-based derivatives for commercialization is reviewed in Section 2.4.This leads to a review of the key factors and frameworks developed by industrialists and researchers for use in the selection of biochemicals for commercialization in Section 2.5, and subsequently an analysis of areas of improvement within all the techniques reviewed.

In Section 2.6, data driven forecasting techniques to address the gaps in the existing screening methodologies are reviewed. Lastly, Sections 2.7 to 2.8 provide a summary of key findings, the detailed project objectives and key questions, respectively.

## 2.1 Transforming sugarcane into sugar

Sugar, as referred to in the present day, encompasses an entire category of carbohydrates of the general formula $C_n(H_2O)_n$ which are present in a wide array of both natural and synthetic types of food and beverages. Colloquial use of the term sugar, however, invariably refers to 'table sugar' or crystalline sucrose; a disaccharide composed of one molecule of glucose connected to one molecule of fructose via a glycosidic bond and having the chemical formula $C_{12}H_{22}O_{11}$.

In recent years, sucrose has gained a level of notoriety and has become synonymous to some degree with terms such as 'artificial' and 'non-nutritive' as a result of its current excessive use in its refined form in food products and the increased health consciousness and marketing targeted to combat obesity epidemics worldwide. Contrary to modern beliefs, however, sucrose functions as a natural beneficial source of energy for both plants and animals, being formed from glucose created via photosynthesis in leafy green plants. The glucose produced is either stored as a polymer in the form of starch or is transported for use in the plant as sucrose.

Sucrose is therefore found in almost all plants but is not present at high enough concentrations in most for economically viable recovery, except in sugarcane and in sugar beets. The sucrose extracted from either of these plants is chemically identical, but the differing spectrum of accompanying non-sugars from each raw material distinguishes the final sugar profiles. The raw sugar yield from sugarcane is typically 7-18%, and 8-22% from sugar beets ("Sugar," 2016). Sugarcane grows as tall, leafy stalks in tropical and subtropical regions, preferring areas with a high exposure to sunlight and either heavily seasonal rainfall or adequate irrigation.

In South Africa, approximately 432 000 hectares of land are dedicated to the growth of sugarcane, of which approximately 325 000 are harvested annually. SASA (2005) reports that between 8.3 -10 tonnes of sugarcane are needed to produce 1 tonne of sugar, and that the average sucrose content of sugarcane in South Africa is 13.5%.

#### 2.1.1 Growing conditions

In a set of sugarcane production guidelines published by The Department of Agriculture, Forestry and Fisheries (Department of Agriculture Forestry and Fisheries, 2014) detailed instructions are provided on growing sugarcane in South Africa. The warm South African climate is ideal for sugarcane production, which favours temperature ranges of 20-35 °C and prefers long sunlit periods of 12-14 hours. High humidity areas such as the KwaZulu Natal province allow rapid cane elongation during high growth periods. The sugarcane plant prefers soil to be kept loosely packed and requires a high moisture content in the soil during planting till full growth has been achieved. For this, growth periods need between 1100 and 1500 mm well distributed rainfall, and a dry period for ripening. During a drought period, adequate irrigation is required to maintain the plant's health.

The average sugarcane yield is reported as 60 tons/hectare/annum in the KwaZulu-Natal province (TongaatHulett, 2020) and approximately 67 tons/hectare/annum on the South Coast. These yields are reported for a minimum annual rainfall of 900 mm. The yield of sugarcane reduces as the moisture level decreases (Schulze et al., 2007).

To encourage tall sugarcane stalks and a high sugar content, growers are encouraged to apply fertilizer rich in Nitrogen, Phosphorus and Potassium to the soil. Growers are further advised to adjust the ratio of these elements in the fertilizer according to the plant's growth phase. In general, it is advised to apply Phosphorus within four months of planting, Nitrogen within six months and Potassium within seven months. Soil sampling throughout the growth phase can allow growers to ascertain fertilizer needs.

Along with catering to the plant's nutritional requirements, it is vital for growers to spray herbicide to prevent the sugarcane plant having to compete for space and nutrients with weeds, especially during the earlier growth phases. Growers may also need to use insecticides as sugarcane is prone to becoming infested with caterpillars, moths, beetles, ants and termites, amongst others. Insecticide use can be supplemented by growers leveraging natural predators' activities by them planting varieties of sugarcane which have been proven to be less susceptible to some infestations, practising proper field hygiene and removing infested cane.

Planting of sugarcane, fertilisation and irrigation typically occur from February till May, after soil preparation and sampling in the previous month. This is followed by pest control, disease control and weed control, which take place from April till June, coinciding with the first three harvesting months. Harvesting and marketing continue till December, after which a new season starts.

### 2.1.2 Sugarcane processing

There are five major steps in the production of raw sugar from sugarcane: extraction; juice clarification; concentration; crystallization, and separation of the crystals from liquid. Unlike in sugar beets, the sucrose in sugarcane is prone to rapid deterioration after harvesting, therefore care is taken to minimize storage time prior to extraction ("Sugar," 2016).

The two main by-products from sugarcane processing to refined sugar are molasses and bagasse, which are both utilized in secondary industries. Bagasse refers to the fibrous material remnants post-extraction and which has a multitude of uses including functioning as a fuel source on sugarcane mills, manufacturing animal feeds, producing paper, as well as being a key component in the manufacture of construction materials and biodegradable plastics ("Bagasse", 2016).

Molasses is a thick, dark syrup which is derived from the sucrose-poor concentrate collected after each sucrose extraction stage, and has several different grades depending on where in the extraction process it was collected. Late stage or blackstrap molasses are typically used in animal feeds or in the manufacture of vinegar and other products; lighter grades of molasses can be used in baking, alcohol production and in confectionaries ("Molasses," 2018).

## 2.2 Global trends in the production of and price of sugar

The major producers of cane sugar include Brazil, India, China, Thailand, South Africa, Guatemala and Mexico. Brazil has historically been the primary producer of sugar from sugarcane, averaging over 25 000 kilotons per annum between 1990 and 2018 (FAO, 2019), but the increased profitability of diverting Brazilian sugarcane towards bioethanol has resulted in India becoming the principal provider of sugar from sugarcane into the global market since 2017 (FAO, 2018).

The production of sugar, like any other agricultural product, is influenced by environmental factors such as droughts, floods, abnormalities in temperature, infestation and disease, as well as political and economic dynamics. Nazir et al. (2013) also report high prices of inputs such as urea, land preparation and seed, as well as delays in payments as factors influencing sugarcane production and profitability, and consequently sugar production. Moreover, in countries like South Africa where specific physical and political infrastructures are present, delays in land reform and labour disputes can further limit sugar output (OECD-FAO, 2015).

Fluctuations in sugar production as well as changes in global demand for sugar and sugar-related products have influenced the global trading price of sugar. As Figure 3 shows, the price of raw sugar on the global market has become increasingly volatile in the last decade. Between 1989 and 2009, the price of sugar fluctuated between a maximum of US$ 0.30/kg sugar and a minimum of US$ 0.11/kg sugar; however, this was followed by unprecedented fluctuations between 2009 and 2011 and a surge price of sugar to US$ 0.65/kg sugar in 2011. Maitah and Smutka (2018) attribute this volatility to speculative hedge funds as well as a growing demand for biofuels, which has resulted in periods with an oversupply of sugar and periods of shortage.

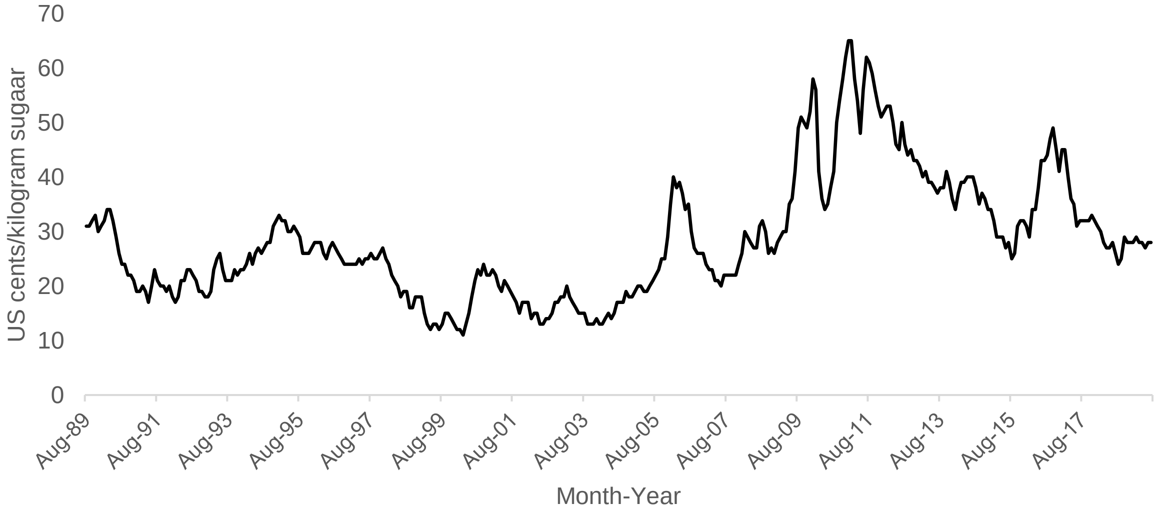


Figure 3: Historical global sugar prices (Data adapted from ("Sugar Monthly Price", 2019) )

The price of sugar continues to be influenced by policy changes such as the elimination of the sugar quota system in the European Union, which was implemented in October 2017, as well as the removal of production quotas in countries such as Thailand. In the medium term, therefore, future prices of sugar are expected to increase only moderately as supply is expected to exceed demand (OECD-FAO, 2019).

In light of the volatility of global sugar prices and the availability of relatively cheaper sugar from countries such as Brazil, a grouping of southern African countries, including South

Africa, Botswana, Lesotho, Namibia and Eswatini (formerly Swaziland) have entered into a trade agreement known as the Southern African Customs Union (SACU) which encourages interchange of goods between member countries at a single tariff with no customs duties between them.

SACU members are unified in their lobbying efforts to protect regional markets, where sugar can be traded at higher prices than on the global market. The regional sugar industry is also protected by a dollar-based reference price tariff system that is based on the long-term average world price of sugar, which comes into place when world price drops below the reference price.

## 2.3 Key drivers of sugar value chain diversification

The survival and success of any industry has historically been known to be a combination of a strong business strategy, adequate investment and a willingness to adapt to the ever-changing needs of consumers and policy makers.

The continued presence of sugarcane industries around the world is thus an example of them having progressed from fulfilling customers' basic needs to expanding their product offering by adapting to changes in consumer preferences and by incorporating technological advancements. Even so, sugarcane industries have been forced to invest in diversification research in recent years as a result of mandates implemented out of necessity by global leaders to address issues which are impacting the environment and societies worldwide at a grander scale than previously imagined.

The key drivers of change within the sugar industry are discussed in this section, followed by an overview of which product diversification routes have been explored. Decision making frameworks previously used by policy makers are discussed. Finally a review of techniques which can improve these frameworks is presented.

### 2.3.1 Cost of sugar production

The availability of low-priced subsidized sugar on the global market has severely impacted the price of sugar in the South African market, reducing the profit margin which domestic producers can apply to local sugar, according to a report published in 2017 (Department of Agriculture Forestry and Fisheries, 2017).

Further, between 2001 and 2014, the annual recoverable prices of sugar have not matched the increases in production costs and farming inputs such as pesticides, fuel and fertilizer. The economic threat to the local sugar industry is further compounded by major setbacks such as drought and larval infestation which has led to severe damage to crop yield in recent years (Harrison et al., 2016).

Of all the other factors discussed in this section, the fact that the sugar industry may soon no longer be able to compete at all with global sugar prices is perhaps the most important and relevant to discussions on value chain diversification.

If the local sugar industry is to remain a viable revenue generating and job providing sector, it is necessary for the sugar value chain to diversify and so increase the demand for sugar.

#### 2.3.2 Sugar tax

Besides global competitive prices, the he most recent driver of diversification in the sugarcane industry is the implementation of the Health Protection Levy in South Africa, or sugar tax, adopted by many countries subsequent to the World Health Organization (WHO) advocating for taxation on sugar-sweetened beverages (SSBs) to reduce consumption of sugary drinks.

The WHO reports the worldwide prevalence of obesity to have nearly tripled since 1975. Some 41 million children under the age of 5 were declared obese in 2011 alone. Consequently, obesity-related diabetes has placed a great burden on national health budgets; the WHO estimates the loss in gross domestic product, including direct and indirect costs of diabetes worldwide to amount to US$ 1.7 trillion between 2011 and 2030 (WHO, 2016).

Although the WHO advises countries to raise the price of SSBs by at least 20%, the nature of the tax varies, with some countries adopting a flat percentage tax on all sugary drinks with a sugar content above a stipulated level irrespective of volume, whereas most other countries charge a fixed rate per unit volume. Beverages with a high sugar content but with an obvious health benefit are exempt from the sugar tax in some countries. In South Africa for example, fruit and vegetable juices are exempt (Cawley et al., 2019) .

Although the implementation of the sugar tax has shown benefits such as a reduction in adults' consumption of some taxed SSBs, Cawley et al. (2019) report an increase in cross-border buying from untaxed jurisdictions. Moreover, the sugar tax has forced the sugarcane industry to find alternative routes to divert sugar into as the use of sugar itself becomes unfavourable to beverage manufacturers.

Despite sugarcane production in South Africa being estimated to be over 19 kilotons in the most recent season, the sugar industry is under a serious threat from the implementation of the Health Protection Levy, implemented in April 2018, and will likely not produce as much sugar in future. Originally stipulated as 2.1 cents per gram of the sugar content in beverages that exceeds 4 grams per 100 ml, the levy has been revised to 2.21 cents per gram of sugar above the allowed limit.

It is therefore imperative to explore and invest in alternative uses for sugar to increase its demand in the long term and with it, assist with job creation.

### 2.3.3 Climate change

Amongst the causes of global warming, as noted throughout the series of Intergovernmental Panel on Climate Change (IPCC) Assessment reports, the use of fossil fuels remains the highest contributor of greenhouse gases and, more specifically, the release of carbon dioxide. Between 1970 and 2010, carbon dioxide emissions from fossil fuel combustion and industrial processes contributed about 78% of the total greenhouse gas emissions (Pachauri et al., 2007). Rising populations and economic growth remain drivers of growth in energy use for the foreseeable future; however, the Fifth Assessment report has stressed the crucial need for policy makers to adopt faster adaptation and mitigation efforts.

The integration of sugarcane industries towards lessening the reliance on fossil fuels may have opportunities within the platform chemical space, especially where the biochemicals can replace fossil fuel based key intermediary chemicals.

## 2.4 Strategic valorisation of sugar into biofuels, biomaterials and platform chemicals

In the manufacture of sugar, sugarcane juice is the primary resource, but the process also generates several waste streams which can be further valorised. In a conventional biorefinery, however, the utilization of waste streams is generally limited to the burning of bagasse in boilers to generate steam used to operate turbines onsite, and the further processing of molasses into a saleable version.

Production of value-added products by sugar manufacturers has required a transformation of existing systems from manufacturing only sugar into integrated biorefineries capable of multi-product outputs. A biorefinery differs from a traditional refinery in its focus on utilising only biomass from natural sources such as sugarcane, instead of petroleum based starting materials. While many use the word ‘biorefinery’ to address only the processing of woody biomass, it is used here in the broadest sense to refer to conversion of all renewable organic resources.

Beyond the conventional use of sugarcane waste streams, there exists a wider scope to utilize these and other waste streams from sugar production to build a biorefinery with a greater focus on valorisation, which can create higher value-add products and diversified markets. Figure 4 overleaf maps out the most widely researched valorisation options as reported in recent literature. The following subsections describe these in further detail.

### 2.4.1 Categories of bio-products

Biorefinery outputs are categorised into first, second or third generation bioproducts depending on which starting material is used. In the case of first-generation products, the starting material is edible feedstock such as cane juice, whereas second generation feedstocks are lignocellulosic materials such as bagasse and products created via algal biomass or by utilizing carbon dioxide or other waste products as a feedstock are classified as third generation.

Moreover, bioproducts with a high potential of directly substituting fossil-based counterparts are classified as drop-in chemicals, whereas chemicals with multiple functional groups, which can be subsequently transformed into an array of higher-value bio-based products are labelled as platform chemicals. The term ‘platform chemicals’ was made popular by the United States Department of Energy’s publication of two reports in 2004 ((EERE), 2004; Bozell G.R., 2010), respectively. The first focused on the potential of integrated biorefineries using sugar and the second addressed lignin-based value-added products.

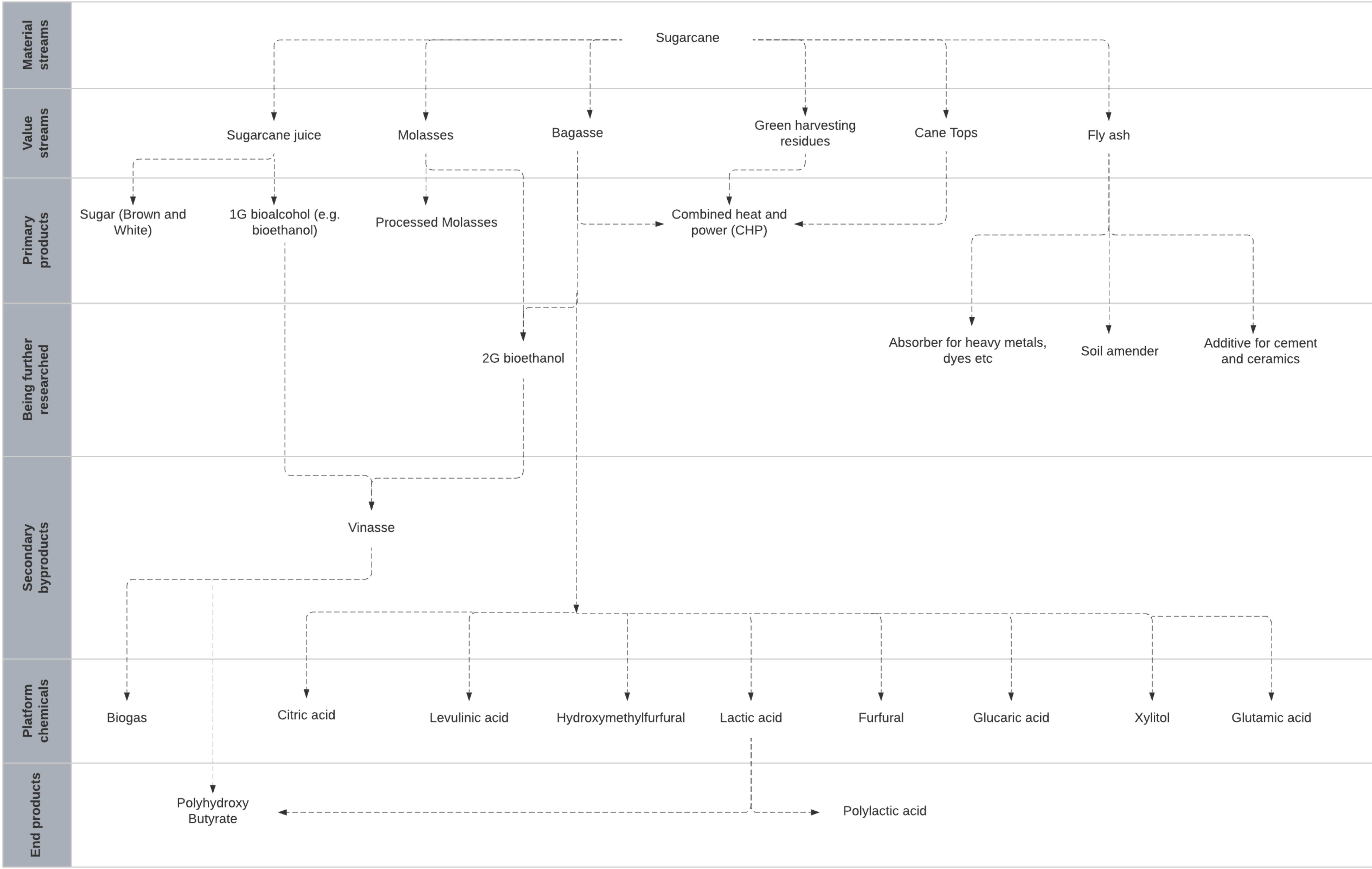


Figure 4: A schematic showing the current and potential valorisation routes for sugarcane and the waste streams from the sugar production process (compiled using Pachon et al. (2018), Losordo et al. (2016), Olivera et al. (2018), Ong et al. (2019), David et al. (2019), Lee et al. (2017), Iryani et al. (2013), Akaraonye et al. (2012), Moraes et al. (2015) and Cavalett et al. (2012)

### 2.4.2 Lignocellulosic materials

The fibrous sugarcane remnants collected after juice extraction are known as bagasse; a type of lignocellulosic material. This, and green harvesting residues left in the field post-harvest collectively comprise a large percentage of the total annual lignocellulosic output in South Africa. Sugarcane bagasse is one of the largest flows of lignocellulosic material in the country (Pachon et al., 2018); about 280 kg of bagasse is generated per tonne of harvested cane (Farzad et al., 2017), amounting to 6.3-8.16 million tonnes produced annually (Özüdoğru et al., 2019).

Bagasse is typically burned in low efficiency boilers onsite, whereas harvesting residues are either left in the field or burned before harvest. This is because neither of these materials are of high value before extensive processing, and so their use is limited to low value disposal treatments. However, burning the cane in the fields releases large amounts of gaseous emissions and soot particles which cause respiratory health problems in neighbouring communities (Özüdoğru et al., 2019).

Harvesting residues can be further classified as either green tops, referring to the top-most part of the plant, and brown leaves which are attached to the stalk itself. It is common practice to separate the green tops from the stalk and spread these across the sugarcane fields to assist in soil fertility, while the brown leaves are separated and transported for burning together with the stalks (Cerri et al., 2011).

Considered as second generation (2G) feedstocks because as waste streams they do not compete with the primary input of the sugar process, bagasse and harvesting residues are promising renewable biomass sources for their lower cost, relative abundance and lack of competition for food-designated land (Pachon et al., 2018). However, due to their chemical composition, transformation of these materials into high value products is limited by cost intensive processes.

Valorisation of bagasse has been extensively researched in recent years to direct the feedstock into the production of 2G biofuels such as bioethanol. However, 2G ethanol technology is still not cost efficient enough to be considered mainstream on its own; several studies propose the integration of first and second generation ethanol processes to leverage the existing first generation infrastructure while further research is conducted on processing lignocellulose (Losordo et al., 2016; Oliveira et al., 2018).

Compared to first generation substrates, such as the sugars in cane juice, lignocellulosic materials are more recalcitrant due to their heterogenous composition of cellulose and hemicellulose, which are difficult to break down into sugars. The average chemical composition of bagasse and brown leaves in South African sugar mills is 40.7% cellulose, 21.9% lignin, 27.1% hemicellulose, 3.5% ash and 6.7% extractive and total water content of dry mixture of 42% (Farzad et al., 2017). Biological conversion routes of lignocellulose therefore often require multiple steps including thermochemical pre-treatment, enzymatic hydrolysis and fermentation (Losordo et al., 2016).

***Lignocellulosic pre-treatments***

Bagasse is particularly recalcitrant because of strong intra and intermolecular hydrogen bonds maintaining the crystalline regions, making the cellulosic material highly resistant to acid, alkaline and enzymatic hydrolysis.

Conversion of bagasse into ethanol therefore requires pre-treatment, hydrolysis then fermentation. In the pre-treatment step, lignin and hemicelluloses are altered or removed, thus increasing the surface area of the cellulose and decreasing the degree of crystallinity and polymerisation of cellulose, thus making it more accessible to the subsequent hydrolysis agents (Mosier et al., 2005).

Pre-treatments can be physical, physicochemical, chemical, biological or a combination of techniques. Physical pre-treatments are further classified into mechanical and non-mechanical. Mechanical pre-treatments involve grinding and/or milling of the lignocellulosic material, which can be followed by some form of separation technique to isolate the cellulose.

Physicochemical pre-treatments such as steam explosion and liquid hot water treatments work by exposing the lignocellulose to a very high temperature either in combination with or in the absence of an acid or base catalyst. Compared to steam pre-treatments, steam explosion and liquid hot water have lower environmental impacts, are more cost effective and have low to no toxic chemical usage. Steam explosion is, however, associated with the partial degradation of hemicelluloses and the formation of toxic components but generally has a higher sugar yield compared to the liquid hot water on an equivalent exposure time basis (Hassan et al., 2019, 2018; Mosier et al., 2005).

Chemical pre-treatments involve the use of dilute or concentrated acids or bases, or the use of aqueous organic solvent mixtures with or without using acid or alkali catalysts. Acid pre-treatments offer a high sugar yield but require significant volumes of hazardous acids which may require the use of expensive corrosion-resistant reactors. Nevertheless, dilute acid hydrolysis is the most widely used technique.

Alkali pre-treatments also involve the use of harsh chemicals such as sodium hydroxide, which is inexpensive, but requires large volumes of wash water to effectively remove the generated salts from within the lignocellulosic structure. A further drawback of alkali pre-treatments is the potential formation of enzyme inhibitors which can reduce the efficacy of downstream biological treatments.

Biological pre-treatments offer an alternative to chemically intensive processes and are considered cost efficient and less environmentally detrimental than other options. Biological options typically employ filamentous fungi which use lignin-degrading enzymes. As with biological alternatives in general, biological pre-treatments of lignocellulose have lower efficiencies than conventional counterparts and require a long incubation time to achieve an equivalent conversion. A further disadvantage is that not all microorganisms are highly selective, resulting in the unwanted degradation of cellulose (Hassan et al., 2019; Zheng et al., 2014).

In recent years, the use of ionic liquids as pre-treatments have gained traction. Ionic liquids destroy the complex lignocellulosic network of non-covalent interactions and by forming hydrogen bonds with the sugars (Swatloski et al., 2004). The dissolution of lignocellulosic biomass can be enhanced by combining ionic liquids with microwave, ultrasonic and/or thermal technologies to improve the cellulose recovery yield (Montalbo-Lomboy and Grewell, 2015).

Selection of the right pre-treatment option is dependent on several factors such as the physical properties of the lignocellulosic material and selected downstream treatment options. The optimal pre-treatment option will minimize cellulose degradation, maximise sugar yield in subsequent steps, reduce hazardous chemical consumption and be efficient both in terms of energy consumption and cost.

### *Products from lignocellulosic material*

The research into bagasse valorisation is extremely vast and has broadened considerably in recent years. Beyond using bagasse as a source material for ethanol production, Guna et al (2019) have successfully demonstrated using bagasse as part of a composite for biodegradable ceiling tiles, reporting that gluten-bagasse composite is significantly stronger than conventional gypsum-only tiles. Additionally, Hilares et al (2018) have reported the burgeoning potential of bagasse featuring in pigment production, by successfully using it to produce red pigment.

Conversion of bagasse hydrolysate into xylitol, an artificial sweetener has featured in a few studies since 1995, and interest has continued into recent years such as by Gurgel et al (1995), Rao et al (2006) and de Albuquerque et al (2014).

Kumari and Debabrata (2015) have further investigated the use of bagasse in forming hydrogen gas via dark fermentation, a technique of fermenting sugars in the absence of light.

Further work on this valorisation route is limited as it has yet to be proven commercially viable, due mainly to the challenge of identifying a pre-treatment option that does not form any enzyme inhibitors.

Since the publication of potential lignocellulosic based platform chemicals by Bozell and Petersen in 2004, there has been considerable work done in this realm. Ong et al (2019) for example, have explored the co-fermentation of lignocellulosic derived glucose and xylose into succinic acid but have identified the need to further optimize this process via metabolic engineering of the yeast strain to improve the overall yield.

Succinic acid is a versatile platform chemical whose derivatives have applications in cosmetic products, biodegradable polymers, herbicides, food ingredients and pharmaceuticals, amongst others (Lee et al., 2017). Hydroxymethylfurfural is another platform chemical with a wide range of applications, including being a key intermediate in the production of biofuels and polymers (Lee et al., 2017). Li et al (2020) have demonstrated the formation of 5-hydroxymethylfurfural from bagasse pre-treated with ionic liquids and ultrasound. Previous studies on forming HMF from bagasse include those conducted by Iryani et al (2013) and Atanda et al (2016).

Further transformations of sugarcane based lignocellulosic material into platform chemicals include conversions to levulinic acid, which can be further transformed into textiles, plasticizers, resins and animal feeds. Mthembu et al (2020) for example, have reported a levulinic acid yield of 44.8% from bagasse, which can be further improved once the formation of humins is reduced.

Other platform chemicals produced from sugarcane lignocellulose include levoglucosan and citric acid (David et al., 2019). Citric acid production has been investigated since the early 2000s; some studies include the work conducted by Vandenberghe et al (2000), Kumar et al (2003) and Khosravi-Darani et al (2008).

The production of platform chemicals from sugarcane lignocellulose is undoubtedly a valuable valorisation route, as has been demonstrated by the multiple studies published on the myriad of possibilities. A common limitation reported is the cost intensiveness of the lignocellulose pre-treatment which may at times be coupled with the formation of unwanted by-products. Commercialization of any of these routes is therefore blocked until the pre-treatment step is further optimized.

### 2.4.3 Molasses

Sugarcane molasses is considered an excellent carbon source for a biorefinery due to its high sugar content and relatively low price. Essentially the residual syrup from the sugar crystallization step, there is a limited loss of sugar if the molasses being valorised is C molasses which typically has no further easily obtainable crystalline sugar, unlike A or B molasses which still contains considerable value. The composition of sugars in molasses is primarily sucrose, followed by smaller, similar amounts of glucose and fructose (Akaraonye et al., 2012).

Conventional uses of molasses are its use as an animal feed, transformation into bioethanol and its inclusion in food products. Due to molasses not requiring intensive pre-treatments, there are several advantages of valorising molasses instead of lignocellulosic materials, such as the higher product yields, simpler product recovery processes, minimum purification steps and cheaper processing technologies.

Like bagasse, molasses is available for conversion into a wide variety of products and platform chemicals due to the availability of sugars as carbon sources. One of the most commonly researched products formed from molasses is 2,3-butanediol, an alcohol which is used in the production of plasticizers, polyester, drugs, cosmetics and softening agents (Dai et al., 2015; Jung et al., 2013). It can also be used as a starting material for 2-butanone, a liquid fuel additive, and 1,3-butadiene which is used in synthetic rubber production (Lee et al., 2019).

Other platform chemicals can also be formed from molasses, such as 5-HMF as demonstrated by Gomes et al (2017) for example, and lactic acid as reported by Sun et al (2019). There are many avenues into which molasses can be diverted but one of the key limitations of valorising molasses is the presence of non-sugar components, namely organosulfur and organonitrogen, which deactivate solid acid catalysts, resulting in low product yield and selectivity (Tian et al., 2020). Consequently, several studies have been published on optimizing upgrading molasses, including using nickel catalysts to remove catalyst poisons by Yang et al (2019).

### 2.4.4 Vinasse

Vinasse is the residual liquid from ethanol production, and is typically used in field fertigation, providing nutrients and water to crops (Cavalett et al., 2012); the composition contains high levels of organic compounds, especially potassium, nitrogen and phosphorus. While using vinasse as a fertilizer has the benefit of supplementing conventional fertilizers, the limitations include soil salinization, leaching of metals and sulfate, ground water contamination, insect attraction, as well as release of unpleasant odours and greenhouse gases.

If the vinasse is a by-product of 1G ethanol production, it will typically have a higher nutrient content than if it were generated as a result of 2G ethanol production due to the differences in the chemical profiles of the starting material.

Vinasse from molasses generally has a higher chemical oxygen demand (COD) and biochemical oxygen demand (BOD) than vinasse from sugarcane juice. This is a result of the highly concentrated sugars in molasses increasing the content of non-fermentable organics that remain in the vinasse post-fermentation. Regardless of origin however, the main organic acids present in sugarcane vinasse are acetic acid and lactic acid, as well as glycerol, ethanol and a small amount of carbohydrates.

It has been reported that approximately 11 litres of vinasse are produced per litre of anhydrous ethanol (Dias et al., 2012) thus highlighting the need to explore valorisation routes for vinasse as more ethanol is produced in alignment with global initiatives to reduce fossil fuel consumption will result in more vinasse than can be used on the fields safely.

The main valorisation route that most studies are focused on is the production of biogas from vinasse via anaerobic digestion, which is utilizing microorganisms to digest vinasse in the absence of molecular oxygen to produce mainly methane and carbon dioxide gases. The methane can then be used in further processes or can be used directly as a fuel (Espana-Gamboa et al., 2012).

The types of microorganisms used in this process include acidogenic bacteria, acetogenic bacteria and methanogenic archaea. These operate optimally either around 30°C if a mesophilic process is desired, or around 50°C if the process is to be thermophilic, and at a pH between 6.5-8.2. Other environmental factors which need to be maintained to favour anaerobic digestion is the presence of adequate macronutrients (nitrogen, phosphorus and sulfate ions), trace metals as micronutrients, and a carbon source for synthesis and energy (Moraes et al., 2015). In the presence of sulfate, sulphite or thiosulfate ions, hydrogen sulphide gas is generated as well, which is a result of the activity of sulfate-reducing bacteria.

One of the main challenges in commercializing anaerobic digestion for vinasse is the lack of environmental and economic stimuli for investment in large scale plants for vinasse pre-treatment (Moraes et al., 2015).

## 2.5 Decision making techniques used in product portfolio selections

This section discusses the processes used by business decision makers to systematically narrow-down a pool of candidate products to the best one, for further development and commercialization. In the context of diversifying the sugar value chain, the purpose of this section is to identify a technique to select a platform chemical from the myriad of available options, as well as to highlight any gaps in existing processes which this study could potentially fill.

Four main categories of decision-making frameworks (not restricted by industry) were identified:

- Frameworks based on analysing previously launched products; these analysed both successful and unsuccessful product launches
- Frameworks incorporating multiple factors including the analysis of previously launched products, expert opinion and industry performance, for example
- Scoring methodologies constructed with the sole purpose of narrowing down a long list of candidate products based on pre-defined criteria
- Integrated methodologies which incorporate mathematical modelling, market analysis, expert opinion with techno economics.

Besides the above four categories, special attention was also given to the approaches used by two of the most influential publications on the diversification of sugar value chains.

These findings are summarized in Figure 5 overleaf.

| Post-evaluation of successes and failures | Multi-factor screening | Scoring methodologies | Integrated Methodologies |
|---|---|---|---|
| •Analysis of a large portfolio of previously launched products to evaluate factors contributing to their success or failure<br>•Emphasis on the use of surveys sent to senior industry personnel to evaluate individual products<br>•Some studies focus solely on either successful products or failures, whereas others attempt a comparative review in a single study | •Stepwise elimination of possible candidates from a large pool using pre-defined criteria<br>•Incorporation of industry experience via engagement with senior personnel<br>•Evaluation of the level of industry activity by region<br>•Review of available literature, databases, interviews with industry personnel and examining of industry reports to gain an updated perspective on the pool of chemicals and evaluate market potential | •Weighted factor scoring<br>•Portfolio matrices on multiple factors<br>•Iterative interactions between project champions and decision makers<br>•Calculation of market potential, technology substitution potential, economic substitution potential and/or a technology diffusion rate<br>•Use of multiple scenarios to predict poor, modest and advantageous environments for market growth<br>•Use of surveys to elicit industry landscape | •Business aspects combined with engineering aspects<br>•Phase wise approach suggested to diversify product portfolios<br>•Suggested to transition from low risk, established technology products towards more innovative and higher risk products<br>•Consideration of product revenue, margin creation, evaluation of whether product yield will match market need<br>•Mathematical solutions to form part of forecasting strategy<br>•Use of technoeconomics to provide holistic view of projects |

Figure 5: Summary of reviewed product portfolio selection methodologies (compiled using Hopkins, 1981; Cooper, 1994; Dornburg, Hermann and Patel, 2008a; Sammons Jr *et al.*, 2008; Mansoornejad, Chambost and Stuart, 2010; Shen, Worrell and Patel, 201))

The methodologies described in Figure 5 are each distinct in their overall approaches but with some common principles and an observed evolution from rudimentary frameworks, which is discussed in detail below.

Techniques for screening suitable candidates for a company's product portfolio stemmed from a reliance on seeking patterns defining successful and unsuccessful previous product launches. Studies such as those conducted by Cooper (1994) evaluated products post-launch to determine which factors contributed to their success; whereas, other studies such as Cooper (1975) and Hopkins (1981) focused on the opposite side of the spectrum, analysing failed products for defining characteristics.

The idea behind these studies of creating a knowledge base of factors which companies could later use in selecting future products is quite useful but presents a difficulty when the same factor appears to be characteristic of both successful and failed products. As commented on by Zirger and Maidique (1990), this drawback limits the usefulness of these studies, and any conclusions reached from such isolated evaluations of successes or failures must be viewed as tentative at best.

A natural evolution of this technique thus emerged in the form of studies evaluating successes and failures as pairs of products launched within the same industry or by the same company, but no longer considering each separately. In so doing, a greater degree of comparison became available and key factors affecting product outcome could be identified. Zirger and Maidique (1990) for example, examined over 330 new products in the electronics' industry and found there to be distinct factors contributing to a product's eventual success, which were either not entirely present in failed product launches, or were completely absent. These included a high degree of competency and accountability at the managerial level, correctly identifying the product's benefit to customers, and focusing products for early entry into large and growing markets.

In a similar comparative study of 43 successful and failed product pairs in the chemical and scientific instruments industry, Rothwell et al. (1974) and Rothwell (1972) found a product's success to be primarily related to a handful of factors including a thorough understanding of the user's needs and an attention to marketing and publicity. Likewise, Cooper (1979) determined similar factors to contribute to a product's success after conducting an extensive survey exercise whereby managers were asked to rate several new industrial products along 77 dimensions.

Table 1 summarizes the primary factors found to increase the chances of a product's eventual success, as identified by the studies discussed.

Table 1: An analysis of factors determined to influence a product's success in the market. This analysis is focused on a general business case and is not limited to bioproducts (compiled using (Cooper, 1994, 1975; Hopkins, 1981; Rothwell, 1972; Rothwell et al., 1974; Zirger and Maidique, 1990)

| **Common Factors** |
|---|
| Understanding users' needs & doing a thorough market research |
| Products address users' specific needs and are evaluated beyond their technical merit |
| Investment in marketing |
| Detailed planning and strategic focus on product development |
| **Unique Factors** |
| Detailed planning and strategic screening of products and building business cases |
| Managerial accountability |
| Comprehensive analysis of competitors |
| Enter high need, high growth markets |
| Accurate product pricing |
| Correctly planned and efficient product development |
| Avoiding markets saturated with new products |
| Early stage entry into large and growing markets |
| Early definition of product requirements |
| Focused, cross-functional team approach and accountability |

As Table 1 highlights, despite the evolution over time in the approach taken to identify success factors of products post-launch, the common factors deemed important are identifying the users' needs through a thorough market analysis, designing and selecting products which address this need, having accountability at a senior level and having this person champion the product through its stages of development. Significant too is the need for a detailed plan of development and the aim to enter markets which are likely to grow. It is also important for products to address market needs rather than follow a technology driven push. as the latter was commented on by Myers and Marquis as early as 1969, and repeated in later studies, including Gerstenfeld (1979), and Zirger and Maidique (1990).

A common thread observed in many of these studies is the reliance on surveys to gain expert industry input on what was deemed to contribute to a product's success or failure. These surveys were generally delivered by mail to the relevant company personnel and contained many questions for senior managers to answer about products already launched. One of the drawbacks of collecting information in this way is its time-consuming nature. Another set of methodologies applied beyond 1990 to incorporate industry input collected via personal communication or via surveys includes scoring techniques and scenario-based frameworks.

In their 1999 study for example, Archer and Ghasemzadeh (1999) sought to present a streamlined process of selecting new product portfolios. Their proposed scoring model embedded within a larger decision-making framework would allow users to yield an overall benefit measure for each proposed project. Using weighted factoring of pre-defined criteria, combined with iterative interactions with decision makers, companies would be able to compare projects fairly.

Their approach consisted of scoring a small group of factors such as cost, available work force, resource availability, probability of technical success then combining these in a weighted factor scoring based on weights determined through interactions with industry personnel. By iteratively considering the weighted scores, the portfolio of products for a company could be narrowed down to the highest rated products, increasing their chances of eventual success. Of note too within this selection framework is the inclusion of portfolio matrices, which allow a graphical representation of the products on two dimensions, enabling a comprehensive understanding of the dynamics of each product and allowing decision makers to select the best products till the available resources were exhausted.

The overall selection methodology as described by Archer and Ghasemzadeh (1999) is depicted in Figure 6.

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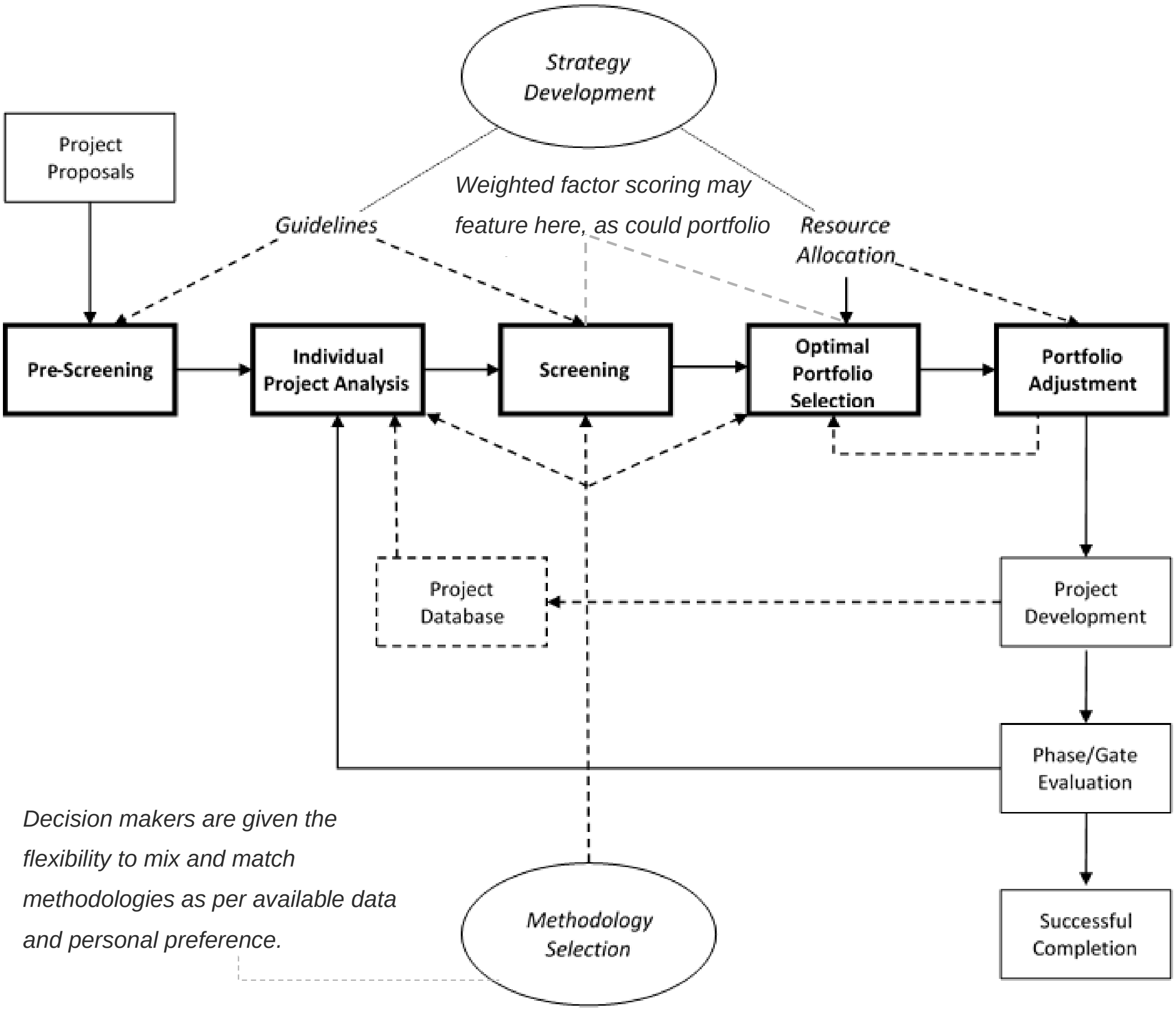


Figure 6: An example of an integrated product portfolio selection framework (adapted from Archer & Ghasemzadeh (1999))

Whereas previous studies have utilised once-off industry expert input to guide the selection of products, the framework presented in Figure 6 emphasises the iterative nature of project portfolio selection, which Archer and Ghasemzadeh (1999) suggest should be done in conjunction with input from decision makers. Unlike previous frameworks too, this study equips decision makers with a flexible approach and does not prevent them from adapting the process as per their available data or other factors such as their company's funding or available manpower.

Similar to portfolio matrices used to evaluate products as described by Archer and Ghasemzadeh (1999), studies conducted by Dornburg et al. (2008) and Shen et al. (2010) both utilise scenario based environments to project long term market potentials for bio-based products. Table 2 summarizes Dornburg et al's (2008) approach to calculating future market potentials based on 'unfavourable', 'moderate' and 'optimal' conditions as per the scenarios used in these studies. Figure 8 provides a similar summary of Shen et al's (2010) approach.

Note that while both studies use scenarios to evaluate their chemical candidates, Dornburg et al's approach is far more generalized than Shen et al. (2010), who focus primarily on bioplastics.

Table 2: Calculation of market potentials for bio-based chemicals (Dornburg et al., 2008a)

| Step | Description |
|---|---|
| **1** | Chemicals selected as those analysed by Hermann and Patel (2007) to be economically favourably and those estimated by industry experts to have relatively low future production costs and high market shares |
| **2** | Petrochemical counterparts for each selected bio-based chemical, based on expert opinion |
| | In most cases one main reference petrochemical was identified, although two may be specified to account for different target markets |
| **3** | Market potential calculated in kton |
| | First the technical substitution potential was estimated as a function of the chemical similarity between the biochemical and petrochemical counterpart |
| | An estimation of the economically viable part of the technical substitution potential was estimated |
| | An estimation of the time it would take to achieve the economic substitution potential |
| **4** | Based on the estimated growth rate for each scenario, the market potential of each biochemical was projected from 2007 to 2050 |
| | The observed dynamics of each biochemical would assist decision makers in selecting a product portfolio |

Along with forecasting the market potentials of the selected bio-based chemicals according to the methodology described in Table 2 above, the authors also forecasted the production of the petrochemical counterparts, enabling a comparison of both products at different time points for each scenario. This is shown in Figure 7. Figure 8 provides a summary of the approach taken by Shen et al (2010

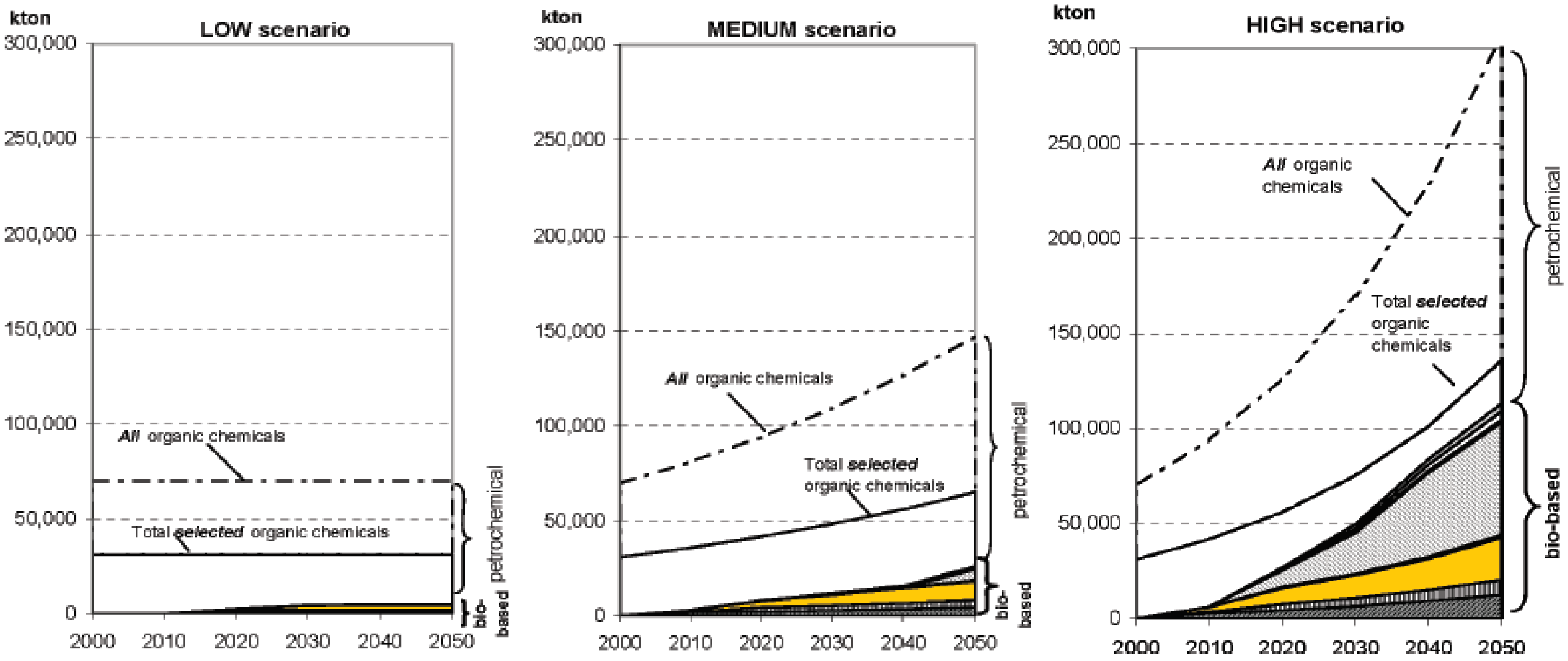


Figure 7: Scenario based projections for bio-based chemicals and petrochemicals counterparts (adapted from

Naturally, the 'High' scenario representing the favourable scenario in which fossil fuel costs are high, technology development of biochemicals and uptake is significant, subsidies are available and the chemical market is growing well relative to the other scenarios, the production of biochemicals is predicted to be feasible for more than one of the selected candidates.

**Market Projection 1**

- Companies' expected production capacity of bioplastics gaining research attention determined via surveys, personal communication with companies and industry associations and publicly available

**Market Projection 2**

- Companies were also asked for expectations of growth rate of bio-based plastics for the next 10-20 years in the surveys
- Average growth rates were used to estimate the projection between 2009 and 2020

**Market Projection 3**

Three scenarios were constructed not only considering company announcements and their expectations, but also considering technical barriers, estimated market size for bulk applications, cost competitiveness

Multiply technical substitution potential by the expected production volume of each bio-based plastic as determined by each method. A comparison of all methods was then conducted at the end.

Figure 8: Calculation of market potentials by Shen et al (2010)

The similarity between these two studies extends beyond them both using three scenarios to simulate future conditions; both utilised surveys to elicit market growth rates of their respective industries, and selected a limited number of bio-based chemicals to compare to their respective petrochemical counterparts in terms of market growth rate and other potential markers. Both studies agree too, that if a bio-based chemical is completely identical technically to its petrochemical counterpart, the substitution potential is assumed to be 100%.

Where the biochemical is not completely identical, a substitution potential lower than 100% was estimated by Shen et al. (2010) by evaluating its technical properties and consulting industry experts. This substitution potential was then multiplied by the projected production capacity of the reference petrochemical to obtain an estimate of the expected volume of bio-based chemical production over the next 20 years. The expected production capacity for petrochemicals was calculated from information gathered via surveys mailed to companies, via personal communication with senior company personnel, and through publicly available announcements.

Similarly, Dornburg et al. (2008) estimated the technical substitution potential for a biochemical using expert opinion where the biochemical presented some differences to its reference petrochemical counterpart. Unlike the relatively straightforward calculation of market potential used by Shen et al, Dornburg et al. (2008) calculated each biochemical's overall market potential as a function of its technical substitution potential, economic substitution potential and its technology diffusion rate. The overall potential was then scaled up or down as per each created scenario.

For the economic substitution potential, the authors calculated the product value for both the bio-based chemical and the reference petrochemical as the sum of the production costs and profits. The production cost was inclusive of variable costs, fixed costs, taxes, insurance feeds, plant overheads, marketing, administration, research and development, depreciation and profits. Where the bio-based chemical is chemically identical, the economic substitution potential is assumed to be 100%, else, if the product value of the bio-based chemical is lower than the petrochemical, then the economic substitution potential is assumed to be 0%. Table 3 compares the three scenarios used by the two studies.

While the use of scenarios to create 'unfavourable', 'moderate' and 'favourable' projections for bio-based chemicals may be of use for decision makers, the construction of each scenario needs to be simple enough for easy repeatability but thorough enough to capture the market's dynamics. The scenarios as presented by Shen et al. (2010) and Dornburg et al. (2008) are both sensible yet present the challenge of being overly complicated and heavily reliant on the use of expert opinion to estimate future production volumes, as is acknowledged by the authors.

Within the realm of focused studies on diversifying sugar value chains, two of the most comprehensive and systematic approaches are those described in the 2004 study conducted by the United States' Department of Energy (US DOE; (Werpy and Petersen, 2004)) and the 2015 study on sugar based platform chemicals conducted by the European Union (EU; (Taylor et al., 2015)). A key similarity between these two studies is the selection of a few sugar based chemicals from an initially large pool of candidates using stepwise selection based on pre-defined criteria.

The initial screening criteria used by the Werpy and Petersen (2004) to narrow down its pool of over 300 potential sugar based building block chemicals was unable to sufficiently distinguish candidates solely on the basis of cost of feedstock, estimated processing costs, current market volumes and prices, as well as relevance to current or future biorefinery operations. Knowing that at the time of publication in 2004, many of the products being considered were in the early phases of commercialization or still being researched, it is not surprising that there was little differentiation based on factors such as processing costs and market volumes.

Their revised screening tool thus addressed the products' infancy by incorporating the industry experience of the research team involved, like the approach taken by Taylor et al. (2015). By iteratively reviewing the feedstock, primary chemical derivative, market production data, estimates of material and performance properties as well as projected production volumes based on industry experience, the pool of over 300 chemicals was successfully reduced to just 50. Table 3 below summarizes the approach taken by Taylor et al. (2015).

Table 3: The selection methodology used by the European Union's 2015 review of sugar-based platform chemicals (adapted from Taylor et al. (2015))

| Step | Description |
|---|---|
| **1. Mapping of value chains** | Analysis of a wide array of products by mapping their starting raw material, pre-treatments, number of carbon sugars, treatment pathways, 1st derivatives, downstream catalysis and 2nd derivatives |
| **2. Focus on 94 products** | Populated a database with details of 94 products which were in some form of development |
| | Details included company name, location, products made, process technology used, Technology Readiness Level (TRL), total production capacity |
| **3. Selection of 25 products** | Market potential calculated in kton |
| | Inclusion of chemicals suggested by US DOE in 2004 |
| | Chemicals have a high level of industry activity |
| | Mostly primary products |
| | Multifunctional intermediates |
| **4. Final selection of 10 products** | Chemicals are at least at TRL 5 (pilot phase) |
| | At least one developer exists within the European Union |
| | Industry opinion suggests significant room for market growth |

Notably, the starting point of Taylor et al.'s study in 2015 was at a much later date, and thus the products being considered were at a more developed stage than in 2004. Taylor et al. (2015) therefore created an initial pool with chemicals already in some form of production, and thus had a much smaller starting pool of just 94 products.

In the first screening stage of both studies, each chemical was rigorously analysed as part of a flowchart to identify its pre-cursors, source materials, functionalities and any useful intermediates. Considering too that even in 2015 not all the proposed chemicals by the US DOE in 2004 had been fully commercialized, these too were incorporated by default within the narrowed selection.

Of note too is the classification system used by the two studies to indicate either a level of chemical functionality, or a product's position on its trajectory towards commercialization. Werpy and Petersen (2004) allocated a carbon number to each chemical indicating its potential functionality as a building block, with a higher carbon number suggesting a greater functionality; whereas Taylor et al. (2015) assigned a technology readiness level (TRL) indicating the stage of development.

In the final down-selection process, the two studies differ in that Werpy and Petersen (2004) simply continued iteratively reviewing each chemical till only 12 chemicals remained, while Taylor et al. (2015) selected only those which were at least a TRL 5, had at least one EU developer and their research indicated a significant potential for market expansion. Both studies made a point of not selecting super-commodity chemicals, as their room for further market expansion would be limited. Figure 9 overleaf summarizes the approach taken by Werpy and Petersen (2004).

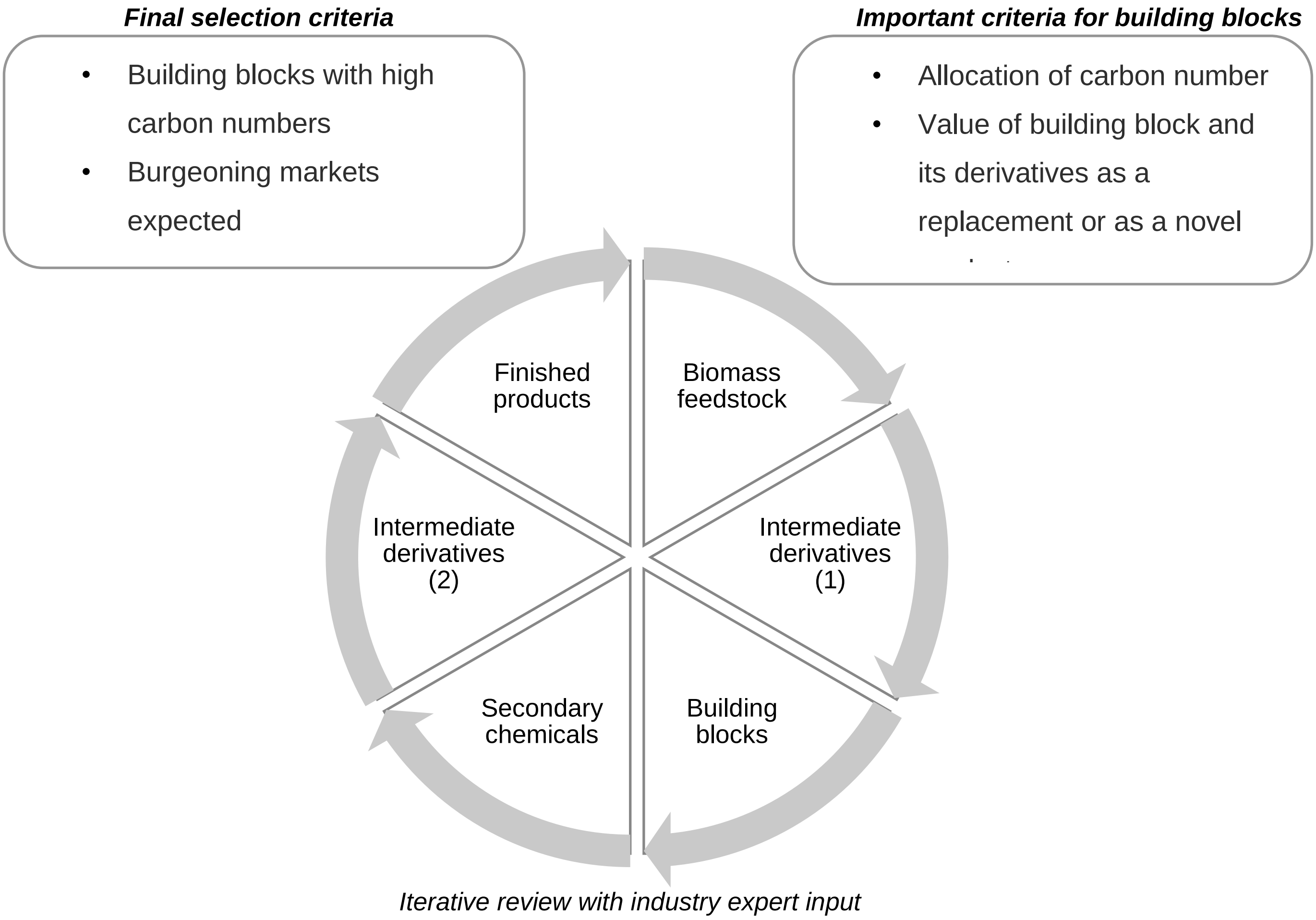


Figure 9: The selection methodology used by the US DOE's 2004 review of sugar-based platform

The screening methodologies adopted by the US DOE and by the EU are both systematic, comprehensive and are easy to understand. The major downside, however, is that despite being highly detailed, these processes will not be easily repeatable due largely to the substantial influence of industry input to select certain chemicals over others based on previous experience and to predict market growth, the revision of which would be time consuming and extremely dependent on people to respond timeously and correctly.

Moreover, a heavy reliance on industry input via personal communication and surveys features in many of the methodologies discussed, such as those used by Archer and Ghasemzadeh (1999), Dornburg et al. (2008), Shen et al. (2010), and Åstebro (2004). While some of the authors acknowledge the dependence on industry experience and the limitations it presents, it remains a highly popular method of collecting projections and estimations of a product's success. Shen et al. (2010) comment that only 7 companies completed the questionnaire sent to them, out of the total 50 companies contacted. Balachandra and Friar (1997) also comment that using surveys to collect information may not be the most reliable of methods as personal experiences and certain biases may not provide objective predictions.

### 2.5.1 Model based decision making

As an alternative to using surveys to predict future volumes of chemicals, Sammons et al. (2008) suggest using a quantitative and mathematical optimization framework which offers a high degree of repeatability, objectivity and time efficiency. Zacharakis and Meyer (2000) also promote the use of statistical models to aid in product selection and demonstrate the superiority of such models in predicting the success of a product over the estimations of industry personnel. In their study, senior industry personnel were only able to achieve a maximum of 40% accuracy of correctly classifying the success of a previously launched product, whereas the statistical models used by the authors were accurate within the range of 40% to 60%.

The mathematical optimization framework proposed by Sammons et al. (2008) is designed to include profitability within an engineering environment. Their proposed framework for allocating products for biorefining processing facilities thus combines a process system engineering approach with a business approach.

The use of such mathematical frameworks is further supported by Mansoornejad et al. (2010) in a methodology incorporating both process design and supply chain optimization in a design decision framework. Their framework builds off the example of the pulp and paper industry's decision framework as described by Chambost and Stuart (2007), which is one cited again by Batsy et al. (2014).

The three-phase methodology as described by Chambost and Stuart (2007) proposes that facilities looking to diversify their product portfolio first invest in a low technology risk product and continue then to generate revenue for diversification into more innovative and lucrative products. In so doing, the intrinsic risks associated with switching to a relatively unknown product can be mitigated.

The selection strategies available to screen chemicals then come nearly full circle as integrated methodologies such as those described by Mansoornejad et al. (2010) propose the evaluation of factors such as market growth, mirroring those approaches of earlier studies. The modern uptake of such methodologies in an engineering capacity must, however, utilise techno-economic evaluations to further aid in the selection of chemicals.

Figure 10 describes the integration of the suggestions put forward by Sammons et al. (2008) and Mansoornejad et al. (2010) with the three-phase methodology described by Chambost and Stuart (2007).

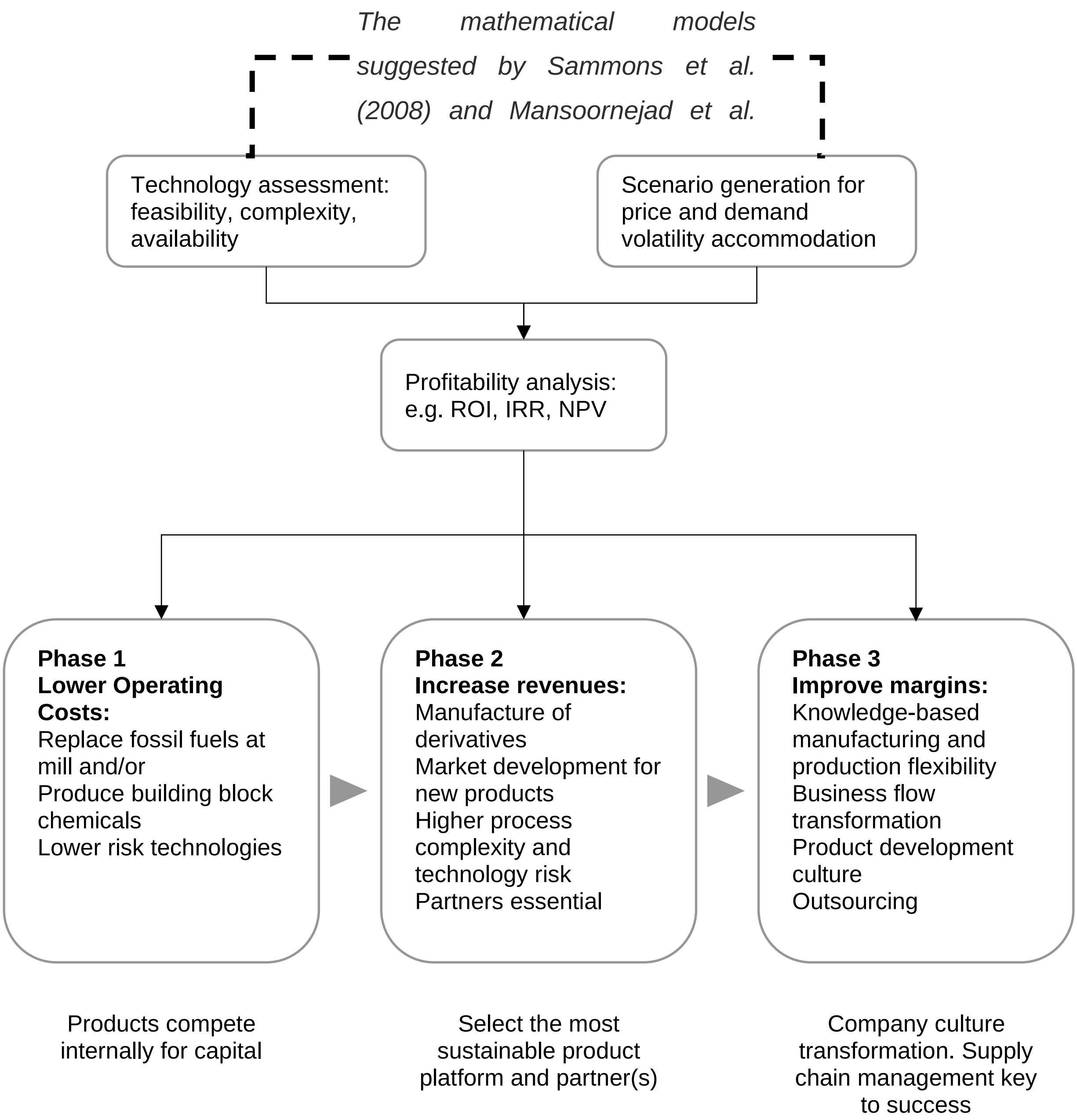


Figure 10: Three phase integrated methodologies as described by Chambost and Stuart (2007) , Mansoornejad et al (2010) and Sammons et al. (2008) (Adapted from Batsy et al. (2014))

The incorporation of mathematical models early in the process of project selection can aid decision makers to use available data to forecast market growth for both bio-based products and petrochemical counterparts, incorporating even scenarios such as those used by Dornburg et al. (2008) and Shen et al. (2010). In so doing, an integrated methodology such as the one described above removes the heavy reliance on surveys to provide key decision-making information and can remain flexible enough as suggested by Archer and Ghasemzadeh (1999).

Furthermore, such a methodology ensures that companies approach the selection of products in a holistic manner, taking into consideration not only the technical merits of products, but also use business principles to define their eventual product selection. This framework also highlights the mitigation of risk for companies, especially in the beginning phases of transitioning sugar processing facilities towards diversifying into bio-based products. In so doing, the selection of products for any portfolio should therefore be varied by technology risk, investment requirements and market growth, in effect a company should be considering more than one product at a given time for effective future planning.

## 2.6 Quantitative forecasting to improve screening techniques

The use of any of the selection frameworks discussed in Section 2.5 serves to attempt to predict which product or portfolio of products could make the best return on investment, and in some cases, have a high likelihood of sustainable demand in a growing market. A similar approach could be used to maximising environmental responsibility of the project portfolio.

The use of mathematical models as included in more recent frameworks aims to improve the accuracy of the prediction, thus building investors' confidence in the chosen product. The evolution of the selection frameworks has also manifested a flexibility of approach which had been previously limited. It gives decision makers the opportunity to customize the chosen framework as per their available data and to choose a forecasting technique at their discretion.

Sections 2.6.1 and 2.6.2 provides detail on qualitative and quantitative models as applied in the context of business decision scenarios, followed by an explanation of the mathematical structure of time series analyses, exponential smoothing, classical decomposition models and ARMA/ARIMA models.

Forecasting is a tool which uses historical data to predict the future performance of a given variable. The application of forecasting features in many key industries such as in the prediction of stock prices and can play a key role in allocating resources and budgets within a business. There exist two main categories of forecasting techniques; namely, qualitative and quantitative.

Figure 11 below summarizes the various models discussed in this section and which models would be applicable for specific applications.

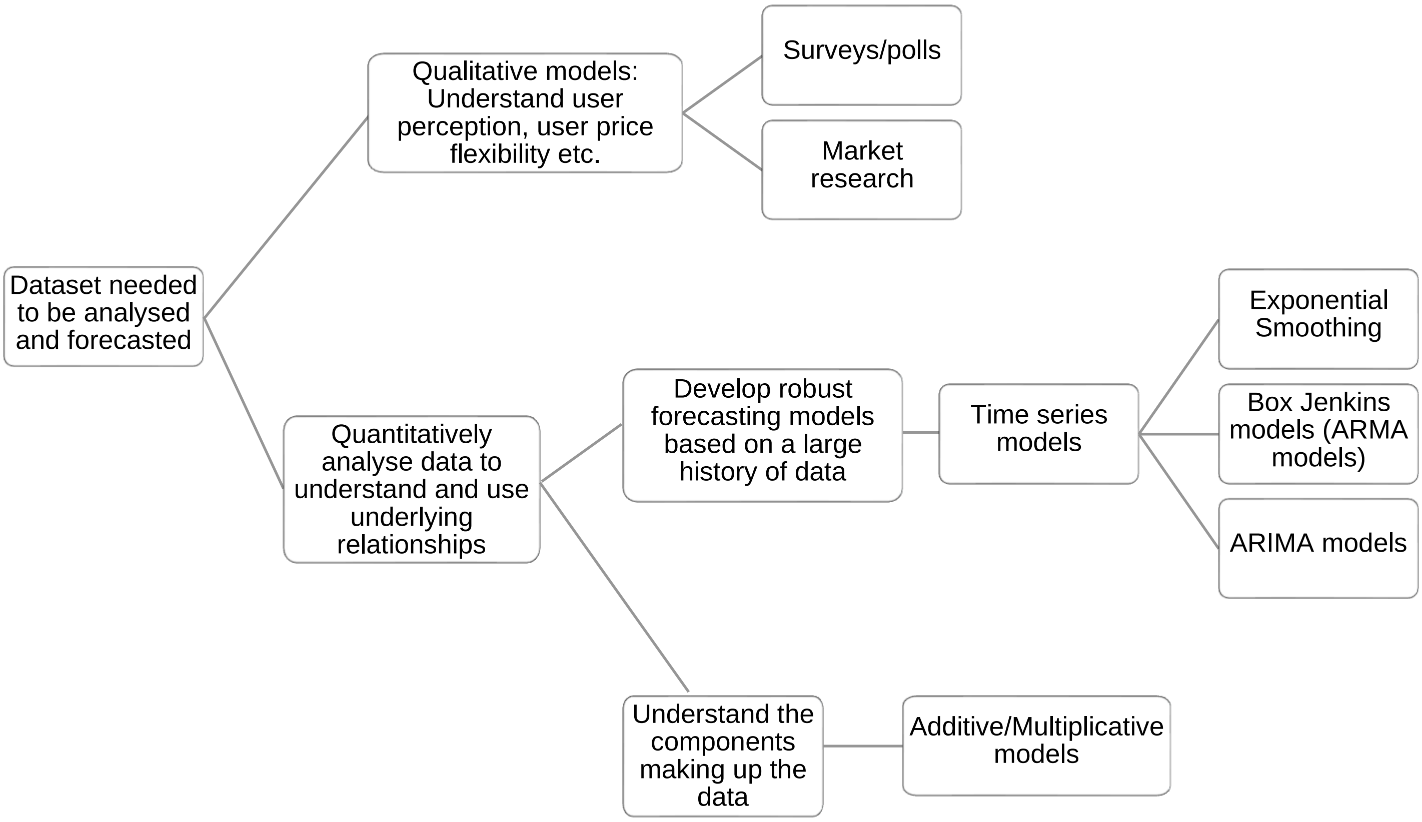


Figure 11: Decision tree of how a user may make a decision between the models discussed in

### 2.6.1 Qualitative models

Qualitative forecasting encompasses the use of surveys, polls, and market research; the objective being to collect as much relevant information as possible on factors such as consumer perception to make an informed prediction in a business scenario. The Delphi method, which is the formal classification of forecasts obtained through multiple rounds of questionnaires sent to experts, is a key qualitative forecasting technique which featured extensively in earlier studies such as those conducted by Cooper (1979, 1975).

The advantage of qualitative forecasting is its accessibility even in the absence of enough historic data and may be superior to quantitative forecasting in the short term if an unprecedented economic event is on the horizon, for example. The weaknesses are its time-consuming nature, lack of exact repeatability if a certain expert becomes unavailable, and the personal experience bias which may influence an expert's forecast.

### 2.6.2 Quantitative models

Conversely, quantitative forecasting techniques rely mainly on statistical analyses of data to generate a prediction based on historical observations. There are numerous techniques available within this category, with an increasing number having been developed with the advent of machine learning in recent years. Some common methods include time series analysis, discounting, indicator models, and econometric modelling. The latter three model types are applied extensively in investment analyses and in evaluating the economic performance of countries. They are not described in further detail here as they are outside the scope of this study. Table 4 summarizes the function of each type of quantitative model discussed and their advantages and disadvantages.

Table 4: Summary of the functions, advantages and disadvantages of the quantitative models discussed

| Model | Description | Advantages | Disadvantages |
|---|---|---|---|
| **Classical decomposition** | Decompose data into trend, seasonality and noise. Can use additive or multiplicative based on what the data looks like. | Useful when trying to isolate different components of the data in order to model them separately. | Not designed specifically for forecasting data. |
| **Exponential Smoothing** | Allocates weights to recent data points | Often used in conjunction with other models. Simple to understand. Does not require a lot of data. | May or may not be applicable for future data. |
| **Box-Jenkins (ARMA)** | Rigorous time series modelling which does not necessarily incorporate seasonality. | Able to thoroughly analyse underlying relationship between data points. Considers the entire dataset when a model is built. Able to incorporate trend, seasonality and noise. Able to be used for forecasting | Time consuming. Requires a large set of data. |
| **ARIMA** | Rigorous time series modelling incorporating seasonality. | | |

***Time series analysis***

Time series analysis is the generation of predictions based on the underlying dynamics in a set of observations recorded over time. Data may either be recorded discretely as one observation at every fixed time interval, or continuously over a specific time interval. Discrete time series are more common than continuous series in real life and will thus be the focus of the following discussion. Furthermore, while captured data may record the values of multiple variables simultaneously, the ensuing discussion will only be concerned with univariate datasets.

The objective of time series analysis is two-fold; the first being the identification of the relationships and dynamics within the sequence of observations, and the second being forecasting the variable using a model incorporating the observed patterns (Hill and Lewicki, 2013).

***Exponential Smoothing***

Exponential smoothing methods are a family of forecasting methods which have a wide application, and feature in the forecasting of deconstructed time series. The technique works by assigning weighted averages to past observations in order to forecast new values. Generally higher weights are assigned to more recent values, although this is not a fixed rule. There exist three main types of exponential smoothing; namely, single, double, and triple.

Single exponential smoothing refers to the application of the technique when there is no definitive trend or seasonality present; it is the most basic form of exponential smoothing. Double exponential smoothing is an extension of the basic technique to accommodate time series with a clear trend component, while triple exponential smoothing is the most advanced variation, and is used when there are clear trend and seasonal components (Brownlee, 2018).

In the case of combining the forecasts of the individual components through a decomposition model, the use of exponential smoothing has featured in many studies. Hilas et al. (2006) for example, utilized exponential smoothing as one of their methods to develop forecasting models for the monthly outgoing telephone calls for a university campus. Taylor (2003) also utilized double exponential smoothing to forecast short term electricity demands.

Forecasting using exponential smoothing can be done using in-built functions in statistical packages, such as with the ETS() function in R. The ETS() function is the naming convention given to exponential smoothing models accommodating Error, Trend and Seasonality in time series. Many variations of the ETS() function exist, depending on whether an additive or multiplicative decomposition breakdown best describes each component.

In R, the ETS() function is built to address Error, Trend and Seasonality additively or multiplicatively in the form of ETS(Error $_{\text{Additive/Multiplicative}}$, Trend $_{\text{Additive/Multiplicative}}$, Seasonality $_{\text{Additive/Multiplicative}}$). Using the ETS() function allows the user to obtain a single forecast value, or series of forecast values. Detail on the mathematics driving the ETS() function are available in literature.

Exponential smoothing offers a degree of complexity above other smoothing techniques such as simple moving average or centred moving averages which, when used to describe an entire time series rather than just in isolating the trend, have several limitations. In addition to simplifying the time series to such a degree as to ignore rapid rises or falls due to exogenous factors, moving average smoothing techniques have the further drawback of making the first and last few observations unavailable except as part of an averaged value. This could make explaining the trajectory of a time series difficult if presented to investors, for example. Exponential smoothing may be used as a standalone model or may be incorporated as a smoothing technique as part of another model, such as classical decomposition models.

### ***Classical decomposition models: Additive and Multiplicative***

Classical decomposition methods are some of the most common techniques used to generate forecasts in a wide variety of applications.

In the field of epidemiology for example, Dominici et al. (2002) and Stieb et al. (2003) utilized classical decomposition models to analyse the effect of air pollution on health and mortality rates. Likewise, Deng and Jirutitijaroen (2010) also used classical decomposition models to predict the load on the Singaporean electric grid; while Prema and Rao (2015) used similar models to predict solar generated electric power capacities. Box-Jenkins models feature prominently in the sphere of forecasting too, with studies ranging from predicting household electric consumptions to analysing the symptoms of diseases, such as in the studies conducted by Chujai et al. (2013) and Andersson et al. (1997), respectively.

Classical decomposition models essentially deconstruct a time series into its components of trend, seasonality and noise to examine the individual behaviours and apply a suitable model to each. Forecasts of the overall series are then generated by combining the forecasts of the individual components, as per the specific model fitted to each. In the context of time series, trend is the general systematic upwards or downwards movement of the data, which may be linear or non-linear, and which may change direction as the series progresses. Seasonality is an observed systematically repeating pattern at regular intervals, which may or may not appear throughout the series. Notably, seasonality is distinct from a business cycle, which is a non-recurring undulation of the series due to an unexpected factor. Finally, noise, or residual, quantifies the part of the data which the trend and seasonality cannot account for.

There are two types of decomposition methods: additive and multiplicative. Additive models work based on an observed measurement being equal to the sum of its trend, seasonality and noise components. Conversely, the basis of multiplicative models is an observed measurement being equal to the product of its trend, seasonality and noise components. The equations for the two models are shown below.

Additive decomposition model:

$$Equation\ 1: y(t) = Trend(T_t) + Seasonality(S_t) + Noise(R_t)$$

Multiplicative decomposition model:

$$Equation\ 2: y(t) = Trend(T_t)\ x\ Seasonality(S_t)\ x\ Noise(R_t)$$

In determining which of the two models is best applicable to a dataset, the series is first deconstructed into its individual components, which can be done using the decompose() or STL() functions in R Studio, for example. When decomposing a time series, the trend is the first component to be isolated and analysed. It is then removed from the series to result in a set of observations known as de-trended values, which are comprised of the seasonal and noise components. Next, the seasonal component is isolated from the de-trended data, and finally the residuals are evaluated.

The key steps for decomposing a time series are as follows:

1. Extract the trend component
2. This is to isolate and quantify the trend component from the overall series
3. This can be done via smoothing methods such as centred moving average, simple moving average and weighted moving average
4. Remove the smoothed trend component from the series (de-trending)
5. In additive decomposition, de-trended series = time series – trend
6. In multiplicative decomposition, de-trended series = time series/ trend
7. Extract the seasonal component
8. If an obvious seasonality is present at regular intervals, the seasonal component can be calculated as the seasonal average from the de-trended data for every period (e.g. the seasonal component for February in an annual period is the average of all the observations recorded for February in the entire series)
9. Calculate the residuals
10. In additive decomposition, residuals = time series – trend – seasonality
11. In multiplicative decomposition, residuals = time series/(trend x seasonality)

When comparing additive and multiplicative decomposition for a time series, the best model would be the one which most resembles the original series when its decomposed components are used to reconstruct the series, and the residuals are minimized.

In general, an additive model best describes a series which has a linear trend, seasonality which does not change in magnitude over time, and residuals which also have a fixed variance over time. In case of the trend being non-linear, and/or the seasonality increasing or decreasing in the size of variation with time, a multiplicative model would be better suited. The figure below illustrates this point in more detail.

Ultimately the choice between an additive model and a multiplicative model depends on which of the models produces a fitted time series using the individual components most resembling the original time series.

While decomposition models are popular because of their relatively simple nature, which allows for a straightforward explanation to non-specialists, they may not be best suited to real life scenarios where trend and seasonality may exhibit changes in direction and magnitude on multiple occasions throughout a time series. It is also possible for real life scenarios to contain periods of irregular seasonality, which cannot be adequately explained by an additive or multiplicative decomposition model either (Hyndman and Athanasopoulos, 2018a).

Moreover, as Theodosiou (2011) notes, decomposition models were not primarily developed to serve as prediction tools, but were targeted instead to aid in the understanding of the individual components. The shift toward utilizing these models in forecasting arose with research indicating the advantage of combining forecasts of the individual components to improve forecast accuracy, particularly in time series with high levels of noise.

Decomposing the time series into its individual components thus allows forecasters to apply a model of their choice to each component and combine the individual forecasts to obtain a single, overall value. Clemen (1989) reports that in so doing, the forecast accuracy can be improved relative to that obtained by using a single model to forecast the entire series. Such claims may be true in the case of the forecaster being well-versed in the range of models and forecasting techniques available, as Clemen (1989) also notes that the accuracy gain is due in part to the strength of the individual forecasting methods.

***Box-Jenkins models/ARMA models***

Box-Jenkins' models are a class of models and forecasting techniques commonly used as an alternative to exponential smoothing and classical decomposition models. While smoothing methods assign a relative weight to each observation in a time series, Box-Jenkins' models assess the correlation between observations and their historic counterparts at certain lags; this is known as autocorrelation. These models also analyse, and may incorporate, the relationship between an observation and residual errors generated from a moving average model applied to lagged observations.

Box-Jenkins models require time series to satisfy two conditions in order to generate a suitable model; namely, the mean and variance must both be stationary, i.e. their magnitudes must not be time dependent (Stava, 2015). Figures 12 and 13 below describe these two conditions in more detail.

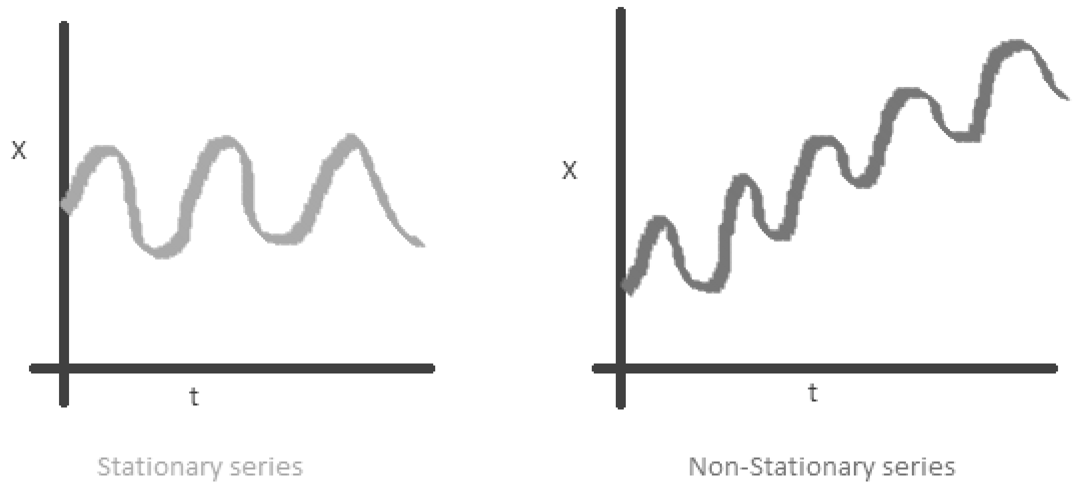


Figure 12: A diagrammatic representation of time series which have a stationary mean (left) and a series with a mean which changes with time (right) (adapted from Stava (2015) )

In Figure 12 above, the left hand side time series shows a time series which has a mean that is not time dependent, therefore the mean will remain the same regardless of where in the time series it is calculated. In the right-hand side diagram however, the series has a mean which increases with time and will be different at every point along the series, making it non-stationary.

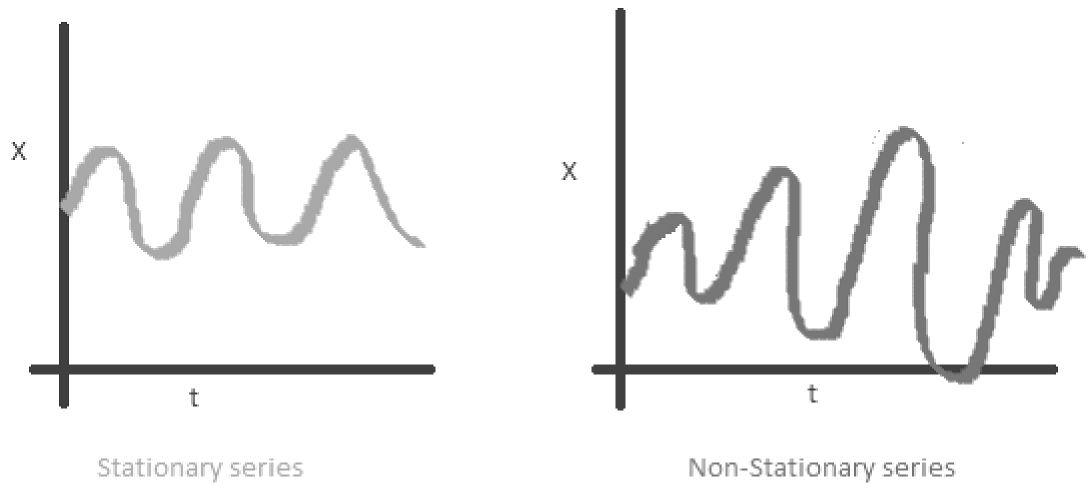


Figure 13: A diagrammatic representation of time series which have a stationary variance (left) and a series which has a variance that changes with time (right) (adapted from Stava (2015))

The left hand side diagram in Figure 13 is an example of a time series which has a stationary variance as well as a stationary mean; the magnitude of its amplitude does not vary with time nor does its calculated mean change at any point along the time series. Conversely, the right-hand side diagram shows a time series which may or may not have a stationary mean, but more importantly, has a variance which is not stationary as the amplitude of the series increases and decreases with time.

The generalized form of Box-Jenkins models is known as Auto-Regressive Moving Average, or ARMA models. These models assign a coefficient to each of the auto-regressive and moving average terms of the model and are used when the series has a stationary mean.

In the case of the time series not having a stationary mean, as is the case with many real-life datasets, Box-Jenkins models transform the series into a stationary one by a method known as ‘differencing’. One step differencing computes the differences between consecutive observations, and this can be repeated until the mean becomes stationary. Equation 3 describes how differencing creates a new series, with one less observation than the original time series.

$Equation\ 3: y_t' = y_t - y_{t-1}$

A Box-Jenkins model which takes differencing into account is said to be ‘Integrated’, thus transforming the ARMA model into an Auto-Regressive Integrated Moving Average (ARIMA) model. An ARIMA model also assigns coefficients to each of its parameters, and is generally specified as ARIMA (p,d,q)(P,D,Q)$_m$. The graphic below (Figure 11) explains each of these parameters in greater detail. In The ARIMA notation is seen to have two parts to it, the seasonal and non-seasonal coefficients which may or may not all be included in the model, depending on the time series. Table 5 explains each parameter in more detail.

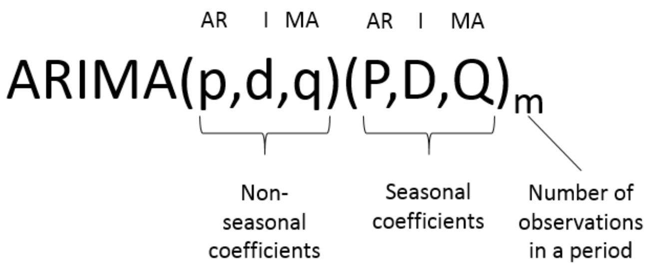


Figure 14: An explanation of ARIMA notation

Table 5: A summary of the coefficients included in an ARIMA model

| Parameter | Definition |
|---|---|
| **p** | Number of non-seasonal AR lags included in the model |
| **d** | Number of times that the raw series is differenced to make the mean stationary |
| **q** | The order of the moving average |
| **P** | Number of seasonal AR lags |
| **D** | Number of seasonal lags |
| **Q** | Number of seasonal MA lags |
| **m** | Number of observations per seasonal period (e.g. 12 monthly observations in a year) |

There is a wide variety of automated Box-Jenkins' model building functions in statistical programs such as Python and R, which can determine all the above coefficients automatically once the raw data is in a suitable format. Manual determination of the coefficients is also possible and requires careful observation of plots of the Auto-Correlation Function (ACF) and Partial Auto-Correlation Function (PACF) to determine the AR and MA coefficients. The automated programs have the advantage of being time efficient as the manual process can often be iterative in nature. Nevertheless, both approaches require a thorough understanding of the basic principles of time series and the interpretation of the ACF and PACF plots.

Figure 15 overleaf summarizes the steps needed for both the automated programs as well as the manual process.

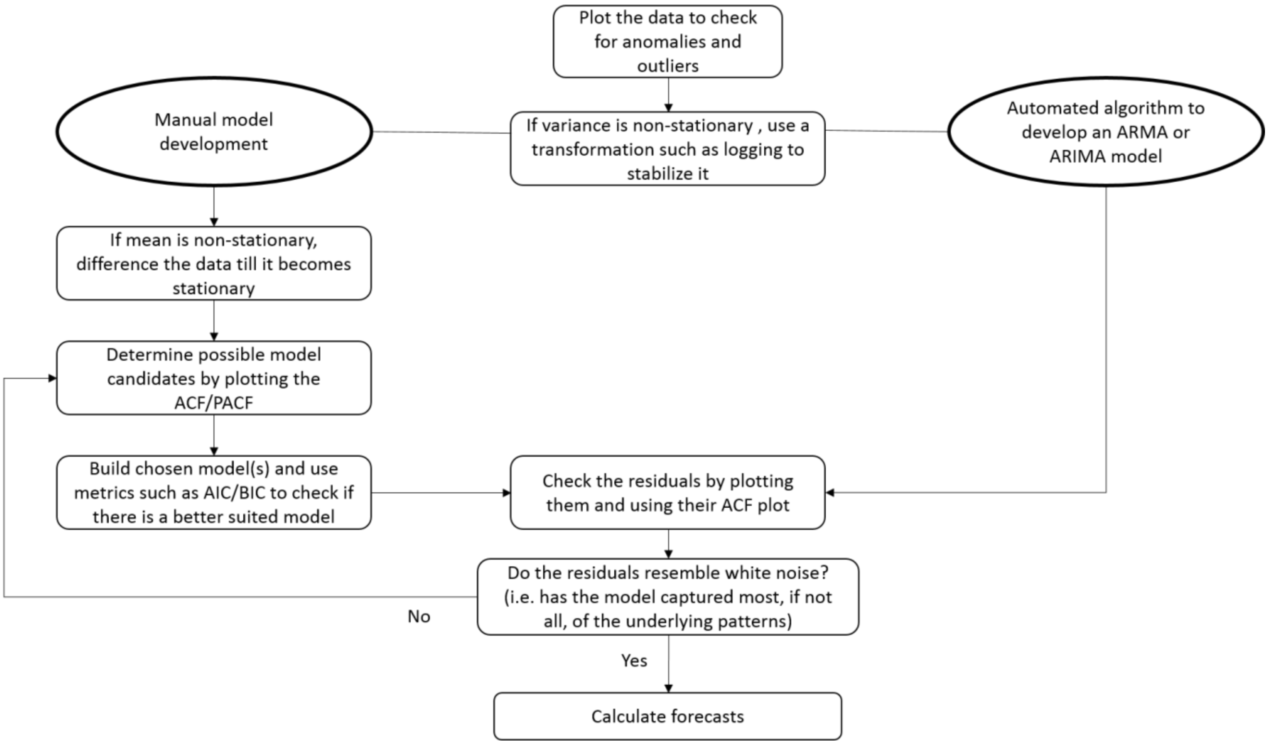


Figure 15: High level sequence of steps needed to build an ARMA/ARIMA model manually or using an automated algorithm (adapted from Hyndman & Athanasopoulos (2013)

As Figure 15 shows, the manual process of building a Box-Jenkins model is more time consuming but can offer the user a thorough understanding of why certain models are superior to others, owing to their having to investigate each in much detail. The automated algorithm essentially uses the same criteria of determining the best model from a large initial pool of possible models, but provides an output of only one model, the residuals of which are then checked. If the user desires to check the background detail on why the suggested model was deemed superior to the rest, additional steps may need to be taken.

At times the model suggested by the automated algorithm may not be in complete agreement with a manually created one despite them using the same starting dataset. One reason for this may be that the automated algorithm is able to check a larger pool of models quickly, compared to the fewer number of models which a user may be able to consider within a reasonable time. Furthermore, manual determination of a model is largely dependent on the user's experience as well as their personal judgement in choosing between models.

A common feature of both the automated and manual routes is the aim of minimizing the Akaike Information Criterion (AIC) or the Bayes Information Criterion (BIC), both of which are an indicator of the likelihood of a model to predict future values (Busemeyer and Diederich, 2014; Tran et al., 2015).

In R, it is possible to manually specify the estimated ARMA/ARIMA coefficients using the ‘Arima’ function; alternatively, it is possible to use ‘auto.arima’ function to determine an appropriate model. Auto.arima works by using a variation of the Hyndman-Khandarkar algorithm, and uses the following high level steps (Hyndman and Athanasopoulos, 2013):

1. Select the number of differences needed to make the mean stationary
2. Fit four initial models and evaluate the AIC
3. Select the model with the lowest AIC from step 2 and vary each of the autoregressive and moving average coefficients by ± 1 and evaluate each AIC
4. Continue steps 1-3 till now lower AIC can be found

### 2.6.3 Model evaluation

Regardless of the chosen model building route, in all cases of modelling it is necessary to validate the result. A popular strategy in model validation is to split the original dataset into a training set which is used to build the model, and a test set which is used to check the model’s forecasting abilities. The original dataset can be split into ratio of observations making up the training and test sets, although care is needed to ensure both that the model is built using enough data as well as avoiding overfitting the model.

In the case of overfitting, the model is not flexible enough to provide adequate forecasts outside of the original dataset, and therefore has limited usability (Cawley and Talbot, 2007). Similarly, under-fitting the model using insufficient data may also lead to limited flexibility outside the training set. Common ratios of training to test sets is to use 70:30 or 80:20, which allows sufficient data for the built model to be flexible enough to handle new data as well as being able to adequately capture the underlying model in the original data (Jank, 2011).

Once the model has been built on the training data, it can be used to forecast ahead and be validated against the test set. This is used to evaluate the model’s forecasting accuracy and can be done using a combination of residual analyses as well as quantifying metrics such as the Mean Average Percentage Error (MAPE). The MAPE is the mean of the absolute percentage errors of forecasts, where an error is defined as the difference between an actual value and the corresponding forecast. Since it is expressed as a percentage, communicating the reliability of a forecast is easily done using MAPE in business scenarios (Swamidass, 2000).

Analysis of the residuals, which are the differences between actual values and their corresponding forecasted values as output by the model, is done to verify whether any major feature of the dataset has not been captured fully. Ideally, the residuals of a well built and comprehensive model should resemble white noise, where the residuals have a mean of zero and lack of any distinct patterns.

The main features necessary for residuals to resemble white noise are:

- The residuals as plotted against fitted values should be symmetrically distributed around the zero axis, thus showing the model to be correct on average for all fitted values
- The residuals should be clustered around low y-values, thus showing the residuals to be relatively small
- There should be no clear patterns in the residual distribution, thus indicating constant variance

Like the automated packages available for model building, the analysis of residuals can be done with ease in R using automated graphical plots.

## 2.7 Gaps in current knowledge

Based on the existing literature on product selection models used in the context of bioproducts applicable to the South African sugar industry, the key points are:

- Limited work has been done on exploring less commercialized or researched platform chemicals as solutions to the sugar value diversification problem
- Application of forecasting models using time series, especially ARIMA models has not been reported in the context of bioproducts
- No work has been done on devising a solution for South Africa's sugar industry based on overall manufacturing activity in the country

## 2.8 Defining the research project

### 2.8.1 Problem Statement and objectives

The South African sugar industry requires diversification of its value chain mainly due to financial difficulties resulting from competitive global prices, droughts in South Africa and changing consumer buying patterns.

To date, the solutions put forth on valorizing sugar value chains globally have not made extensive use of mathematical forecasting models, especially those based on time series. Furthermore, the diversification routes focused on thus far have been on highly commercialized chemicals or those close to commercialization.

Continuing operations of the local sugar industry without diversification runs a high risk of the industry's collapse and the loss of countless jobs. Thus, exploring the diversification using mathematical forecasting and potentially identifying a non-mainstream and less commercialized chemical for investment can create avenues for the industry's ultimate survival.

The objectives of this study are therefore to:

- Find a dataset that will be suitable for modelling South Africa's manufacturing industry and that can be used for forecasting the potential demand of sugar- based chemicals
- Evaluate at least three mathematical modeling techniques using the above identified dataset to be used in forecasting chemical demand in South Africa
- Forecast manufacturing activity in South Africa forward 20 years using the best performing model and identify the industry which would be best suited for a sucrose-based chemical investment

- Analyse the research progress made on sugar-based biochemicals which have been deemed not ready for commercialization in recent studies
- Evaluate the most progressed chemicals in the context of being implemented in South Africa’s manufacturing sector using the industry forecasts
- If implementing one of the lesser commercialized chemicals in South Africa is not supported by the industries’ forecasts, then a chemical should be selected for the identified best performing industry
- Select one main sucrose-based chemical for the sugar industry to invest into the identified industry
- Evaluate the various technologies available to produce the chosen chemical
- Perform an economic analysis for the chosen technology
- Conduct one optimization to evaluate the effect on the plant profitability over 10 years

### 2.8.2 Research aims and key questions

The aim of this study is to use mathematical forecasting to identify the best possible industry for sugar to be re-routed in to manufacture a chemical which can help sustain the South African sugar industry financially.

The key questions are therefore:

1. What are the key attributes of a dataset which can be used to analyse the historic production level data of manufacturing industries in South Africa?
2. What do the production profiles of manufacturing industries in South Africa look like?
3. Which one model is most appropriate to characterize and forecast all industries’ production level data?
4. Which industry does a selection matrix factoring in the production forecast and growth rate identify as being best suited for an investment?
5. Are chemicals previously deemed not commercially ready now ready for commercialization and do they fit within the identified industry?
6. Does the technoeconomic analysis reveal this chemical to be profitable over a plant life of 10-15 years?

# 3 Data selection

One of the key findings from the literature review was the clear lack of studies on valorising sugar in South Africa without making use of forecasts based on a dataset focused on South Africa's economy. In order to address this gap and create a sugar chain diversification solution for South Africa, a dataset that best describes the potential market success of a sugar- based product needed to be found.

The purpose of this dataset is to describe the production trend over a period of at least ten years since the present day for key manufacturing industries. This data will then be used to forecast trends forwards in time to identify the best industry for product placement and thus choose a suitable product to divert sugar into.

Manufacturing activity was chosen as the focus of the selected data because this metric provides insight into historic production outputs, and therefore represents a measure of potential future consumer demand in domestic markets as well as in international markets to a smaller extent.

## 3.1 Characteristics of the target dataset

The following set of criteria was used to evaluate datasets and choose the one best suited to characterizing the South African market and which has the most reliable datapoints for forecasting:

1. The data needs to have a reliable and reputable source; preferably published by a known public entity
2. There needs to be historic data available of at least ten years in order to build a model
3. There need to be clear explanations of:
    a. How the data was collected
    b. Whether any alterations or omissions had been made
    c. Any missing data points
4. The data needs to represent manufacturing activity in South Africa for at least five industries
5. The data needs to be easily accessible for future analyses
6. The data needs to specific to individual industries and not grouped together as a single metric to represent production activity

## 3.2 Datasets considered

A range of datasets were considered for use in this study. Table 6 summarizes the findings from each.

Table 6: A comparison of the datasets considered

| Data source | Description | Advantages | Disadvantages |
|---|---|---|---|
| **Trading Economics** (Trading Economics, 2019) | Manufacturing statistics in South Africa, including some forecasts | 1. Specific to South Africa<br>2. Wide array of metrics available<br>3. No omitted data reported | 1. Unclear explanation of how and on which metrics the data was collected.<br>2. Full dataset not available for free to the public<br>3. Not broken down by industry<br>4. No schedule set for updated publications |
| **The World Bank** (The World Bank, 2018) | Industrial production in South Africa | 1. Specific to South Africa<br>2. 10 years' worth of data available to forecast with<br>3. Published by a well-known source | 1. Unclear explanation of how and on which metrics the data was collected.<br>2. Not broken down by industry<br>3. No schedule set for updated publications |

| Data source (contd.) | Description | Advantages | Disadvantages |
|---|---|---|---|
| **The Organisation for Economic Co-operation and Development** ((OECD), 2018) | Industrial production in South Africa | 1. Specific to South Africa<br>2. Published by a well-known source | 1. Unclear explanation of how and on which metrics the data was collected.<br>2. Incomplete dataset<br>3. Not broken down by industry<br>4. No schedule set for updated publications |
| **Statistics South Africa** (Statistics South Africa (Stats SA), 2016) | Manufacturing production data dating back to 1998 | 1. Generated from within South Africa<br>2. Freely available to the public<br>3. Schedule of future releases available<br>4. Broken down into individual industries (more than five available)<br>5. Deemed reliable as it is used by the government for their policy making<br>6. Clear explanation of how the data was sourced | 1. Smaller industries could have been included too<br>2. Some of the industries could have been broken down further |

Considering the set evaluation criteria, three of the four datasets considered were deemed inappropriate for use in this project. Datasets from Trading Economics, The World Bank and the OECD-FAO were ruled out based on them not having clear and easily available explanations of how the data had been collected.

Furthermore, while these sources are widely considered to be of good repute and often cited when assessing a country's overall economic performance, the datasets offered only high-level statistics of overall industrial or manufacturing production. For the purpose of this project, it was preferred to use more granular data such as statistics by manufacturing industry in a country.

Moreover, while Trading Economics had a database of extensive historic data as well as forecasts, these were available only after payment, which was unavailable for this research. Additionally, the OECD-FAO database was deemed questionable when the statistics to produce sugar was investigated, as their data suggested South Africa only began to produce sugar from 2001 onwards. This is clearly untrue, and thus contributed to the argument against using this dataset.

Of the sources considered therefore, the manufacturing production statistics in South Africa as published by Stats SA was deemed best suited for this project for several reasons. Besides the data being available at a granular level to assess the manufacturing production output of individual industries, there is a clear explanation of how the data was collected as well as an identification of the limitations of that method. There are no missing data values, as well as an absence of outliers and the data goes as far back as 1998. It is also publicly available in both MS Excel and ASCII formats which makes data manipulation easy. Since the data is updated monthly, it is likely to be easily accessible for any future analyses like this project or even the updating of the results herein.

As the publication explains, the main purpose of the data is to estimate Gross Domestic Product (GDP) which in turn is used to develop and monitor government policy. The data is therefore structured to estimate the true level of manufacturing activity in the country, and thus can be considered reliable.

### 3.2.1 Details of the chosen dataset

The manufacturing production dataset published monthly by Stats SA includes three types of data:

1. Seasonally adjusted indices of physical production volume (All indices in the chosen dataset are based relative to values in 2015; i.e. 2015 production = 100 points)
2. Unadjusted actual indices of physical production volume
3. Seasonally adjusted value of sales; represented as Rand values in R 1000 units
4. Actual value of sales; represented as Rand values in R 1000 units

In accordance with international practices, the indices in the dataset are rebased every five years. The Rand values are current values at the time of publication. For the purposes of this study, it was decided to use the actual value of sales as these data would provide an easy interpretation of future production volume without reference to a base year, as well as being without any seasonal adjustment which may or may not comply with the chosen forecasting technique.

The scope of the dataset is to report the results of a questionnaire-based survey which is sent out to a large sample of companies in South Africa. The large sample survey (LSS) covers enterprises registered for Value Added Tax with the South African Revenue Service (SARS), and which are mainly engaged in manufacturing activities. The survey sample is meant to gain a representative view of the overall manufacturing activity, because sending a survey to every single enterprise would be overly complicated.

The dataset includes results from South African based activities of enterprises which operate in multiple countries but does not include the activities of South Africa based companies in other countries. The collected data is inclusive of purchases of raw materials as well as the income from a company’s own manufactured products.

There are 55 industries in total reported on in the manufacturing data but only eight were selected for use in this study. These included beverages; basic chemicals; other chemical products; rubber products; textiles; motor vehicles, parts and accessories and other transport equipment; petroleum, chemical products, rubber and plastic products; and plastic products.

These industries were selected because of their broad classifications which would allow a variety of chemicals to be considered as substitutes within them. Furthermore, it was difficult to imagine how sugar-based chemicals would be able to penetrate industries such as furniture; glass and non-metallic mineral products or footwear, for example.

The industries whose data was not used were thus considered to be too niche or without an obvious prospect for chemical substitutions.

## 3.3 Observed trends of industries in South Africa

To understand the manufacturing trends in South Africa, the sales data was plotted for the following industries using Stats SA's dataset:

- Beverages
- Textiles
- Motor vehicles
- Plastics
- Rubber
- Basic chemicals
- Other chemicals
- Petroleum

Data for other industries reported in the dataset was not used as they were considered unlikely to feature a potential market for sugar-based chemicals (such as furniture or leather industries).

The graphs of the historic trends for each of these industries are available in Appendix A.

The highest value industry in terms of sales in USD million is petroleum which recorded its peak sales in 2014 at approximately USD 3 billion, whereas the lowest value industry is the textiles industry which recorded its peak of approximately USD 60 million in 2003.

Of all the industries, the beverages industry demonstrates the most consistent year on year growth in sales and a predictable seasonality, of higher sales during the summer months and lower in winter. Some industries such as the basic chemicals' and the petroleum industry show peaks between 2008 and 2009 which interestingly coincide with the financial crash around the same time.

There is an overall growth in sales observed for all industries except for the textiles and rubber industries, both of which are also the lowest value manufacturing sectors in South Africa according to the dataset. Neither industry shows drastic peaks or spikes, but rather show stagnancy since 1998, which may be reflective of the lack of investment in these industries and the global purchasing trend for these products.

Section 4 will explore forecasting methods for this dataset. The results will form the basis on which a valorisation solution is proposed for the South African sugar industry.

# 4 Predictive model selection and build

Having selected a suitable dataset, the next step was to choose an appropriate forecasting technique. It was desired to find a forecasting technique which would be suitable for most, if not all, of the industries' data in order to generate highly comparable forecasts.

This section describes the findings from exploring various modelling techniques and the subsequent model building process with the selected model type.

## 4.1 Methods explored

### 4.1.1 Naïve method

The Naïve method is one of the most basic forecasting techniques which can be used with time series data and requires setting the forecast value to be equal to the last data point in the dataset (Hyndman and Athanasopoulos, 2018b). The forecast can effectively be extended to as far as desired but will remain unchanged from a flat line.

An example of the Naïve method as applied to the beverages industry's data is shown in Figure 16 below.

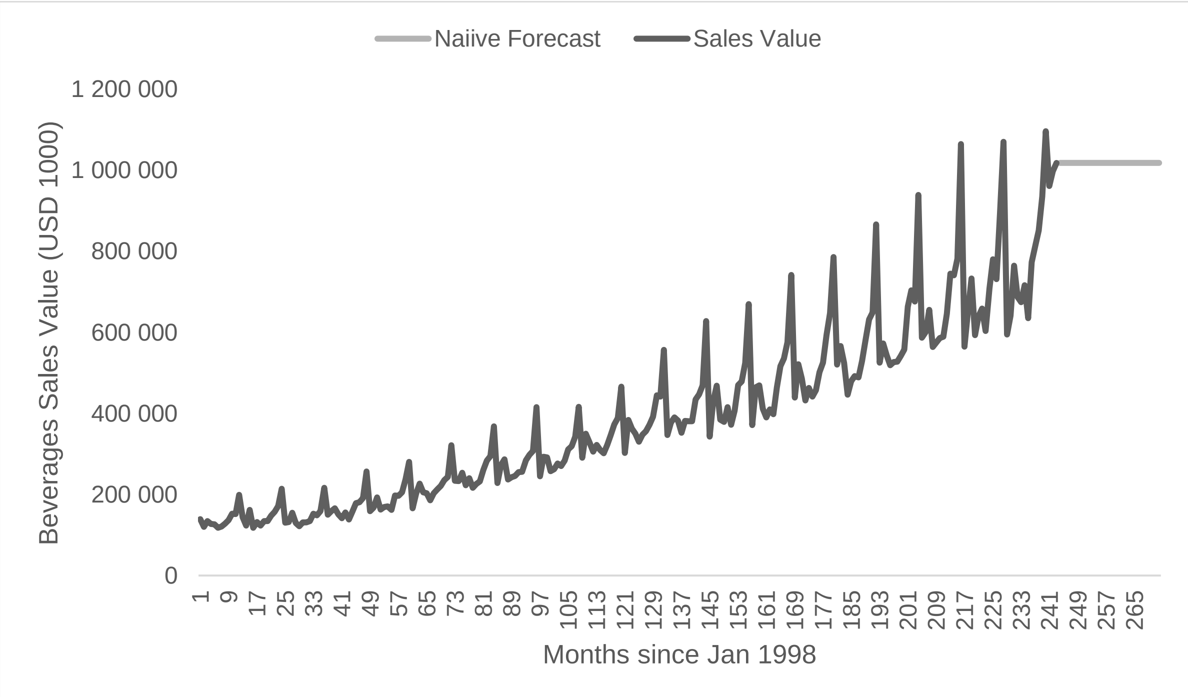


Figure 16: An example of the Naïve method applied as a forecasting technique to the beverages' industry data

This model was considered too simplistic for this study as it would be unable to capture any of the trend or seasonality of the data and would not provide enough information to decide between industries for chemical product placement.

#### 4.1.2 Simple moving averages

The technique of using simple moving averages to forecast the industries' data forward was applied to each of the chosen eight industries based on 3-month, 6 month and 12-month averages to compare the forecasts achieved from a quarterly, biannual and annual basis.

The technique involves calculating the average of a set number of consecutive historical points and continuing this till the last data point is reached and if a forecast is needed, extending the forecast forward the same number of points (Hyndman and Athanasopoulos, 2018c). For example, on a 3-month basis, the first simple moving average point would be calculated at the fourth month point of a dataset comprising of monthly data points. The model could be calculated for every subsequent month by averaging the previous three months' data points.

The graphs of each industry's forecasts using simple moving averages can be found in Appendix B.

This technique can generate quick forecasts based on the available data and works well with the time series at hand. The drawbacks in the context of this study are firstly that the forecast generated is entirely smoothed out and does not capture any of the seasonality that is highly characteristic of some industries' data. While this will still allow a conclusion to be made based on which industry is likely to demonstrate rapid, sustainable growth, the other drawback is that simple moving averages can only provide a very short range of forecasts.

While using 3 months as the basis of a quarterly averaging technique, the most the forecast can reach to is 3 months beyond the last datapoint. Thus, the maximum forecasting horizon achievable with this technique is 12 months ahead of the last data point, unless a much lower averaging frequency such as 24 months is used to extend the forecast. Such an unusual averaging frequency would run the risk of oversimplifying any unusual peaks or spikes in the data.

Consequently, this technique was considered unsuitable to adequately represent the available data and would essentially only make use of the last few datapoints to provide an extremely limited forecasting view. Furthermore, it would not represent any seasonality or unusual events observed in the data thus oversimplifying the overall history of each industry.

### 4.1.3 Weighted moving averages

The application of weighted moving averages would involve applying the same technique as for simple moving averages except for assigning a greater weight to more recent data points. Considering that the same limitations as simple moving averages would apply to using weighted moving averages, namely having only a very short forecasting horizon and the risk of oversimplifying the data, this technique was decided as not being suitable for the purposes of this study.

### 4.1.4 Simple exponential smoothing

In simple exponential smoothing, the forecasted value is based on the last value as well as the last forecasted value, as per Equation 4. The error term is calculated as the difference between the forecast and the original data point.

$Equation\ 4\ y_n = y_{n-1} + \alpha error_{n-1}$

Given its wide application, simple exponential smoothing was considered a possible modelling technique for the given dataset.

A major limitation of this technique, however, is that is works best in forecasting data with no clear trend or seasonality (Hyndman and Athanasopoulos, 2018d). The datasets for the rubber industry and for the textiles industry could be a suitable candidate for this model's application; however simple exponential smoothing would not be a universal solution to all the datasets at hand.

### 4.1.5 Holt's method and Holt-Winter's method

The next technique considered to model and forecast the data was Holt's linear trend method, or double exponential smoothing which allows forecasting data with a trend (Hyndman and Athanasopoulos, 2018e). The limitation of this method is that while it may be suitable for industries with a strong trend, it will not be a suitable model for some of the industries' data which does not show an upward or downward trend.

Furthermore, Holt-Winter's method, or triple exponential smoothing, is also not a suitable model because it is designed to accommodate data with strong seasonal patterns. Some industries' data in the chosen dataset does display strong seasonality but since neither of these modelling techniques would be the best option to apply to all the datasets, it was therefore decided not to apply these.

### 4.1.6 ARIMA

Having considered several traditional models which are used for forecasting time series data, it was found that these would be unsuitable for the industries' data which are included in the chosen dataset for this study. There exists a large amount of variability in the amount of trend and seasonality that each of the eight industries' data displays, which makes it challenging to use many of the straightforward conventional techniques.

Further research into this problem suggested that a class of Box-Jenkins' models called Autoregressive Integrated Moving Average models may be a suitable fit for the dataset. This is because unlike other models which use the trend and seasonality in data, ARIMA models aim to describe the autocorrelations, or correlations of the data points to their own deviation from the mean, in the data and thus do not require the raw data to meet trend or seasonality criteria.

ARIMA models require a large amount of reliable data, which in this case was available in the chosen dataset. Furthermore, the models are known to provide stable estimation of time-varying trends with relatively few parameters.

The limitations of the models include the risk of overfitting the data, mis-identifying an appropriate model, and the need to spend a lot of time understanding the data and explaining the results in an easy to understand manner.

## 4.2 Application of ARIMA models to the dataset

R was selected as the software of choice in which to develop the Box-Jenkins models and forecast them. It was also decided to use the auto.arima function in R to build the models as per the technique described in the literature review. The reason for choosing the automated algorithm over a manual development of each model was because the algorithm's ability to traverse a wide range of possible models in a short amount of time, whereas a manual development would be slower and carries a risk of not arriving at the optimal model in the given time.

Once the models have been created and validated, the next step is to select the industry whose forecasts suggested the most sustainable growth and market demand for the sugar industry to invest sugar based biochemical in. For this a type of selection matrix will prove useful.

The aim of using these selection matrices was to add a degree of refinement in choosing a champion industry beyond just observing the prospective sales. In so doing, each industry was evaluated with a combination of weights assigned to both the sales values as well as to the growth rates so that the champion industry would be selected on the basis of it outperforming the rest on both the growth rate aspect as well as on the predicted revenue generation.

Finally, after analysing the matrices and choosing the industry with the highest overall scores across the three milestone years, the last step was to select a chemical to evaluate the techno-economics for in the chosen industry. This is described further in section 4.2.1.

### 4.2.1 Model construction

Figure 17 describes the high-level methodology of building the models:

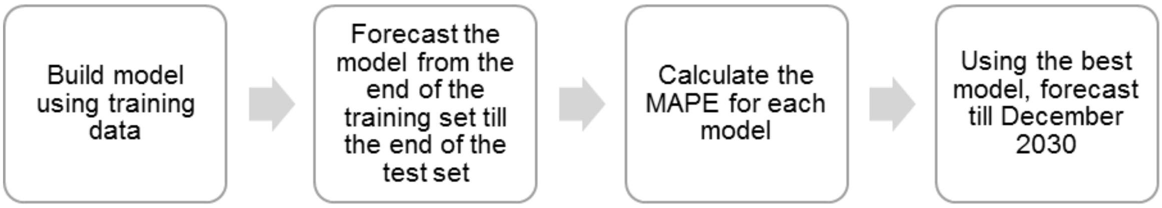


Figure 17: A high level summary of the model building process using auto.arima

As Figure 17 describes, there are four main steps in obtaining forecasts of the sales values for each industry. After building each model using auto.arima, validation is performed by forecasting the model from the end of the training set till the end of the test set then the Mean Absolute Percentage Error is calculated. Once all the MAPE values have been calculated, one single model is selected for each industry which is then used to forecast the training data till December 2030.

The procedure followed using auto.arima to build each model was the following:

1. Load the training sales value dataset for each industry from an MS Excel file
2. Define the data as a time series object in R
3. Plot the data to note any anomalies, missing values or outliers
4. Where a non-stationary variance is observed in the training data, the variance is stabilized by applying the $\log_{10}$ function
5. Apply the auto.arima function to the transformed training data
6. Check the residuals for each model using the checkresiduals() function

Once the models were built using the training data, validation was conducted using the test data set as per the steps below:

1. Load the test sales value dataset for each industry from an MS Excel file
2. Define the data as a time series object in R
3. Plot the data to note any anomalies, missing values or outliers

4. Forecast each model to predict sales values from the end of the training set to the end of the test set in order to compare
5. Apply the antilog to the forecasted data to re-establish the correct variance
6. Plot the test set and the forecasted values on the same set of axes to visualize the closeness of fit
7. Export the forecasted data to MS Excel
8. Calculate the Mean Absolute Percentage Error (MAPE) for each model

The above steps were repeated using training to test ratios of 70:30; 80:20 and 90:10. The first two combinations, namely 70:30 and 80:20, are commonly used in literature, and the additional combination of 90:10 was added in case the other two ratios were unable to produce a model with a tolerable MAPE.

The tolerance level was arbitrarily chosen as an MAPE of 10%.

Once all three training to test ratios had been used to build models for each industry, one model was chosen to represent each industry. In order to minimize error and obtain an accurate a forecast as possible, the model with the lowest MAPE for each industry was selected.

Exceptions were made if the 90:10 split had the lowest MAPE but either the 70:30 and/or 80:20 also had MAPE values below 10%, in which case the next best ratio was given preference over the 90:10 to reduce the risk of overfitting.

### 4.2.2 Selection matrices

Performance matrices were constructed to compare industries based on growth rate as well as projected sales values.

The matrices were constructed for the selected milestone years of 2022, 2025 and 2030 and the results then compared across all industries. First, factors ranging from 10-100 were assigned to intervals of sales values via the following:

For each milestone year, the sum of all the forecasted monthly sales values for each industry were added together to generate a cumulative value representing January - December

Next, the range of sales values for all industries was analysed to identify the minimum and maximum for each milestone year

Intervals of sales values spanning a range from the minimum to the maximum were created

A factor between 10-100 was assigned to each interval, with higher sales value intervals being assigned higher factors

For example, if between January and December 2022, the range of sales values for the eight industries ranged from R 6 million to R 367 million, then the sales value intervals would be assigned factors such as in Table 7.

Table 7: An example of factors assigned to sales value intervals for a milestone year in the creation of selection matrices

| Sales Value Range | Factor |
|---|---|
| 0-5 | 10 |
| 5-10 | 20 |
| 10-50 | 30 |
| 50-100 | 40 |
| 100-150 | 50 |
| 150-200 | 60 |
| 200-250 | 70 |
| 250-300 | 80 |
| 300-350 | 90 |
| 350-400 | 100 |

Next, the growth rate for each industry was calculated for the three milestone years relative to the sales value achieved between January and December 2018 for the same industry. This was done to have the same basis for comparison for all industries. The following steps were followed to generate intervals for the growth rate, like the procedure followed for the sales value ranges.

1. For each milestone year, the sum of all the forecasted monthly sales values for each industry were added together to generate a cumulative value representing January – December
2. Each cumulative sum was divided by the cumulative sales in the period of January – December 2018
3. Next, a range of growth rate intervals was created to accommodate the minimum and maximum calculated growth rates from the previous step
4. Each growth rate interval was assigned a factor between 10-100, with higher intervals being assigned higher factors

Once both the sales values as well as the growth rates had been assigned factors, matrices such as the one below was constructed for each industry, for each of the three milestone years. Figure 18 outlines this process for one milestone year.

| | | Growth Rate Factor | | | | |
|---|---|---|---|---|---|---|
| | **2022** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| Sales Value Factor | 0.2 | | | | | (0.8 x GRF) + (0.2 x SVF) |
| | 0.4 | | | | (0.6 x GRF) + (0.4 x SVF) | |
| | 0.5 | | | (0.5 x GRF) + (0.5 x SVF) | | |
| | 0.6 | | (0.4 x GRF) + (0.6 x SVF) | | | |
| | 0.8 | (0.2 x GRF) + (0.8 x SVF) | | | | |

GRF: The value of the Growth Rate Factor between 10 -100 as determined by the industry's particular growth rate interval
SVF: The value of the Sales Value Factor between 10 -100 as determined by the industry's particular sales value interval

Figure 18: A demonstration of how a selection matrix was constructed using the sales values and growth rates

### 4.2.3 Model build and validation

The models built for each of the eight industries using auto.arima were evaluated based on their Mean Absolute Percentage Error (MAPE). The validation is summarized overleaf for each industry.

There are three MAPE values for each industry; one for the model built using 70% of the training data, one for the model built using 80% of the training data and one for the model built using 90% of the training data. The table was used to determine which model would be used to forecast each industry's sales from December 2018 to December 2030.

As the validation results in Table 8 show, there is a large variation in the MAPE values for most of the industries, with no clear pattern as to whether a larger training data set corresponds to a higher or lower MAPE value. Furthermore, many of the MAPE values exceed the assumed threshold of 10%, with the highest value being 24.7% calculated for the ARIMA model built using 80% of the plastics' industry's training data. The lowest MAPE value is 3.32%, calculated for the ARIMA model built using 80% of the Other Chemicals' training dataset.

The model chosen to forecast each industry's sales data was that having the lowest calculated MAPE, unless if the 90:10 split had the lowest MAPE but either the 70:30 and/or 80:20 also had MAPE values below 10%, in which case the next best ratio was given preference over the 90:10 to reduce the risk of overfitting.

Table 8: Summary of the MAPE values used to assess each ARIMA model built for eight of South Africa's manufacturing industries

| **Beverages** | | **Basic Chemicals** | | **Other Chemicals** | | **Petroleum, chemical products, rubber and plastic products** | |
|---|---|---|---|---|---|---|---|
| **70% training/test split** | | | | | | | |
| **Number of training points** | 168 | Number of training points | 168 | Number of training points | 168 | Number of training points | 168 |
| **Number of test points** | 72 | Number of test points | 72 | Number of test points | 72 | Number of test points | 72 |
| **MAPE** | 5.74% | MAPE | 20.0% | MAPE | 3.39% | MAPE | 15.87% |
| **80% training/test split** | | | | | | | |
| **Number of training points** | 192 | Number of training points | 192 | Number of training points | 192 | Number of training points | 192 |
| **Number of test points** | 48 | Number of test points | 48 | Number of test points | 48 | Number of test points | 48 |
| **MAPE** | 4.68% | MAPE | 22.1% | MAPE | 3.32% | MAPE | 24.7% |
| **90% training/test split** | | | | | | | |
| **Number of training points** | 216 | Number of training points | 216 | Number of training points | 216 | Number of training points | 216 |
| **Number of test points** | 24 | Number of test points | 24 | Number of test points | 24 | Number of test points | 24 |
| **MAPE** | 6.70% | MAPE | 7.2% | MAPE | 2.88% | MAPE | 5.09% |

| **Plastic products** | | **Rubber products** | | **Motor vehicles** | | **Textiles** | |
|---|---|---|---|---|---|---|---|
| **70% training/test split** | | | | | | | |
| Number of training points | 168 | Number of training points | 168 | Number of training points | 168 | Number of training points | 168 |
| Number of test points | 72 | Number of test points | 72 | Number of test points | 72 | Number of test points | 72 |
| MAPE | 20.26% | MAPE | 17.93% | MAPE | 23.8% | MAPE | 17.7% |
| **80% training/test split** | | | | | | | |
| Number of training points | 192 | Number of training points | 192 | Number of training points | 192 | Number of training points | 192 |
| Number of test points | 48 | Number of test points | 48 | Number of test points | 48 | Number of test points | 48 |
| MAPE | 19.63% | MAPE | 8.19% | MAPE | 6.62% | MAPE | 17.9% |
| **90% training/test split** | | | | | | | |
| Number of training points | 216 | Number of training points | 216 | Number of training points | 216 | Number of training points | 216 |
| Number of test points | 24 | Number of test points | 24 | Number of test points | 24 | Number of test points | 24 |
| MAPE | 8.63% | MAPE | 4.53% | MAPE | 7.46% | MAPE | 11.2% |

Table 9 shows which ARIMA model was used for each industry to forecast with.

Table 9: Selected ARIMA models for forecasting manufacturing sales

| Industry | Selected ARIMA model | MAPE |
|---|---|---|
| Beverages | 80% training data | 4.68% |
| Basic Chemicals | 90% training data | 7.20% |
| Other Chemicals | 80% training data | 3.32% |
| Petroleum | 90% training data | 5.09% |
| Plastics | 90% training data | 8.63% |
| Rubber | 80% training data | 8.19% |
| Motor Vehicles | 80% training data | 6.62% |
| Textiles | 90% training data | 11.2% |

The limitations of this approach are that in using 90:10, there is a risk of overfitting the model. It is also possible that other ratios such a training to test ratio of 60:40 could be better suited to some industries' data than those combinations considered here.

### 4.2.4 Forecasts

Forecasts generated for each industry from December 2018 till December 2030 using the models selected in the previous section are shown graphically in Appendix A, along with the historic data series used to build each model. Each forecast is plotted alongside its upper and lower 80% confidence bands.

Based on these plots, it can be observed that the ARIMA models are a good fit for most of the industries but there are some instances where perhaps an alternative ARIMA model or another type of model altogether may be better suited to some industries' data.

The beverage industry's data for example is observed to have a very regular seasonal pattern of sales increasing during the summer months, and a dip is observed during the cooler months. This is expected as consumers generally purchase fewer cold drinks during winter, of which the juices and soft drinks form a large part of the beverages' sales. Considering the steady year-on-year increase in beverage sales, which has also never experienced a dip in any year, the forecasts are therefore in line with what would be expected in future too; that is, the forecasts are for continued growth at a linear rate year-on-year with the same seasonal pattern as observed in the training data.

Similarly, the other chemicals' and plastics' industries also have consistent historical upward growth trends, albeit not as predictable as the beverages' industry's data. Their forecasts too reflect a continued steady upward growth pattern with regular seasonal variations. Based on these results, it can be concluded that ARIMA models may offer a high level of confidence when used to forecast data which has a strong consistent history, and which may or may not have seasonal variations which also grow proportionally with the overall trend.

There are some historical data which have a spike in sales followed by a steep decline, as is observed in the basic chemicals' and petroleum historic data between 2008 and 2009, which could be related to the global credit crash during that time. In these instances, the forecasts reflect the continued seasonality of these industries' data, but the year-on-year growth rate is lower than in the historic data. Of note too is the declining forecasts which are observed for the basic chemicals' industries, despite most of the historic data being on an upward trend, bar the 2008/2009 spike. There is however, a sharp decline in sales between 2014 and 2015, which is close to the end of the training data and since such a dip had not been observed since 2008/2009, this may have influenced the forecasts not growing at the same rate as the historic data.

All the forecasts were between their 80% confidence intervals, but notably the upper 80% confidence interval grew at a much faster rate than the forecasts and lower 80% confidence band for the motor vehicles' industry. Further research is needed to determine the cause of this variation and whether another model may provide better results for this industry.

#### 4.2.5 Industry chosen using selection matrices

Following the model forecasts, selection matrices comparing the sales value factor and the growth rate factor of each industry were constructed to choose a champion industry to investigate potential chemical investment opportunities in.

The individual selection matrices can be found in Appendix B. Below is a comparison of the beverages' industry and the motor vehicles' industry, both of which scored the highest in all three milestone years (2022, 2025 & 2030).

The table summarizes the comparison between the two industries by showing the ratio of the beverages' industry's score to the motor vehicles' industry's score in every category.

Table 10: A summary of the comparison between the beverages' industry and the motor vehicles' industry

| | Growth Rate Factor | | | | | |
|---|---|---|---|---|---|---|
| Sales Value Factor | **2022** | **0.2** | **0.4** | **0.5** | **0.6** | **0.8** |
| | 0.2 | | | | | 1.24 |
| | 0.4 | | | | 1.07 | |
| | 0.5 | | | 1.00 | | |
| | 0.6 | | 0.93 | | | |
| | 0.8 | 0.81 | | | | |
| | **2025** | **0.2** | **0.4** | **0.5** | **0.6** | **0.8** |
| | 0.2 | | | | | 1.29 |
| | 0.4 | | | | 1.17 | |
| | 0.5 | | | 1.12 | | |
| | 0.6 | | 1.07 | | | |
| | 0.8 | 0.98 | | | | |
| | **2030** | **0.2** | **0.4** | **0.5** | **0.6** | **0.8** |
| | 0.2 | | | | | 1.63 |
| | 0.4 | | | | 1.37 | |
| | 0.5 | | | 1.27 | | |
| | 0.6 | | 1.18 | | | |
| | 0.8 | 1.02 | | | | |

Although the beverages' industry was found to be the overall champion as seen in the table above, the motor vehicles' industry was a close second.

The results identify the motor vehicles' industry as a close contender in being considered the manufacturing sector of choice for the sugar industry to invest in. In the short term (2017-2022), the motor vehicles' industry shows more promise than the beverages' industry when the sales factor is higher than the growth rate factor, but the beverages' industry clearly outperforms the other in the moderate (2017-2025) and long term (2017-2030).

It is possible for the motor vehicles' industry to gain traction in future due to a change in consumer preferences, greater investments available for biofuels, for example. This industry should therefore be closely monitored for burgeoning opportunities for product portfolio diversification.

# 5 Investigating low TRL chemicals

Having identified the beverages' industry as the best placed for sucrose-based product placement in South Africa, it was desired to first explore chemicals which could feature in this industry, but which are more future-focused than mainstream valorisation options. That is, to align with the initial objectives of this study, it was desired to find a chemical which is not yet commercialized but which has enough research and interest being shown in it to reasonably expect it to be commercialized in at least five years.

The purpose of not focusing solely on mainstream options is to increase the number of valorisation options for the sugar industry to consider, and to potentially uncover any overlooked opportunities.

In order to fairly classify chemicals based on their progression towards commercialization, a metric known as the Technology Readiness Level (TRL) was applied. There are a number of studies that have included TRL as part of their evaluation criteria for a pool of products being considered for further investment, such as by Badr et al (2018) in their study on integrated biorefineries and by Stadler and Chauvet (2018) in their research into innovative bioeconomy solutions to be implemented in France.

At the time of conducting this study, the most recently published studies using TRL to as an evaluation metric for sugar based chemicals included two studies published by the European Commission; one on sugar based platform chemicals to bio products and bio fuels (Taylor et al., 2015) and another on benchmarking bio-based industries (Parisi and Ronzon, 2016).

Since the sugar based platform chemicals report was more in alignment with the focus of this study, included detailed methodologies of classifying the products using the TRL metric, and had a more extensive range of products on all TRL levels, this report was chosen to be explored further for chemicals which may align with the industries' trends identified in Section 4.

The TRL scale as used in the report classifies products based on their current development status, ranging from TRL 1 describing products which have had only their basic principles observed to TRL 9 which classifies commercialized products. Table 11 below breaks this down further.

Table 11: TRL definitions (adapted from Taylor et al 2015)

| TRL | Plant stage | Description |
|---|---|---|
| **1** | Basic research | Basic principles observed |
| **2** | Technology formulation | Technology concept formulated |
| **3** | Applied research | Experimental proof of concept |
| **4** | Small scale prototype | Technology validated in the laboratory |
| **5** | Large scale prototype | Technology validated in an industrially relevant environment |
| **6** | Prototype system | Technology demonstrated in an industrially relevant environment |
| **7** | Demonstration system | Operating in an operational environment at a pre-commercial scale |
| **8** | First of a kind commercial system | Manufacturing issues resolved |
| **9** | Full commercial application | Technology commercially available |

The focus was to be on those chemicals which the 2015 study had deemed to not be technologically advanced enough for commercialization in the near present; namely those chemicals which were classified as being at a Technology Readiness Level (TRL) of 5 or below. This is because a chemical classified at a TRL of 5 or below are less likely to have been considered as part of the mainstream valorisation routes than ones which were already beyond the prototype phase.

An extensive literature review was conducted, including referencing journal articles, patents, press releases from production facilities, and reports published by research companies. These findings were compiled to identify those chemicals with increased interest towards being commercialized.

The chemicals which had demonstrably risen in their TRL rank were subsequently further examined to determine their production routes, intermediary products, end products and which industries they could potentially supply. With the knowledge that the initial identification of these chemicals in the 2015 study was done in a European context, it was important to assess whether, regardless of the demonstrated technological developments, these chemicals would serve as a realistic solution for the South African sugar industry to invest in.

The chemicals were therefore then assessed on two criteria:

- Can these chemicals be utilized in a South African manufacturing industry whose historic manufacturing data indicates growth?
- Are these chemicals able to be utilized in more than one industry in order to reduce investment risk?

## 5.1 Expansion of knowledge on low TRL sugar-based biochemicals

The first set of results obtained in this study were based on a market analysis of chemicals identified with a Technology Readiness Level (TRL) below 5 in the European Commission's 2015 study on sugar. The list of chemicals is included in Table 12**Error! Reference source not found.**.

Table 12: List of chemicals identified for review (Taylor et al., 2015)

| Chemical | TRL | TRL definition |
|---|---|---|
| Caprolactam | 4 | Small scale prototype |
| Dodecanedioic acid | 4 | Small scale prototype |
| Gamma-butyrolactone | 4 | Small scale prototype |
| Malic acid | 4 | Small scale prototype |
| Furoate esters | 4 | Small scale prototype |
| Iso-pentanol | 4 | Small scale prototype |
| Fumaric acid | 3-4 | Applied research/small scale prototype |
| Glycolic acid | 3-4 | Applied research/small scale prototype |
| Iso-propanol | 3-4 | Applied research/small scale prototype |
| Methyl levulinate | 3-4 | Applied research/small scale prototype |
| Muconic acid | 3-4 | Applied research/small scale prototype |
| PMMA | 3-4 | Applied research/small scale prototype |
| Heptanone | 3 | Applied research |
| HMDA | 3 | Applied research |
| Hexane | 3 | Applied research |
| PA 6,6 | 3 | Applied research |
| Diaminopentane | 3 | Applied research |
| N-propanol | 2 | Technology formulation |

At the time of conducting this section of research in 2016, no updates had been published on the TRL status of the chemicals listed in Table 7. The following section outlines the key findings from a literature review focused on identifying the technological progression of the chemicals. The approach included reviewing journal articles, patents, press releases, and reports from research companies.

The key finding of the qualitative analysis is that in 2016, the chemicals in Table 7 which were higher up on the TRL scale had significantly more research funding invested into them; whereas the chemicals classified as being at the Applied Research phase or lower in 2015 had still not developed enough to be considered commercially viable or viable even to advance to the small scale prototype stage.

Despite the lack of research investment in most of the other chemicals on the list, however, four chemicals did prove to have multiple research interests. The four chemicals, Muconic acid, Caprolactam, Adipic acid and Dodecanedioic acid, are detailed in 5.1.1-5.1.4, with a focus on their individual uses, production pathways, market segmentation and developing commercial or research interest as of 2016.

Specific attention was also given to the opportunities for bio-based technologies to feature in the production of each of the four chemicals.

### 5.1.1 Caprolactam

***Uses***

Caprolactam is largely used as an intermediate in the production of nylon 6 fibres and resins. It was reported that in 2008, 68% of the caprolactam produced globally was used in the production of nylon fibres, carpet, and industrial yarns. The remainder was used for engineering resins and films. (ICIS, 2008)

***Current production pathway***

The conventional production of caprolactam involves the intermediate cyclohexanone, which is typically obtained from the oxidation of cyclohexane, but may use phenol or toluene as alternatives. Additionally, production uses hydroxylamine sulphate, which requires the oxidation of ammonia to nitrous oxide, followed by hydrogenation in the presence of sulphuric acid.

One of the major disadvantages of the existing technology is the production of a tonne of ammonia for every tonne of caprolactam manufactured. Several attempts have been made to reduce or even eliminate the production of ammonia by companies such as DSM (ICIS, no date). Adopting a biological approach may address the issue of unwanted by-products, as well as volatile prices in the fossil fuel market.

***Market segmentation and growth***

Grand View Research Incorporated speculate that the global caprolactam market will reach $ 15.3 billion by 2022. (Grand View Research, 2015a)

The growth will be driven largely by the rising demand for nylon 6 resin and fibre, particularly due to the growing electronics and automotive sector. Nylon-6 resins are expected to grow in demand by 5.1 % between 2015 and 2022, with an increasing consumption in the manufacture of engineering plastics.

PCI Nylon report the global production of caprolactam to have been 6 247 kton in 2014, and anticipate a 2.1% growth between 2015 and 2022, in line with the growth of the overall nylon-6 market. (PCI Wood Mackenzie, no date)

***Interest and development***

The biggest investor in the production of bio-based caprolactam at present, is the American company, Genomatica.

In a 2014 press release, Genomatica announced their interest in developing complete process technologies for caprolactam, hexamethylenediamine, and adipic acid. Interest in these particular chemicals stems from Genomatica's development program to replace fossil-based nylon intermediates with their bio-counterparts. At the time of the statement's release, the development of the commercial processes for the nylon intermediates was expected to take several years. (Genomatica, 2014)

Subsequent press releases have shown significant progress, in the shape of eight issued U.S. patents and several pending worldwide applications. Supporting experimental proofs of concept have successfully demonstrated metabolic pathways, methods to produce the proposed nylon intermediates, and the recovery of intermediates. (Genomatica, 2015)

### 5.1.2 Dodecanedioic acid

***Uses***

Dodecanedioic acid (DDDA) is primarily used in the manufacture of high-performance nylon-6,12, moulding resins, adhesives, and powder coatings.

Everyday applications include toothbrushes, cosmetics, paints, lubricants, and corrosion-inhibitors. (Verdezyne, no date)

***Current production pathway***

The production of DDDA starts with the conversion of 1,3-butadiene to 1,5,9-cyclododecatriene (a tri-merization), using a $TiCl_4$ and $AlCl_3$ catalyst. Thereafter, a catalytic hydrogen-reduction takes place, then an oxidation using nitric acid and copper-vanadium catalysts yielding a final mixture comprising DDDA (Faber, 1983)

***Market segmentation and growth***

The global DDDA market is anticipated to grow as a result of increasing demand for nylon 6,12; adhesives, powder coatings, and paints.

In 2014, the largest application of DDDA was attributed to nylon-based resins (over 60%) and Nylon has been increasingly used in fibres, screws and gears, which Grand View Research predicts will drive further demand for DDDA in this segment.

Furthermore, the presence of bio-based polymers such as nylon 6,12 is anticipated to grow, in line with growing demand for bio-based products. Grand View Research anticipates bio-based products to replace approximately 30% of their fossil-counterparts between 2015 and 2022. (Grand View Research, 2015b)

While the growing demand for bio-based products may appear significant in countries where consumers are more brand and sustainability conscious, the introduction of bio-based DDDA will need to be justified more from an economic perspective as well as be in line with national sustainability initiatives.

***Interest and development***

Verdezyne, a bio-technology company, agreed with Bio-XCell to construct a commercial-scale renewable chemical manufacturing plant. The construction was due to begin in 2015.

The plant will be designed to produce 30 million pounds per year of di-acids, including DDDA. This will be the first plant to produce bio based DDDA, to be used as a drop-in replacement for its petrochemical counterpart. The manufacture will proceed via yeast fermentation technology, designed to utilize low cost plant-oil sourced feedstocks. (Vedezyne, 2015)

Cathay Industrial Biotech is a Chinese based company which has developed technology for fermentation of paraffin to produce dodecanedioic acid (Biotech, no date).

While the technologies described for the bio-production of dodecanedioic acid are focused on plant-based oils, further work should be done to investigate their flexibility towards sugar-based feedstocks. The nylon-based textile industry is predicted to expand, therefore applicability to South Africa needs to be further investigated.

### 5.1.3 Adipic acid

***Uses***

In 2014, it was reported that approximately 58% of total adipic acid demand came from nylon 6,6 and engineering fibres; while the remainder was allocated to polyurethanes (8-12%), plasticizers (5-8%), food additives (5-10%), and miscellaneous items such as cosmetics (10-12%) (IHS, no date)

***Current production pathway***

The petrochemical production of adipic acid involves the conversion first of benzene to cyclohexane, then oxidation of cyclohexane to a mixture of cyclohexanone and cyclohexanol. Nitric acid is used as an oxidant in the final step to produce adipic acid. A notable drawback of this method is the release of the greenhouse gas, nitrous oxide, which has a Greenhouse Warming Potential (GWP) of 300 times more than that of carbon dioxide (Diamond *et al.*, 2014).

***Market segmentation and growth***

Prospects for adipic acid demand in the future are promising, with its global market anticipated to reach around USD 7,200 million by 2020 according to a 2014 study done by Grand View Research ( Grand View Research 2014).

The growth is largely driven by major end use industries such as the automotive and electronics industries in the BRIC nations (Brazil, Russia, India and China). Nylon 6,6 can provide light weight, high-performance materials for use in vehicles, which will reduce their overall weight. Polyurethanes are also expected to grow at an estimated CAGR of 5.4% between 2014 and 2020.

Although these industries are expected to grow, concerns over the continued use of petroleum-based adipic acid may divert increased investment into bio-based adipic acid development.

***Interest and development***

Deng et al. (2016) discuss some of the progress for adipic acid, and report that the bio-based production of adipic acid is currently in its development phases, with some technical problems yet to be resolved. Production is being investigated via biological pre-cursors such as D-glucaric acid and cis,cis-muconic acid, which can then form adipate.

There is also some interest in the production of adipic acid directly from substrates, such as coconut oil or glucose. To date, coconut oil has proven to deliver higher yields of adipic acid than glucose has.

Rennovia partnered with Johnson-Matthey in 2015 to co-develop catalytic technology to produce adipic acid from glucose-derived glucaric acid (Digest, 2015).

### 5.1.4 Muconic acid

***Uses***

Muconic acid is a dicarboxylic acid and is present in its various isomeric forms, namely cis,cis-;trans,trans-; and cis,trans-muconic acid. It is widely used as an intermediate in the manufacture of adipic acid, HMDA and caprolactam, among others. It can therefore play a key role in the manufacture of fibres and plastics such as nylon 6,6 and polyethylene terephthalate (ResearchMoz, 2013).

***Current production pathway***

The petroleum-based production mechanism falls into the overall mechanism described for the manufacture of adipic acid; namely that involving benzene.

The majority of muconic acid-only mechanisms are bio-based, but some patents exist such as that to produce muconic acid via selective catalytic dihydroxylation from aldaric acid ("Method for producing muconic acid and furans from aldaric acid," n.d.)

***Market segmentation and growth***

Muconic acid is never referenced as a standalone chemical, rather it features heavily as an intermediate in the production of chemicals such as adipic acid. Its market segmentation and growth patterns are therefore in line with those described for adipic acid and caprolactam in the previous sections.

***Interest and development***

Myriant is one of the companies developing its technology for bio-based muconic acid production. In a patent application filed in 2013, Myriant disclosed its technology for producing cis,cis-muconic acid form non-aromatic carbon sources such as sugar, using a genetically modified strain of Escherichia coli ("Production of muconic acid from genetically modified microorganisms," n.d.).

In July 2015, Deinove announced its successful proof of concept for the production of muconic acid by a Deinococcus bacterium, following which the company has decided to perform extensive R & D in this field (Deinove, no date).

### 5.1.5 Assessment of the qualitative analysis of chemicals

Assessing all four chemicals in terms of their uses, production routes, opportunities for biotransformation and reported interest in research and commercial development reveals that all four address largely the same market, that is, the production of some form of nylon. The primary placement for the four chemicals is therefore focused on resins, textiles and some plastics.

A disadvantage of pursuing all four of these chemicals is that there is limited risk diversification as they address largely the same market. Considering too that the list of chemicals was generated in the context of European markets, the reported interest in research and development may not be suitable for South Africa's markets. Furthermore, as Figure 19**Error! Reference source not found.** below shows, the textiles manufacturing industry in South Africa has declined since 2003 and has shown slow growth since. This is also in alignment with the findings in Section 4 which did not identify the textiles industry as one which is forecasted to show significant growth or sales potential.

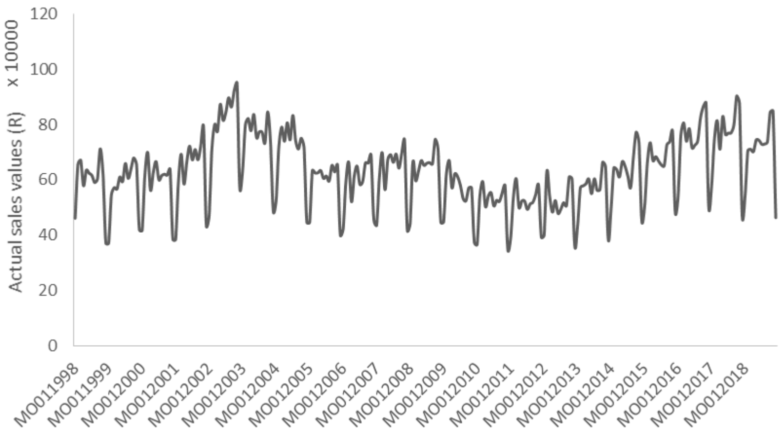


Figure 19: Sales values of the South African textile manufacturing industry (Stats SA., 2020)

It is possible for the sugar industry to consider muconic acid, adipic acid, dodecanedioic acid or caprolactam as investments if the textile industry receives legislative incentives which will boost its growth or if the industry accelerates organically as a result of customer demand for local textiles. In the current state of the market, however, it is unadvisable for the sugar industry to invest in these chemicals as Figure 19 highlights, the slow growth of the industry, which is not aligned with the sugar industry's need to diversify in order to protect jobs and generate revenue sustainably.

The objective to identify a sugar-based chemical which is future focused was therefore unsuccessful using this approach. Firstly, the market for which these chemicals were investigated is markedly different from the European market on the basis of consumer awareness around sustainability measures which may incentivise bio-based production;

therefore it is highly possible that if a list of chemicals were developed in the African context, it would be significantly different to the European Commission's list.

Second, there are far fewer cases in South Africa than in Europe where commercial production has already been rerouted from traditional fossil fuel based processes into bio-based alternatives, which presents a high barrier to entry in this market on a bio-tech perspective, which may be coupled with a high cost of entry should a company decide to do so. Moreover, the textiles industry in South Africa is one which has exhibited slow growth, and which is not anticipated to change based on the historic sales values.

Furthermore, the four chemicals which have shown the most commercial development do not have major applications in the beverages' industry which the analysis in Section 4 identified as the best industry to position chemicals in. There is therefore a need to focus specifically on chemicals which could easily be positioned in the South African beverages' industry. This will the topic of Section 6.

# 6 Chemical selection

This section describes categories of beverages commonly available as well as the main constituents. This is followed by an assessment of which constituent category presents the best opportunity for placing a sugar-based chemical, and subsequently, an assessment of the various options within the chosen category on the basis of selling price, safety and applicability.

There is a multitude of products which form part of the beverages' industry. Common materials and ingredients include plastic bottles, metal cans, sugar, carbon dioxide, flavourants, dyes, sweeteners, water, alcohol, acids, bases, stabilizers and emulsifiers. Although this list is not exhaustive, it represents many of the essential components found in most beverage products.

It is possible for the sugar industry to consider investing in one of the more researched products such as bioplastics, which has been studied numerous times, such as by Coles and Kirwan (2011) and Iles and Martin (2013). However, as one of the aims of this study is to investigate chemicals which fall outside of mainstream bio-products, bioplastics were not considered.

The criteria set to evaluate possible chemical candidates are whether:

1. The chemical is reported being safe for human consumption in the form that it is typically used
2. The chemical is multi-purpose
3. There is a clear need for this chemical both currently and in the foreseeable future
4. The selling price of the chemical is competitive with other options in its category

## 6.1 Types of beverages

According to Buglass (2015), there are four main categories of drinks in most markets, as depicted in Figure 20. The following subsections all directly refer to Buglass (2015) and the references therein, unless explicitly stated otherwise.

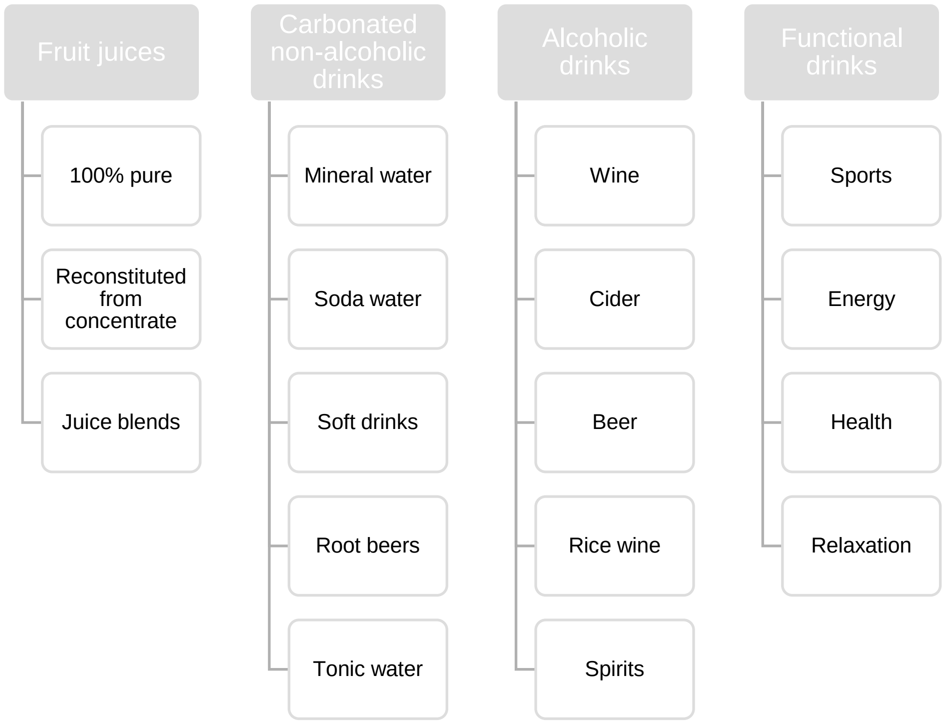


Figure 20: Categories of popular beverages. Adapted from Buglass (2015)

### 6.1.1 Fruit juices

Whole fruit can be pressed to extract the juice which can then be either packaged as is, mixed with additives, or concentrated for reconstitution with water later. Fruit juices can also form the base of many carbonated drinks and of wines.

Fresh juices are the purest form of juice and are often extracted for immediate consumption as no preservatives have been added. For commercial markets however, fruit juice is generally processed further to extend the natural shelf life, improve colour, cloudiness and flavour.

### 6.1.2 Carbonated non-alcoholic drinks

This category of drinks includes mineral water, tonic water, soft drinks and root beers, all of which have dissolved carbon dioxide, giving them their characteristic fizzy and bubbly appearance, the result of the gas rising to the surface upon the pressure reduction as the bottle or can is opened.

Mineral water is the only product in this category which is naturally carbonated as a result of its contact with natural carbon dioxide at above atmospheric pressure usually in mineral springs. This type of water is usually promoted for its high mineral content as a result of the water remaining in contact with mineralized rock for an extended period, and thus is commonly viewed as beneficial for the health. Carbonated mineral water is also sold in flavoured variations in which flavourants have been added, and sometimes colourants as well.

Tonic water is another form of carbonated water but has added quinine and is generally sweetened with sugar or another sweetener.

Finally, soft drinks and root beers are those drinks which have a base of carbonated purified water which is then further enhanced by sweeteners, acids, alkalis, colourants, flavourants and preservatives. These types of drinks are formulated to provide enjoyment rather than to serve a primary nutritional requirement in the average diet, and the exact formulation of many of these drinks are trade secrets. Additionally, soft drinks typically have a full sugar variation as well as a diet version which utilizes low-calorie sweeteners instead of regular sugar.

### 6.1.3 Alcoholic drinks

Alcoholic drinks are primarily made up of ethanol which is produced by a variety of methods including the fermentation of fruit or fruit juice or the malting of cereals and grains. The final alcoholic product is dependent on the raw material, processing method, processing time and additives, all of which can be varied to result in the wide variety of alcoholic drinks available.

Besides ethanol, some of the major constituents of these drinks can include acetaldehydes, carboxylic acids, carboxylate esters, lactones, phenols, pyrazines, terpenoids, amines, volatile compounds, minerals and vitamins.

### 6.1.4 Functional drinks

This category of drinks includes those marketed as sports, performance, recovery, health, energy, rejuvenation and relaxation drinks. It also includes fermented drinks such as kombucha, kefirs, fermented whey and fruit vinegars made from fruit wines.

The main selling point of these types of drinks is a possible health benefit in the form of mineral and electrolyte replenishment, stress relief or probiotics for gut health, although none of these claims are usually medically endorsed. A large percentage of these drinks, especially the sports, performance and energy drinks typically have a high sugar concentration in the form of sugar or sweeteners as well as colourants and sometimes stimulants such as caffeine.

## 6.2 Main beverage constituents

The descriptions of beverages in Section 6.1 have highlighted that many beverages have additional chemicals added for a multitude of reasons, which can include extending shelf life or improving the product's appeal to customers based on appearance and potential health benefits.

Due to their wide applicability, consumer acceptance and existing demand, additives are a promising market for sugar-based chemicals which can diversify the sugar value chain.

This section will therefore describe the main additives which are common in functional, non-alcoholic carbonated drinks and fruit juices. Alcoholic drinks were not investigated further because it is considered that the combined markets of the other three categories would form a larger market for a chemical which could potentially be used in all three alternative markets.

The additives which are typically found in most beverages and which form the topic of discussion are:

- Sweeteners
- Flavourants
- Colourants
- Stabilizers
- Clouding agents
- Foaming agents
- Preservatives
- Acids

The following sub sections largely refer to the book on beverages processing by Mudgill and Barak (2018) and the references therein, unless explicitly stated otherwise.

### 6.2.1 Sweeteners

Sweetened beverages all make use of some form of sweetener, which is either natural or artificial. Natural sweeteners such as sucrose or high fructose corn syrup provide energy as well as sweetness and are thus also termed nutritive sweeteners. Conversely, some synthetic sweeteners such as sucralose or xylitol provide little to no calorific benefit are thus termed non-nutritive sweeteners. Examples of non-nutritive synthetic sweeteners are sucralose, acesulfame-K, aspartame and saccharin; nutritive synthetic sweeteners include maltitol, xylitol and isomalt.

Non-nutritive sweeteners are generally used in products marketed as ‘sugar-free’ or ‘diet’ alternatives to regular, sugar sweetened products. Synthetic sweeteners are highly concentrated and thus only small amounts are needed in food and beverages to provide the equivalent level of sweetness as sucrose. Acesulfame-K and aspartame, for example, are each 200 times sweeter than sucrose on a mass basis, whereas sucralose is 600 times sweeter (AlDeeb et al., 2013).

Ultimately, the use of sweeteners is to mimic the presence of sucrose and therefore combinations of different sweeteners may be used to achieve the optimal flavour in any given product.

### 6.2.2 Flavourants

Flavourants are added to drinks to enhance the existing flavour by either replacing any flavour lost during processing or to add complexity to the drink and thus improve its appeal to customers.

There are three main categories of flavourants, namely natural, nature-identical, and synthetic (Bauer et al., 2008). Natural flavours are those extracted from natural raw materials such as bananas or coconuts whereas nature-identical flavourants are formulated to resemble natural flavours. Commonly used nature-identical flavourants include methyl anthanilate (grape flavour), isoamyl acetate (bananas), ethyl vanillin (vanilla), benzaldehyde (almonds) and limonene (oranges).

Synthetic flavourants are those which cannot be easily extracted from raw sources or which do not naturally occur, but which are deemed suitable for human consumption. They are generally made via chemical modification of naturally occurring isolated substances and by fractional distillation. Examples of synthetic flavourants include esters which provide a fruity aroma to drinks and gamma-undegalactone which provides a peach flavour (Karunaratne and Pamunuwa, 2017).

### 6.2.3 Colourants

As the name suggests, colourants are additives which intensify the original colour or provide an alternative colour to products which will be more appealing to consumers. Using colourants also assures uniformity of colour which further increases the consumer appeal (MacDougall, 2002).

In fruit juice for example, not only does processing the raw fruit deteriorate the original flavour, the original colour of the end product may be affected too. Further, it is often costly and time consuming to extract the natural colour of the raw fruit which gives rise to the use of colourants in beverages.

Like flavourants, colourants can be categorized into natural colours, nature-identical and synthetic colourants. Natural colours are those extracted from the raw source, which is usually fruit, and whose addition to beverages is not limited by regulations unlike nature-identical and synthetic colourants which must follow regulated limits. Nature-identical colourants are those formulated to resemble natural colours, and include beta-carotene (orange/yellow colour), riboflavin (green/yellow colour) and canthaxanthin (red colour), for example. Nature-identical colourants are generally cheaper to synthesize than extracting natural colours and are also more stable which makes them more suitable for commercial products (Delgado-Vargas et al., 2000).

Synthetic colourants include water soluble dyes which are stable under a wide pH and temperature range and have a longer storage period than the other two categories. This type of colourant provides the most intense colour and can be combined to produce new shades as per the desired marketing direction. Examples of synthetic dyes which are approved for use in foodstuffs are Brilliant blue FCF (green/blue), Carmosine (red) and Tartrazine (yellow).

### 6.2.4 Stabilizers

Stabilizers have the function of providing suspension stability to mixtures, improving the viscosity and preventing sugar from crystallizing in beverages. They are therefore vital to products aimed to have a long shelf life.

Like other additives, stabilizers can be either natural or synthetic. Commonly used stabilizers include xanthan gum, gum acacia, guar gum, locust bean gum, alginate, pectin and carboxymethylcellulose (CMC) (Saha and Bhattacharya, 2010). Selection of the most suitable stabilizer depends on the desired interaction with the food product and its effect on the product’s appearance and taste as well.

### 6.2.5 Clouding agents

Clouding agents are used in beverages to increase their opacity if that is desired in the product. The agents are usually in form of emulsions which are in two phases, an oil and an aqueous phase, each of which contains a clouding agent (Ibrahim et al., 2011).

### 6.2.6 Foaming agents

Foaming agents are added to beverages to act as a surfactant to stabilize the interface between water and air and helps prevent the bubbles from bursting before the carbonated product is opened.

Examples of foaming agents include xanthan gum, saponins and arabinogalactans (Guclu-Ustundag and Mazza, 2007).

### 6.2.7 Preservatives

Preservatives are added to beverages to increase their shelf life and prevent any change in flavour, nutritive value, colour and appearance caused by microorganisms. Natural preservatives are commonly known as Class 1 preservatives and include salt, sugar, honey, vinegar and certain spices. Class 2 preservatives include synthetic compounds such as sulphites, benzoic acid, propionic acid, and sorbic acid.

Class 1 preservatives are not always suitable for use in beverages because of their associated taste and thus Class 2 options are more appropriate for most commercial applications.

### 6.2.8 Acids

Acids are added to beverages to enhance the flavour, balance the pH, increase the sourness and have a limited preservation effect. The most used acids are malic acid, lactic acid, adipic acid, fumaric acid, phosphoric acid, acetic acid, and the most used of all, citric acid (Booth and Stratford, 2003)

Citric acid is the most popular acid additive because of its low toxicity, high solubility, stability in product and pleasant sourness. Besides the other acids, minor acids such as tartaric acid, ascorbic acid and adipic acid are sometimes used in conjunction with citric acid to enhance the overall acidity (Khatri and Shalini, 2008).

## 6.3 Selection of target additive

In choosing the additive category for sugar to be diverted into as a valorisation route, consideration was given to whether the additive is a constituent of most drinks and whether there is a growing demand for any one of the additive categories. This was done with the perspective of identifying a product which would allow significant amounts of sugar to be utilized in manufacturing the product and whether the valorisation route would be sustainable for the next few years.

Of the constituents discussed in Section 6.2, sweeteners and acids are the most promising categories for further investigation as the other additives may be useful but there exist a wide variety of options within each category which would be difficult to displace unless a significantly cheaper option were developed. Furthermore, the use of sweeteners and acids can be used in more categories of beverages than the other additives and thus have a greater revenue generating potential.

Acids are a multi-purpose product and are used in a wide variety of beverages and have been approved for use in foodstuffs for many years. Citric acid is an extremely popular constituent, but its production is very well established and so it would be difficult to make a high margin due to the large number of providers. The other minor acids are not used in large enough quantities or as standalone acids in many beverages and so would not be a financially sound investment.

Sweeteners also have many options available but their advantage over acids is them providing a solution to beverage manufacturers in South Africa that are reformulating their products with artificial sweeteners to avoid the sugar tax. This then presents an opportunity for sugar to be diverted into a market where there is a growing demand, and which can be used in many products. Furthermore, the use of sweeteners extends to diet-variations of sports and health drinks and could potentially also be used in fruit juices.

Sweeteners were therefore considered to be the most suitable direction for sugar to be diverted towards because of their potential to be used in multiple beverage categories and due to a demand for them by beverage manufacturers in South Africa. This choice is also in line with the recommendations put forward by Batsy *et al.* (2014) for a company to first diversify into lower risk products and then into higher risk products once a capital base has been established.

## 6.4 Comparison of sweeteners

There are numerous sweeteners available in the market for use in beverages so a selection had to be made as to which one sugarcane derived sucrose could be diverted to in South Africa. This was done by assessing the price, the safety and the applicability of each sweetener.

### 6.4.1 Price comparison

The selling prices of the most common sweeteners were identified from suppliers' websites. All prices are those listed as either ≥98%, ≥99% pure or classified as commercial food grade. These categories were chosen specifically because food grade ingredients require a purity of ≥95% as set by the American Chemical Society (ACS) standard (ACS Chemicals, 2017). Table 13 below summarizes the findings.

Table 13: Comparison of the selling price of common sweeteners

| Sweetener | Purity | Source | Price (USD/kg) |
|---|---|---|---|
| Acesulfame-K | ≥99% | (Sigma-Aldrich, 2020a) | 1 198 |
| Aspartame | Commercial food grade | (NuSci, 2020) | 130 |
| Saccharin | ≥98% | (Sigma-Aldrich, 2020b) | 132 |
| Sucralose | ≥98% | (Sigma-Aldrich, 2020c) | 950 |
| Maltitol | ≥98% | (Sigma-Aldrich, 2020d) | 2 439 |
| Xylitol | ≥98% | (Sigma-Aldrich, 2020e) | 328 |

All prices have been adjusted from ZAR to USD using a ZAR to USD exchange rate of 17 (as of 01/08/2020).

Solely based on the selling price, Maltitol would be most lucrative option for the sugar industry to invest in but since beverages are consumable, consideration must be given to the safety profiles of each of the sweeteners as well as the range of applicability for each sweetener.

The following safety profile comparison and investigation into applicability is limited to the three sweeteners with the highest selling prices; namely, Maltitol, Acesulfame-K and Sucralose. The other options are not explored further because of their relatively limited revenue generating potential.

### 6.4.2 Safety profile comparison

The safety profiles of the three sweeteners are compared below in Table 14.

Table 14: A comparison of the safety profiles of the three most lucrative sweetener options

| Sweetener | Advantages | Disadvantages | References |
|---|---|---|---|
| Maltitol | - Non-cariogenic (does not cause dental caries)<br>- Not metabolized<br>- Fewer calories than sucrose.<br>- Safe at doses below 10g.<br>- FDA approved for use in foodstuffs. | - If consumed in excess of 10g, can lead to gas, bloating and diarrhoea.<br>- Not entirely calorie free.<br>- Linked to foetus complications at high doses. | (Das and Chakraborty, 2016; Marcus, 2013; Rapaille et al., 2016) |
| Acesulfame-K | - Not metabolized<br>- Non-nutritive. Does not affect glycaemic response.<br>- FDA approved for use in foodstuffs. | - Linked to impairments in learning and memory at high doses.<br>- Linked to weight gain.<br>- Found in breast milk.<br>- Linked to cancers due to it hydrolysing on the shelf over time. | (Chakraborty and Das, 2019; Oprea et al., 2019; Yalamanchi et al., 2016) |

| | | | |
|---|---|---|---|
| | | - FDA declared cannot be used by anyone with phenylketonuria, a genetic metabolic disorder. | |
| Sucralose | - Non-cariogenic<br>- Leads to no glycaemic response<br>- Non- calorific.<br>- No reproductive, carcinogenic or neurological risk.<br>- FDA approved for use in foodstuffs. | - Linked to insulin increases in obese people. | (AlDeeb et al., 2013; Glória, 2003; Nan, 2015) |

The advantage of all three sweeteners is that they have been approved for use in general foodstuffs and beverages by the United States Food and Drug Administration (US FDA). Furthermore, their use as a food additive is allowed in South Africa too since they are included as part of the CODEX General Standard for Food Additives which South Africa adopted in 2016 (Department of Health, 2016). Moreover, the advantages of each of the three outweigh their limitations but of the three, sucralose has the least health risks associated with it based on the studies published thus far.

Due to Maltitol being a nutritive sweetener, its application is limited to beverages which would not appeal to consumers with a sensitivity to glucose, such as diabetics, and could also be avoided by consumers who have digestive systems prone to bloating and diarrhoea.

Consumers who are obese may avoid sucralose sweetened beverages due to its effect on insulin as well.

Both Acesulfame-K and Maltitol pose a risk to pregnant and lactating women too, which means that their use in mainstream beverages may limit sales. Of the three sweeteners, Acesulfame-K has the most associated health risks, which may further limit its consumption, especially in people looking to maintain or lose weight.

On a safety profile basis, sucralose appears to be the least hazardous and which could be consumed by the greatest number of consumers. Section 6.4.3 will discuss the applicability of each sweetener.

### 6.4.3 Applicability comparison

The applicability and limitation of each sweetener is compared in Table 15.

Table 15: A comparison of the applicability of Maltitol, Acesulfame K and Sucralose in foodstuffs

| Sweetener | Applicability | Limitations | Reference |
|---|---|---|---|
| Maltitol | - Inert<br>- Neutral taste<br>- Can be used to mask the bitterness of other sweeteners<br>- Works well as a preservative in gelatine gums<br>- Can be used as a bulking agent by imparting a creamy texture to foodstuffs<br>- Provides a small cooling effect | - It is less sweet than sucrose and so its taste is less pronounced<br>- It is not usually used in beverages and rather is used in sweet confectionary products<br>- Imparting of a creamy texture may not be desired in all products thus limiting its application<br>- Does not brown upon heating; cannot be used as a caramelizing product | (Grembecka, 2019; Rapaille et al., 2016; Young and O'Sullivan, 2011) |

| Sweetener | Applicability | Limitations | Reference |
| --- | --- | --- | --- |
| Acesulfame K | - Stable<br>- Heat resistant and therefore suitable for use in food and beverages<br>- Aqueous solutions at pH 3 or greater may be stored for extended periods without decomposition. | - May have a bitter aftertaste if used by itself; thus, it is commonly blended with other sweeteners | (Bassoli and Merlini, 2003; Chakraborty and Das, 2019; Lawrence, 2003) |
| Sucralose | - Stable in dry form (for up to 4 years at 20 °C)<br>- Does not interact with food ingredients<br>- Withstands high temperatures thus it is suitable for use in many food and beverage manufacturing processes<br>- Does not have a bitter aftertaste<br>- Commonly used as a sweetener in carbonated, still and alcoholic beverages | - Under extreme temperatures and pH levels, sucralose may be hydrolysed or degraded to release hydrogen chloride | (AlDeeb et al., 2013; Glória, 2003) |

## 6.5 Selection of a final chemical for further investigation

The applicability of Maltitol, Acesulfame-K and Sucralose based on the findings in Section 6.5 is in general quite broad and the three are described to be stable products under normal conditions.

Maltitol has the advantage of being close to sucrose's taste profile but is reported to be less sweet than sucrose itself which means that either more of the product will need to be added to beverages or it would have to be supplemented with a sweeter alternative if the goal is to mimic the sweetness in diet versions. It is popular in confectionary products such as cakes and acts as a bulking agent as well, which may be useful in food products but its application in beverages may be limited. Maltitol's cooling effect may be useful in chewing gum in which it is popular as well, however this quality may not always be desired in beverages.

Acesulfame-K has an advantage over Maltitol due to its wider applicability in foods and beverages and because of it not imparting a bulking quality; however, its bitter aftertaste would require that it be complemented with another sweetener to mask the unpleasant taste. In this regard, a mixture of Maltitol and Acesulfame-K could prove successful in delivering the required level of sweetness and without the bitter aftertaste, but this would require the setup of two production streams.

Unlike Acesulfame-K, Sucralose does not impart an aftertaste and provides a higher level of sweetness than both other options and is commonly used in many foods and beverages. Like the rest, it too is stable under normal conditions, but its applicability would be limited to beverages that are not highly acidic to prevent its degradation.

Overall, sucralose presents the best option to diversify the sugar value chain with, based on both its safety profile and its applicability within food and beverages. Although it is not the most expensive sweetener of those examined, its wide applicability across multiple beverage categories and its appeal to most consumers may compensate for its mid-range selling price. Section 7 will explore the production of Sucralose and its subsequent techno-economic analysis.

# 7 Technoeconomic analysis

In selecting a process to simulate the production of the chosen chemical via existing routes in industrial production, patents were consulted as well as encyclopaedia articles and any other relevant literary material.

All the considered routes were then summarised and analysed to identify which would be the best option to simulate in terms of a preliminary analysis of the catalyst needed, heating and cooling duties and any other factors marking a route as being excessively expensive.

The factors needed to simulate each component were then collected. These included yields or kinetics, temperature, pressure and other relevant properties.

For this purpose, SuperPro Designer V9.5, Build 3 (Academic License) was used to simulate the process and size the equipment. Costing was done in Microsoft Excel.

A summary of the assumptions made in the simulation is available in Appendix B.

## 7.1 Annual production of sucralose

The annual production of sucralose was calculated based on the following calculation. The basis for the calculation was taken as the sugar in a 330 mL can of Coca Cola, which was chosen because of its high sugar content and of the availability of products such as Coke Light which sucralose can realistically be used in.

Table 16: Calculation of the amount of sucralose to be produced per batch

| Description | Calculation |
|---|---|
| Amount of sugar in a litre of Coca Cola | A = (grams of sugar in a 330 mL can of Coca Cola) x 1000 mL/330 mL |
| Amount of sucralose in equivalent sweetness to sugar in a litre of Coca Cola | B = (grams of sugar in a litre of Coca Cola)/600 |
| Amount of sucralose needed to represent 33% of sugar's sweetness in a litre of Coca Cola | 0.33 x B |
| Cost of a litre of Coca Cola in 2030 | C = (Cost of a litre of Coca Cola in 2018) x (1.05)^11 |
| Cost of Coca Cola (L/R) | 1/C |

| | |
|---|---|
| Total forecasted beverage sales in 2030 | D =Sum of monthly sales 2030 forecasts obtained from ARIMA modelling |
| Assuming 50% of total beverage sales in 2030 come from artificially sweetened beverages (R millions represented as R 1000) | E = 0.5 x D |
| Total value of forecasted sales for sweetened beverages in 2030. Inflated from current rand value at an inflation rate of 5% | F = (E x 1000)/1000000x(1.05)^11 |
| Mass of sucralose needed if assumed to fulfil entire market need for sucralose requirements in 2030. Assuming that sucralose fulfils 33% of sweetener requirements in 2030 | G = F x 1000000 x 0.33 x (Cost of Coca Cola (L/R)) x (1kg/1000g) |
| Assuming market capture in the first year is 20% of the total market need for sucralose in 2030 (kg/annum) | H = 0.2 xG |
| Number of reaction batches (not complete cycle time including heating/cooling etc) | I = 8000 hrs / base processing time |
| Mass production sucralose per batch (kg) | J = H/I |

## 7.2 Costing

Costing of the simulated process was done in MS Excel, on the basis of the Lang-Factor approach as described by Seider *et al.*, (2010) and Turton *et al.*, (2018). Assumptions made during the costing calculations are summarized in Appendix C and the purchase prices of raw materials utilities are available in Appendix D.

An exchange rate of ZAR: USD of 15 (as of 15/11/2020) was assumed. All monetary values are henceforth reported in USD. Note that the price of sucralose used in the profitability analysis may vary from that reported in Section 6.4.1 due to currency fluctuations.

The amount of sucralose produced as per the calculation in Section 7.1 amounts to 243 543 kg/year, which subsequently required 601 767 kg/year of sucrose to produce. In the 2018/2019 season, the amount of saleable sugar produced was 2 181 161 tonnes/year across all mills in South Africa (SASA, n.d.). There are 14 mills in South Africa (SASA, n.d.) which on average could be assumed to process 155 797 tonnes/year of sugar each. Thus, the production of the proposed amount of sucralose would only amount to 0.3% of sugar produced at a single mill. It is also assumed that the production of sucralose as per the design in this study is done at a single manufacturing plant.

## 7.3 Techno-economic analysis of sucralose

### 7.3.1 Transformation of sucrose into sucralose

In producing sucralose from sucrose, the overall transformation consists of replacing three hydroxyl groups with chlorine atoms. While conceptually simple, the process is a multi-step synthesis because of the need to only selectively chlorinate some of the hydroxyl groups, and to protect the primary alcohol groups from being chlorinated.

The overall transformation is summarized in the diagram below.

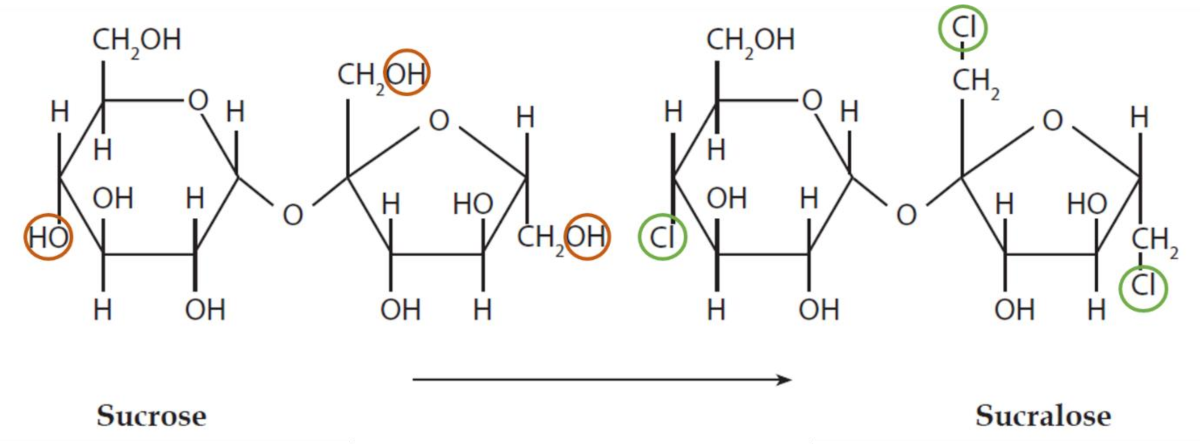


Figure 21: Transformation of sucrose into sucralose by selectively chlorinating three of the original hydroxyl groups (adapted from Sheet et al. (2014))

As Figure 21 above describes, the key difference between sucrose and sucralose is the replacement of two of the primary alcohol groups and one secondary alcohol group on sucrose with chlorine atoms. The selective chlorination process thus refers to only some of the alcohol groups being replaced with chlorine. It is therefore necessary to transform sucrose prior to chlorination in order to protect the primary alcohol on the 6-carbon ring as it would be highly susceptible to chlorination otherwise.

This transformation is typically done via transesterification of the 6-carbon ring; thereafter follows chlorination to form sucralose-6-ester then de-esterification to produce sucralose, and finally a purification step to result in the product of highly pure sucralose, fit for use in food production. The overall process is summarized in Table 17 overleaf.

Table 17: Transformation steps of sucrose into sucralose

| Step 1 | Step 2 | Step 3 |
|---|---|---|
| Transesterification → | Chlorination → | De-esterification |
| Sucrose → Sucrose-6-ester → | Sucralose-6-ester → | Sucralose |

The above process can be represented diagrammatically as well, to highlight where the substitutions take place. In Figure 22 below, an acetate group represents the ester used to protect the primary alcohol in sucrose.

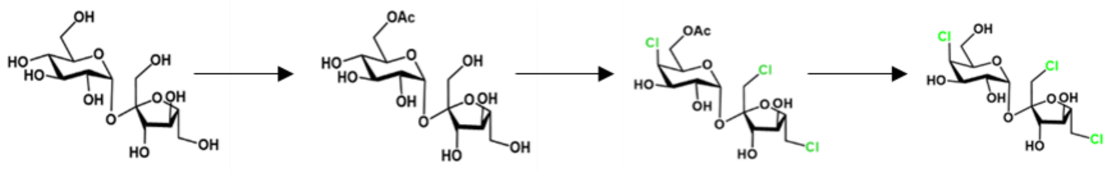

Figure 22: Diagrammatic representation of the transformation of sucrose into sucralose via transesterification

### 7.3.2 Feasibility study of existing synthetic technologies

The design feasibility study was done by evaluating patented technologies for each of the steps of transesterification, chlorination, de-esterification and purification of the product. This section summarizes each of the options considered.

Table 18: Technologies considered for the transesterification process: sucrose to sucrose-6- ester

| Option | Reference Patent | Process | Comments |
|---|---|---|---|
| **A** | US 2008/0103295A1 | Sucrose >> Sucrose-6-acetate<br>Ethyl acetate used in an N-N-Dimethylformamide solvent<br>Catalyst: $SO_4^{2-}$-$TiO_2$/$Al_2O_3$ or $SO_4^{2-}$-$TiO_2$ | a) One step process<br>b) Easy to obtain reagents<br>c) Additional cost of a catalyst |
| **B** | US 5440026 | a) Sucrose + Ketene acetal >> Sucrose alkyl 4,6-orthoester<br>b) Sucrose alkyl 4,6-orthoester + acid hydrolysis >> mix of Sucrose-4-ester and Sucrose-6-ester<br>c) React mixture of Sucrose-4-ester and Sucrose-6-ester + base >> Sucrose-6-ester<br>Ketene acetal: 1,1-dimethoxyethene<br>Organic base or water soluble base recommended<br>Catalyst: p-toluene sulphonic acid and pyridinium chloride | a) Multiple steps<br>b) Extra chemicals involved<br>c) Final product of sucrose-6-acetate may still have a high proportion of sucrose-4-acetate if conditions not carefully controlled<br>d) Hazardous catalysts |
| **C** | US 6939962B2 | a) Sucrose + organotin based acylation promoter + solvent capable of removing water by co-distillation<br>b) Removing water by co-distillation<br>c) Adding a carboxylic anhydride mixture to produce Sucrose -6- ester<br>Recommended solvent: Cyclohexane/toluene/n-heptane/iso-octane<br>Recommended organotin based acylation promoter: 1,3-diacyloxy-1,1,3,3-tetrabutyldistannaoxane | a) Difficult to find safety or cost information for the specified organotin based acylation promoter<br>b) Hazardous recommended solvents<br>c) Added cost of co-distillation |
| **D** | US 7626016B2 | a) Sucrose + N-N-dimethylacetamide dimethyl acetal in N-N-Dimethylformamide solvent to form a cyclic acetal<br>b) Cyclic acetal + mild acid hydrolysis >> Sucrose-6-ester<br>Recommended acid for hydrolysis: Acetic acid/Formic acid/Hydrochloric acid/Sulphuric acid | a) Mild acid hydrolysis suggests moderate temperatures which can lower costs<br>b) The recommended acids are all readily available |

Table 19: Technologies considered for the chlorination process: sucrose-6-ester to sucralose-6-ester

| Option | Reference Patent | Process | Comments |
|---|---|---|---|
| **A** | US 4980463 | a) N-N-Dimethylformamide + acid chloride >> chloroformiminium chloride salt<br>b) Chloroformiminium chloride salt forms a complex with the hydroxyl groups of the Sucrose-6-ester<br>c) Subject reaction mixture to 85°C for long enough to produce a mixture of chlorinated Sucrose-6-ester products consisting of 6-chlorosucrose-6-ester, 4,6-dichlorosucrose-6-ester and 1,6-dichlorosucrose-6-ester<br>d) Subject mixture to 125°C for long enough to convert all Sucrose-6-ester products to Sucralose-6-ester<br>e) Quench with an aqueous solution of Sodium Hydroxide<br>Recommended solvent: N-N-Dimethylformamide<br>Recommended acid chloride: Phosgene | a) Sustained high temperatures suggests a high operational cost<br>b) There is a risk of the product not being sufficiently pure because of an incomplete conversion<br>c) Phosgene is hazardous |
| **B** | US 2006/0205936A1 | a) Thionyl chloride + N-N-Dimethylformamide >> Vilsmeir reagent<br>b) Sucrose-6-acetate + Vilsmeir reagent between -10°C and +10°C<br>c) Temperature of the reaction mixture increased to 50°C-80°C for 1-6 hours<br>d) Temperature of the reaction mixture increased again to 100°C-120°C for 1-6 hours to form Sucralose-6-ester | a) The process of making Vilsmeir reagent onsite is complex and could be costly. There would need to be an analysis of purchasing vs. producing |
| **C** | US 8530643B2 | a) Sucrose-6-acetate + Phosgene/Arnold's reagent + N-N-Dimethylformamide reacted at 85°C-130°C<br>b) A portion of N-N-Dimethylformamide is removed via distillation under reduced pressure at 40°C-150°C<br>c) Removed N-N-Dimethylformamide is reacted with a base and filtered before recycling | a) The process of making Arnold's reagent onsite is complex and could be costly. There would need to be an analysis of purchasing vs. producing<br>b) Phosgene is a hazardous chemical to use |
| **D** | US 7932380B2 | a) Sucrose + chlorinating agent to form chlorinated sucrose at -15°C and 120°C<br>b) React the chlorinated sucrose with a carboxylate salt to form sucralose-6-acetate at 30°C-50°C<br>Recommended chlorinating agent: Thionyl chloride/Phosgene/Solid Phosgene/Phosphorus pentachloride | a) All of the recommended chlorinating agents are hazardous<br>b) The carboxylate salts are readily available |

| | | | |
|---|---|---|---|
| | | Recommended solvent: N-N-Dimethylformamide<br>Recommended carboxylate salt: Sodium acetate/Potassium acetate/Sodium benzoate/Potassium benzoate | |

Table 20: Technologies considered for the deacylation process: sucralose-6-ester to sucralose

| Option | Reference Patent | Process | Comments |
|---|---|---|---|
| **A** | US 8530643 | a) Raise pH of Sucralose-6-ester mixture to between 10.5-11.2 and a temperature of 25°C-35°C (if carried out before the removal of the N-N-Dimethylformamide solvent)<br>b) Raise pH of Sucralose-6-ester mixture to between 10-12 and a temperature of 0°C-40°C (if carried out after the removal of N-N-Dimethylformamide solvent) These conditions do not need to be as strictly controlled as those in the first option<br>c) When the conversion is complete, neutralize using Hydrochloric acid or Carbon Dioxide. pH needs to be 7.5<br>Recommended base: Sodium Hydroxide<br><br>It is possible to perform the quenching after chlorination and the deacylation step in the same vessel by adding base and allowing the pH to rise enough to facilitate deacylation | a) It may be cost effective to perform this process in the same vessel as the chlorination<br>b) The recommended base is readily available<br>c) Removal of the solvent would make the process easier as the pH would not have to be as strictly controlled |
| **B** | US 2006/0276639A1 | a) Sucralose-6-ester + alkaline metal chloride/alkaline earth metal chloride + water in N-N-Dimethylformamide cooled to a temperature between 0°C- 25°C<br>b) Raise the pH to between 12.5 -13.5. Maintain temperature between 5°C-25°C<br>c) Maintain for 1-3 hours for maximum conversion to Sucralose<br>d) Neutralize mixture using Hydrochloric acid<br>e) Remove the N-N-Dimethylformamide<br>Recommended base: Sodium Hydroxide | a) All the reagents are readily available<br>b) The holding temperatures are very mild so would be cost effective |

| | | | |
|---|---|---|---|
| **C** | US 2008/0227971A1 | a) Maintain a solution comprising sucralose-6-acylate in an aqueous N-N-Dimethylformamide solvent at a temperature range of -20°C-20°C and at a pH between 12.2-14<br>b) Maintain the above conditions for between 0.5-8 hours until complete conversion achieved from sucralose-6-ester to sucralose<br>c) Neutralize mixture using Hydrochloric acid<br>d) Remove the N-N-Dimethylformamide | a) Compared to the other options, this option is the simplest in terms of steps and minimal reagents needed<br>b) The pH can be adjusted using NaOH which is readily available |

Table 21: Technologies considered for the purification of sucralose

| Option | Reference Patent | Process | Comments |
|---|---|---|---|
| **A** | US 5498709 | Option 1<br>a) Aqueous solution remaining after ester hydrolysis is concentrated<br>b) Sucralose is isolated by three sequential extractions with ethyl acetate<br>c) The extracts may be combined and optionally, washed with water to remove any remaining N-N-Dimethylformamide<br>d) Concentration and crystallization<br><br>Option 2<br>a) The sucralose contained in the aqueous brine obtained after alkaline de-esterification is extracted into a solvent not miscible in brine, such as ethyl acetate<br>b) The organic extracts may then be backwashed with water to transfer the sucralose back into the aqueous phase<br>c) The aqueous phase is then decolorized, concentrated and sucralose is crystallized out<br>*The authors mention that this process yields a relatively impure product<br><br>Option 3<br>a) Use a double extraction technique with toluene to remove non-polar impurities of the alkaline solution remaining after de-esterification<br>b) The aqueous solution is then extracted repeatedly with 2-butanone<br>c) Combine the 2-butanone extracts<br>d) The solvent is evaporated to yield a reddish syrup containing sucralose | a) Ethyl acetate is readily available<br>b) Option 2 would not be suitable for producing a food-grade product<br>c) Toluene in Option 3 is a hazardous substance and carries a risk of contamination<br>d) Of these, Option 1 is the safest and could produce a food-grade product |
| **B** | US 5530106 | a) After alkaline hydrolysis of sucralose-6-acetate and subsequent neutralization, the aqueous solution is extracted with water saturated ethyl acetate. Some impurities are selectively partitioned to the organic phase by this extraction<br>b) The ethyl acetate is backwashed with water in order to recover a portion of the sucralose that had transferred<br>c) The aqueous solution and the aqueous backwash are combined, concentrated, decolorized<br>d) Sucralose is recovered from the aqueous phase by crystallization | a) The decolorization step would require additional reagents hence making this process costly |

| Option (contd.) | Reference Patent | Process | Comments |
|---|---|---|---|
| **C** | US 2003/0171574A1 | a) Sucralose and impurities in a first solvent (such as water) are contacted with a second solvent (such as ethyl acetate) to remove some of the impurities into the ethyl acetate<br>b) Contact the sucralose and impurities in the first solvent (water) with a third solvent (such as ethyl acetate). Majority of the sucralose is recovered into the third solvent. Majority of the impurities are retained in the first solvent<br>c) The second solvent is recovered by extracting the first solvent, backwashing the second solvent with a new portion of the first solvent, and combining at least a part of this new portion with the composition comprising sucralose and impurities in the first solvent prior to extracting with a third solvent<br>d) Sucralose is crystallized out<br><br>Ratio of second solvent: first solvent; 1:2;1:3:1:4;1:5<br>Extraction can be batch extraction, continuous extraction or continuous counter-current extraction | a) Solvents are all readily available<br>b) Multiple step process may prove to be expensive |
| **D** | US 2003/0171575A1 | a) Subjecting the crude sucralose solution to a non-crystallization purification step (e.g. liquid-liquid extraction, extractive precipitation, chromatography, precipitation followed by solvent washing, derivative formation followed by extraction or distillation) with ethyl acetate and water<br>b) Performing a crystallization procedure on the increased purity sucralose solution to obtain crystalline sucralose and a mother liquor<br>c) Recycling at least a portion of the mother liquor to the feedstock in step a)<br>d) Performing at least three additional sequential crystallization procedures on the crystallized sucralose (by dissolving then re-crystallizing) | a) Recycling of the mother liquor would make this process more cost effective<br>b) Multiple crystallization procedures would be expensive but would yield a high purity product |
| **E** | US 2006/0188629A1 | a) Add alcohol (methanol/ethanol/propanol) at 10°C-90°C for 0.5-30 hours to the mixture of sucralose, polar and non-polar impurities. This will remove at least a portion of the polar impurities<br>b) Mix the resulting solution of sucralose with an aqueous-organic mixture (e.g. ethyl acetate) at 10°C-90°C for 0.5-30 hours to remove at least a portion of the non-polar impurities. This will result in a solution containing 92-96% sucralose by weight, and the total impurities form less than 3% of the solution by weight<br>c) Crystallize the sucralose by seeding | a) Multiple reagents are needed, hence making this option relatively more expensive than the others |

### 7.3.3 Feasibility study of existing biological technologies

In comparison to the number of synthetic routes available to manufacture sucralose, the biological routes are very few. The options which do exist are discussed below.

***Biocatalytic synthesis of sucralose***

In a 1992 study, Bennett *et al.*, (1992) reported the production of sucralose from raffinose as a starting material. The steps are first the chemical chlorination of raffinose to form a tetradeoxygalactoraffinose intermediate, followed by the enzymic hydrolysis of the α-1-6-glycosidic bond to give sucralose and 6-chlorogalactose.

The advantages of this route compared to its synthetic counterparts using sucrose are reported to be a reduction in the number of steps involved when raffinose is used as the starting material, albeit an additional step of forming raffinose from sucrose is required. The exact method used to produce raffinose in this study was that of using saturated aqueous solutions of galactose and sucrose using a selected α-galactosidase from *Aspergillus Niger*.

***Biological production of sucralose intermediates***

In another 1992 study, Jones *et al.* (1992) described the production of sucrose-6-acetate via fermentation of glucose using a strain of *Bacillus megaterium.* Subsequent steps are described to be the same chlorination and deacylation steps as found in the synthetic routes described. A similarity between this process and the above described is that the main reported advantage of this process is the reduction in the number of steps compared to the synthetic route.

In another study on the biological preparation of sucralose, Pengfei *et al.* (2005) also add that the biological route is advantageous too in its use of lower environmental pollution risks, but also reports that current technologies are much more costly than synthetic routes and that there is the added consideration of the difficulty in separating intermediates.

### 7.3.4 Choice between biological and synthetic routes

In selecting a process to simulate to produce sucralose, consideration of the overall cost factors and assumed ease of adoption in South Africa's market based on the historical uptake of biological processes favoured the use of synthetic processes at present.

This is due to the fact that at present there is not extensive research available to support the biological production of sucralose from a commercial standpoint, as well as the fact that in the case of an industry looking to diversify its portfolio for short and long term revenue generation, such as the local sugar industry, the use of biological processes may prove unfavourable investment wise.

However, the advantages of biological production routes offering a safer alternative to existing synthetic routes are not to be ignored, and should biological production become more profitable as a result of metabolic engineering and improved separation technologies, then the case would need to be evaluated.

### 7.3.5 Selected process to simulate

Based on the analysis of the options for each of the four steps involved in the production of sucralose, the selected process as described below was chosen.

Table 22: The production process of sucralose selected for simulation

| Step | Selected process | Description | Reason |
|---|---|---|---|
| 1. Transesterification | US 2008/0103295A1 | Sucrose >> Sucrose-6-acetate<br>Ethyl acetate used in an N-N-Dimethylformamide solvent<br>Catalyst: $SO_4^{2-}$-$TiO_2$/$Al_2O_3$ or $SO_4^{2-}$-$TiO_2$ | This is a single step process which will reduce the number of units needed. It also reduces the number of reagents needed, hence making this the safest and most cost-effective option. |
| 2. Chlorination | US 4980463 | a)N-N-Dimethylformamide + acid chloride >> chloroformiminium chloride salt<br>b) Chloroformiminium chloride salt forms a complex with the hydroxyl groups of the Sucrose-6-ester<br>c) Subject reaction mixture to 85°C for long enough to produce a mixture of chlorinated Sucrose-6-ester products consisting of 6-chlorosucrose-6-ester, 4,6-dichlorosucrose-6-ester and 1,6-dichlorosucrose-6-ester<br>d) Subject mixture to 125°C for long enough to convert all Sucrose-6-ester products to Sucralose-6-ester<br>Recommended solvent: N-N-Dimethylformamide<br><br>Recommended acid chloride: Phosgene | The expense of prolonged heating can be justified by obtaining a high purity product. Phosgene is a hazardous chemical, but any alternative acyl chloride would present the same risk. |
| 3.De-esterification | US 8530643 | a) Raise pH of Sucralose-6-ester mixture to between 10.5-11.2 and a temperature of 25°C-35°C (if carried out before the removal of the N-N-Dimethylformamide solvent)<br>b) When the conversion is complete, neutralize using Hydrochloric acid or Carbon Dioxide. pH needs to be 7.5<br>Recommended base: Sodium Hydroxide<br><br>It is possible to perform the quenching after chlorination and the deacylation step in the same vessel by adding base and allowing the pH to rise enough to facilitate diacylation | This process is cost effective because deacylation can be carried out in the same vessel as the quench after chlorination, as well as using the same alkali. Additionally, performing this process prior to the removal of the<br>N-N-Dimethylformamide solvent results in a reduced risk of solid formation in the steam stripper used to remove the solvent following de-esterification. |

| Step (contd.) | Selected process | Description | Reason |
|---|---|---|---|
| 4. Purification | US 2003/0171575A1 | a) Subjecting the crude sucralose solution to a non-crystallization purification step (e.g. liquid-liquid extraction, extractive precipitation, chromatography, precipitation followed by solvent washing, derivative formation followed by extraction or distillation) with ethyl acetate and water<br>b) Performing a crystallization procedure on the increased purity sucralose solution to obtain crystalline sucralose and a mother liquor<br>c) Recycling at least a portion of the mother liquor to the feedstock in step a)<br>d) Performing at least three additional sequential crystallization procedures on the crystallized sucralose (by dissolving then re-crystallizing) | This process would utilize non-hazardous reagents, which are also readily available. The cost of multiple crystallizations can be justified by obtaining a high purity, food-grade product at the end. |

The high-level selected process is presented as a block flow diagram below. A process flow diagram can be found in Appendix G.

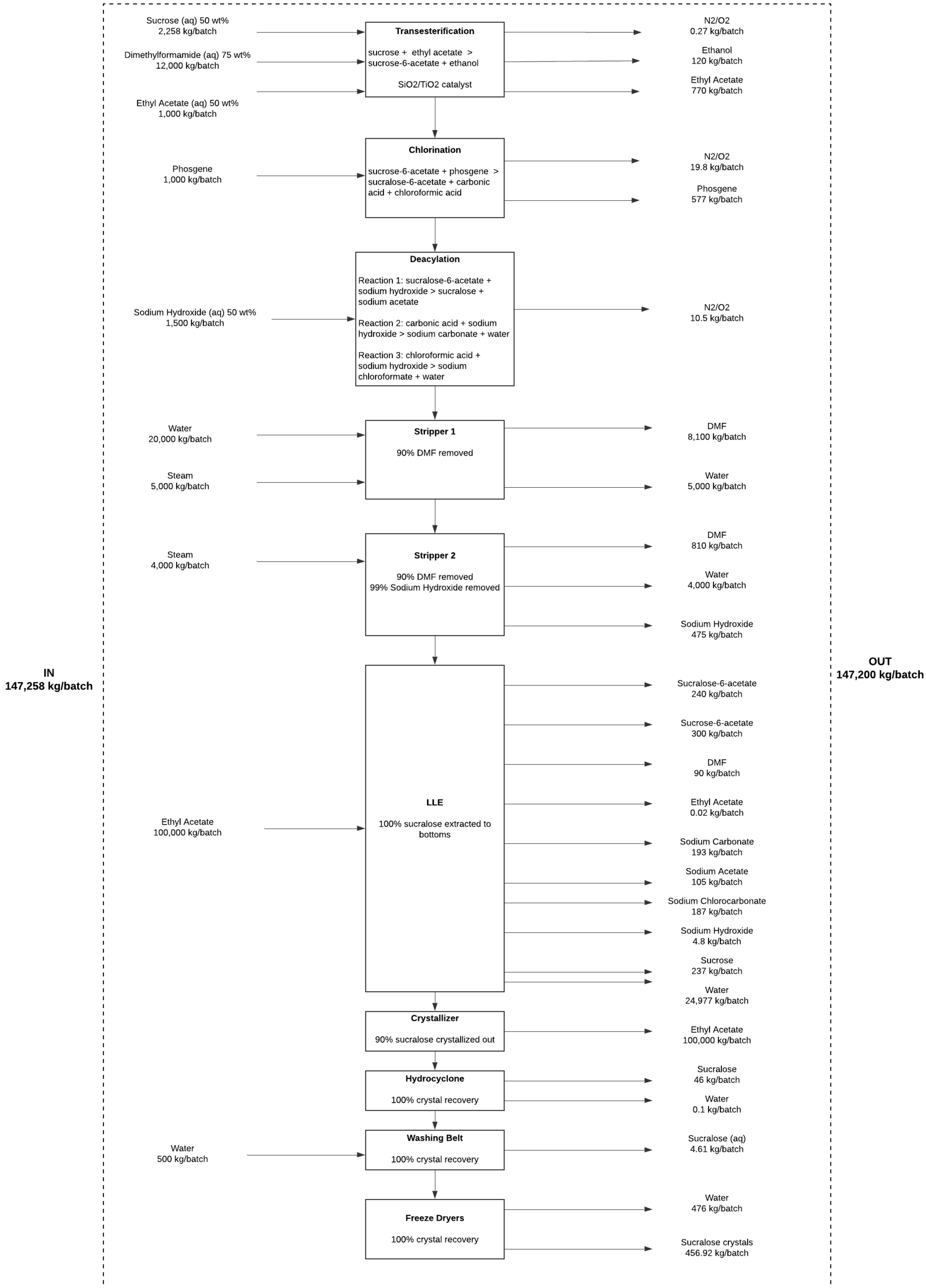


Figure 23: Block flow diagram of the selected process

### 7.3.6 Reactions in the selected process

There are three primary reactions that take place within the selected process, which are:

**Transesterification** (US 2008/0103295A1)

Sucrose + Ethyl Acetate $\longrightarrow$ Sucrose-6-acetate + Ethanol

$C_{12}H_{22}O_{11} + C_4H_8O_2 \longrightarrow C_{14}H_{24}O_{12} + C_2H_5OH$

**Chlorination (**US 4980463)

Sucrose-6-acetate + Phosgene $\longrightarrow$ Sucralose-6-acetate + Carbonic acid + Chloroformic acid

$C_{14}H_{24}O_{12} + 2COCl_2 \longrightarrow C_{14}H_{21}Cl_3O_9 + CH_2O_3 + CO_2HCl$

**Deacylation (**US 8530643)

Sucralose-6-acetate + Sodium Hydroxide $\longrightarrow$ Sucralose + Sodium Acetate

$C_{14}H_{24}Cl_3O_9 + NaOH \longrightarrow C_{12}H_{19}Cl_3O_8 + C_2O_2H_3Na$

### 7.3.7 Plant profitability

An exchange rate of ZAR: USD of 15 was assumed. All monetary values are henceforth reported in USD.

Based on the assumptions made in the simulation of the selected process and the assumptions made in the costing of the plant (see Appendices C,D, E and F), the profitability analysis is as shown in Tables 23 and 24 overleaf. Table 23 is the profitability analysis for the base case and Table 24 is the profitability analysis for a plant configuration using a lower ethyl acetate flow rate with an increased sucrose flowrate.

According to the base case profitability analysis, the production of sucralose in a 10-year plant lifecycle becomes profitable in the first year of operation. This is surprising as most production facilities do not make a profit in the first-year post construction. However, these results may be due to the relatively low fixed capital which is assumed to be solely the purchase cost of equipment and delivery which were calculated as per the methods described by Seider *et al.*(2010) and Turton *et al.* (2018). It can be further substantiated, by the high selling price of sucralose, which retails for close to 8 times the purchase cost of the most expensive raw material (DMF).

Although the base case is already profitable, further refinement was done by examining the raw materials used. The highest expense involved in this process is that of the raw materials, with most of the cost being due to a high flow rate of ethyl acetate. Although ethyl acetate is used in the transesterification reactor, its large flow rate into the liquid-liquid extractor is the biggest bottleneck. However, the flow of ethyl acetate into the LLE cannot be reduced without compromising the recovery of sucralose.

The profitability analysis of a configuration using a lower ethyl acetate flow rate with a higher sucrose flow rate (Table 23) shows a cumulative present value at the project's end of life to be 38% of that calculated in the base case. This is due to the reduced ethyl acetate flow rate which results in a reduced volume of ethyl acetate leaving the system and hence the hypothetical revenue stream reduces, although this would be cleaned and recycled into the system. This is something which future work should investigate.

It is not possible to continue lowering the ethyl acetate flowrate while increasing the sucrose flowrate because realistically there would be a cap on the amount of sucrose available to produce sucralose. To offset the high costs of this process, a cheaper yet still non-toxic solvent can be explored as an alternative to ethyl acetate. One way to consider lowering the costs may be for the sugar industry to partner with key players in the beverages market, such as with Coca Cola. In this scenario an investment from a major industry player may assist the plant in achieving profitability quicker and may also secure a source of subsidized sucralose for the major drinks manufacturers.

It should also be noted that the current configuration does not include any recycle on the assumption that all outgoing streams will be processed further prior to be used again in the next production batch. Recycle was also not added with the consideration of sucralose being a food grade product, which requires a high level of purity. Adding recycle streams at this stage was considered cost intensive and would require the inclusion of onsite recycle stream processing before the streams could re-enter the system. Another option to consider lowering the production costs of this process would be to evaluate the feasibility of adding in recycle streams or at the very least the costs associated with processing exiting streams offsite before re-directing them into the next batch.

Table 23: Profitability Analysis of the Base Case of the sucralose production (All values in USD Million)

| End of year | Land | Fixed Capital Investment | Working Capital | Depreciation | Cost of production excl. depreciation | Sales | Net Earnings | Non-discounted Cash flow | Discounted Cash Flow (PV) | Cumulative PV |
|---|---|---|---|---|---|---|---|---|---|---|
| **0** | -USD 5.00 | | | | | | | -USD 5.00 | -USD 5.00 | -USD 5.00 |
| **1** | | USD 1.46 | | | | | | -USD 1.46 | -USD 1.33 | -USD 6.33 |
| **2** | | USD 0.98 | USD 9.84 | | | | | -USD 10.81 | -USD 8.94 | -USD 15.27 |
| **3** | | | | USD 0.4882 | USD 248.86 | USD 1 930 | USD 1 209.78 | USD 1 210.26 | USD 909.29 | USD 894.02 |
| **4** | | | | USD 0.7812 | USD 339.36 | USD 2 894 | USD 1 839.06 | USD 1 839.84 | USD 1 256.64 | USD 2 150.66 |
| **5** | | | | USD 0.4687 | USD 452.48 | USD 3 859 | USD 2 452.50 | USD 2 452.96 | USD 1 523.10 | USD 3 673.75 |
| **6** | | | | USD 0.28 | USD 452.48 | USD 3 859 | USD 2 452.63 | USD 2 452.91 | USD 1 384.60 | USD 5 058.36 |
| **7** | | | | USD 0.28 | USD 452.48 | USD 3 859 | USD 2 452.63 | USD 2 452.91 | USD 1 258.73 | USD 6 317.09 |
| **8** | | | | USD 0.14 | USD 452.48 | USD 3 859 | USD 2 452.73 | USD 2 452.87 | USD 1 144.28 | USD 7 461.37 |
| **9** | | | | | USD 452.48 | USD 3 859 | USD 2 452.83 | USD 2 452.83 | USD 1 040.24 | USD 8 501.61 |
| **10** | | | | | USD 452.48 | USD 3 859 | USD 2 452.83 | USD 2 452.83 | USD 945.67 | USD 9 447.29 |
| **11** | | | | | USD 452.48 | USD 3 859 | USD 2 452.83 | USD 2 452.83 | USD 859.70 | USD 10 306.99 |
| **12** | | | | | USD 452.48 | USD 3 859 | USD 2 452.83 | USD 2 452.83 | USD 781.55 | USD 11 088.54 |

Table 24: Profitability Analysis of a lowered ethyl acetate flowrate process of sucralose production (All values in USD Million)

| End of year | Land | Fixed Capital Investment | Working Capital | Depreciation | Cost of production excl. depreciation | Sales | Net Earnings | Non-discounted Cash flow | Discounted Cash Flow (PV) | Cumulative PV |
|---|---|---|---|---|---|---|---|---|---|---|
| 0 | -USD 5.00 | | | | | | | -USD 5.00 | -USD 5.00 | -USD 5.00 |
| 1 | | USD 1.48 | | | | | | -USD 1.48 | -USD 1.35 | -USD 6.35 |
| 2 | | USD 0.99 | USD 9.95 | | | | | -USD 10.93 | -USD 9.04 | -USD 15.38 |
| 3 | | | | USD 0.4936 | USD 98.08 | USD 743 | USD 463.80 | USD 464.29 | USD 348.83 | USD 333.45 |
| 4 | | | | USD 0.7898 | USD 133.74 | USD 1 114 | USD 705.29 | USD 706.08 | USD 482.26 | USD 815.71 |
| 5 | | | | USD 0.4739 | USD 178.32 | USD 1 485 | USD 940.80 | USD 941.27 | USD 584.46 | USD 1 400.16 |
| 6 | | | | USD 0.28 | USD 178.32 | USD 1 485 | USD 940.94 | USD 941.22 | USD 531.29 | USD 1 931.46 |
| 7 | | | | USD 0.28 | USD 178.32 | USD 1 485 | USD 940.94 | USD 941.22 | USD 483.00 | USD 2 414.45 |
| 8 | | | | USD 0.14 | USD 178.32 | USD 1 485 | USD 941.04 | USD 941.18 | USD 439.07 | USD 2 853.52 |
| 9 | | | | | USD 178.32 | USD 1 485 | USD 941.14 | USD 941.14 | USD 399.14 | USD 3 252.66 |
| 10 | | | | | USD 178.32 | USD 1 485 | USD 941.14 | USD 941.14 | USD 362.85 | USD 3 615.51 |
| 11 | | | | | USD 178.32 | USD 1 485 | USD 941.14 | USD 941.14 | USD 329.86 | USD 3 945.37 |
| 12 | | | | | USD 178.32 | USD 1 485 | USD 941.14 | USD 941.14 | USD 299.88 | USD 4 245.25 |

# 8 Conclusions and Recommendations

Competitive global prices for sugar, the occurrence of drought and the implementation of the Health Protection Levy have all served heavy blows to the South African sugar industry, severely impacting the revenue being generated from sold sugar. The sugar industry in South Africa thus requires diversification of its value chain to increase demand for sugar, maintain the infrastructure and sustain the many dependent jobs.

Although there exist diversification routes by which sucrose and the by-products of the sugar value chain are being utilized, these are largely low-value options such as the burning of bagasse onsite. The other valorization options are promising but still require research to further optimize the processing costs of some of the materials. For sucrose itself, the main focus is on constructing platform chemicals from it, some of which like citric acid are well established, while others are still at the pilot phase.

The main aim of this study was therefore to find a diversification route for sucrose in South Africa, but to use mathematical modelling of manufacturing data to identify the best performing industry based on its forecast. The use of mathematical modelling in this way is very limited, with most decision-making processes in the bioproducts realm being survey or experience based.

The main objectives of this study were thus to firstly, find a dataset that comprehensively represents manufacturing activity across the main industries in South Africa, then to fit a suitable model to this from which the forecast was to identify one main industry for further research.

To this end, the study successfully considered four datasets published by well-known authorities and identified the individual industries' production data published by Statistics South Africa to be the most robust, clearly explained and well representing of South Africa's markets. Further, more than three mathematical models were evaluated against the dataset and from this, Auto-Regressive Integrated Moving Average (ARIMA) models were found to be the best overall match to the data for the eight main manufacturing industries.

The resulting forecasts from the ARIMA models combined with selection matrices constructed to consider the growth rate and revenue potential identified the beverages' industry as the best possible option to consider placing sugar-based biochemicals in.

Furthermore, the objective of identifying a potential chemical for placement within the beverages' industry was also achieved, albeit the selected chemical was not one which is newly commercialized as was one of the other objectives. While some progress was noted for less commercialized sugar-based chemicals, it was found that the four main candidates would all fall into the textiles' manufacturing sector, which the manufacturing dataset shows to be one of the worst industries to invest in at this time due to minimal growth and a lack of government funding support.

Eight main beverage constituents were then evaluated for suitable chemical candidates, from which the category of non-nutritive sweeteners was found to present the broadest application across the range of commonly consumed beverages and which would provide the South African sugar industry with the lowest investment risk and greatest revenue generating potential.

Six synthetic sweeteners were then evaluated based on their relative selling price, safety profiles and their applicability in food and beverages; the result of which found sucralose to be the most widely used sweetener with the least number of reported serious health risks. Although sucralose is not the most lucrative sweetener of the options considered, its wide application and accessibility to a large percentage of the population make it an attractive option to invest in. Moreover, sucralose presents an opportunity for the sugar industry to leverage beverage manufacturers use of sweeteners to comply with the Heath Protection Levy.

The techno-economic analysis was performed for sucralose using SuperPro Designer, and the selected synthetic chemical process proved profitable in the first year of operation, as did a revised configuration using a lower ethyl acetate flow rate. This is largely due to the retail price of sucralose being close to 8 times the purchase cost of the most expensive raw material used. Although this profitability analysis is promising, further investigation into the fixed capital costs involved should be done prior to the sugar industry investing in sucralose.

Besides achieving the study's objectives, the use of ARIMA models to forecast manufacturing data has demonstrated its usefulness in serving as a tool to assist decision makers. This is also a technique which was not found in literature as having been done before.

The limitations of this study are the consideration of only one synthetic production route to develop sucralose from sucrose, the use of only one data source in creating ARIMA models and only using auto.arima in R to develop the models.

In order to further improve the profitability of the selected production route for sucralose, it is recommended to consider the following:

- Explore alternative solvents to ethyl acetate which are cheaper but still readily available and non-toxic
- Explore alternative synthetic routes of producing sucralose
- Consider biological production routes especially with metabolically engineered species
- Engage in strategic partnerships with key players in the beverage industry to create an ecosystem of dedicated supply and demand, or to consider the subsidization of sucralose production

It is also possible for the sugar industry to delay their investment into the beverages' industry in favour of exploring options for diversification into the motor vehicles' industry which came a close second in the selection matrices. It is also recommended to repeat the methodology described herein using manual development of ARIMA models, which may or may not point towards a different industry to invest in.

The production of sucralose as per the method described in this study has the potential to not only successfully divert sugar into a sustainable revenue generating stream in South Africa, but to also maintain the 1 million livelihoods invested in the industry.

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# Appendix A: Graphs of historic sales and forecasts using ARIMA models

***Beverages***

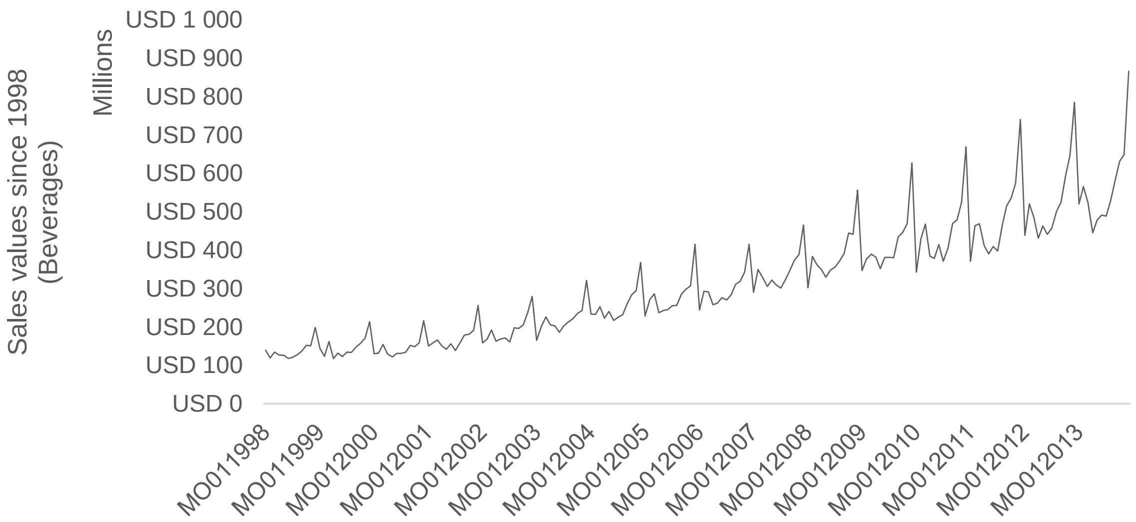


Figure 24: Historic sales values for the beverages' manufacturing sector in South Africa

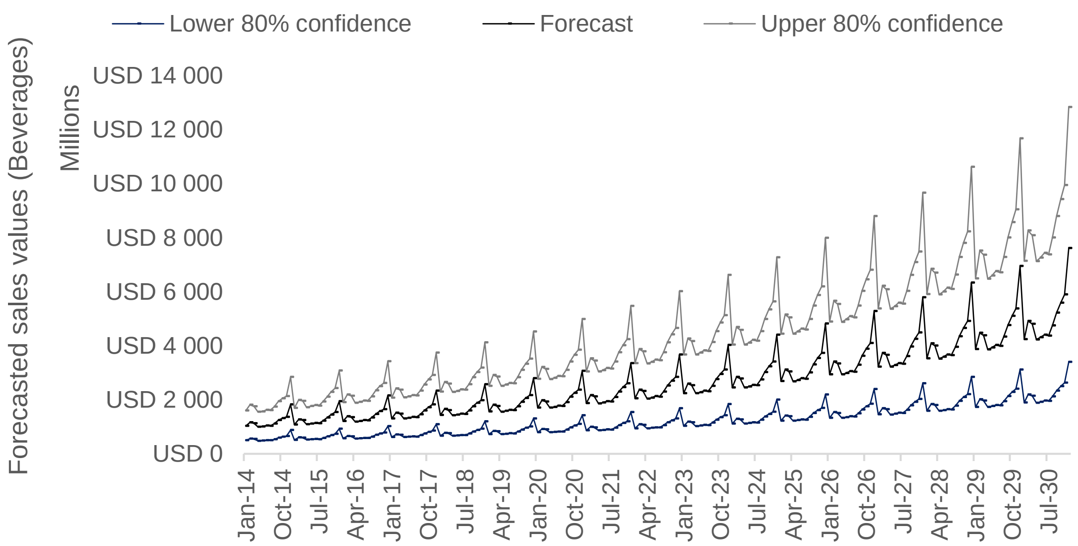


Figure 25: Forecast graphs for the beverages' industry from 2014 till 2030

***Basic Chemicals***

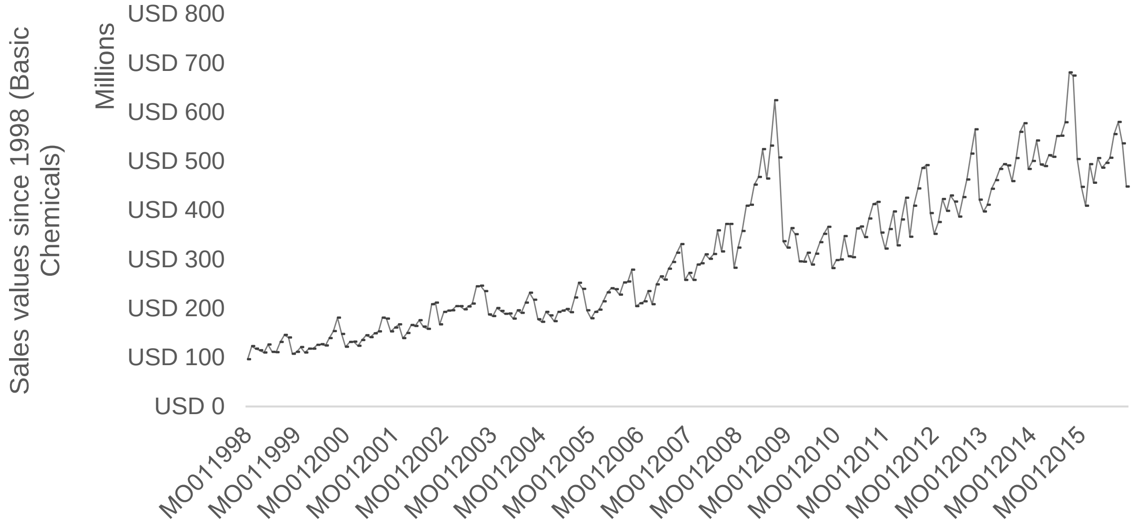


Figure 26: Historic sales values for the basic chemicals' manufacturing sector in South Africa

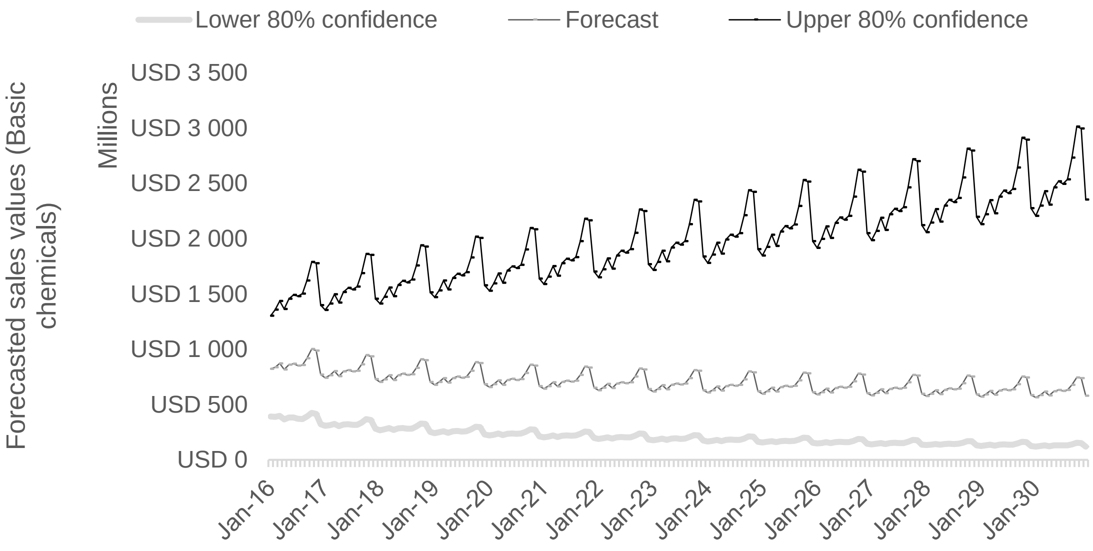


Figure 27: Forecast graphs for the basic chemicals' industry from 2016 till 2030

***Other Chemicals***

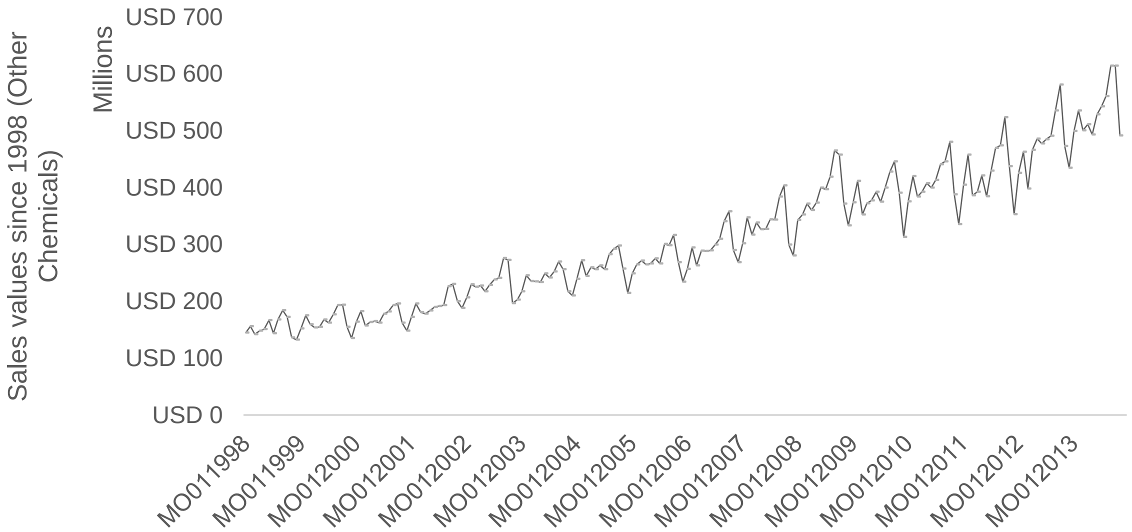


Figure 28: Historic sales values for the other chemicals' manufacturing sector in South Africa

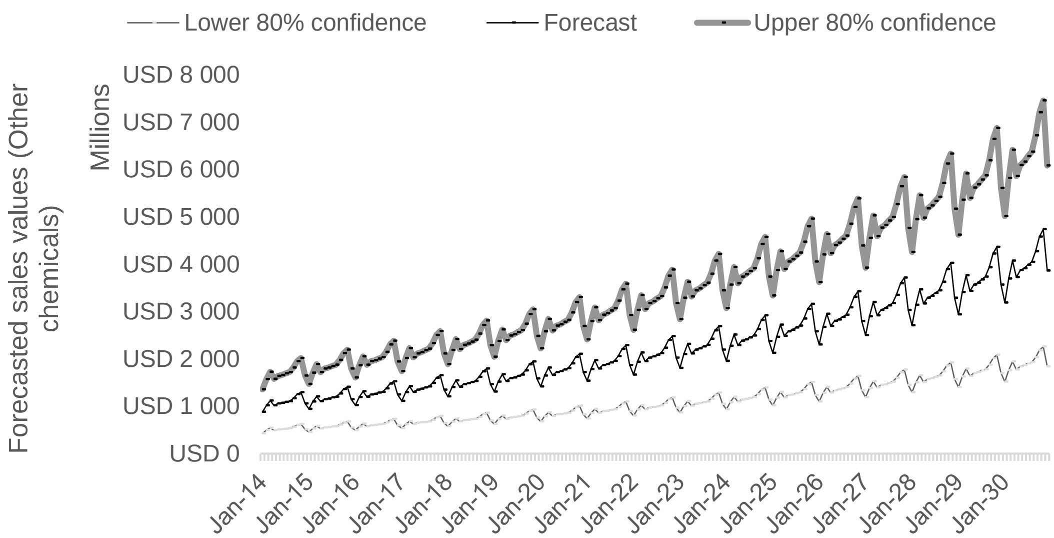


Figure 29: Forecast graphs for the other chemicals' industry from 2014 till 2030

***Petroleum***

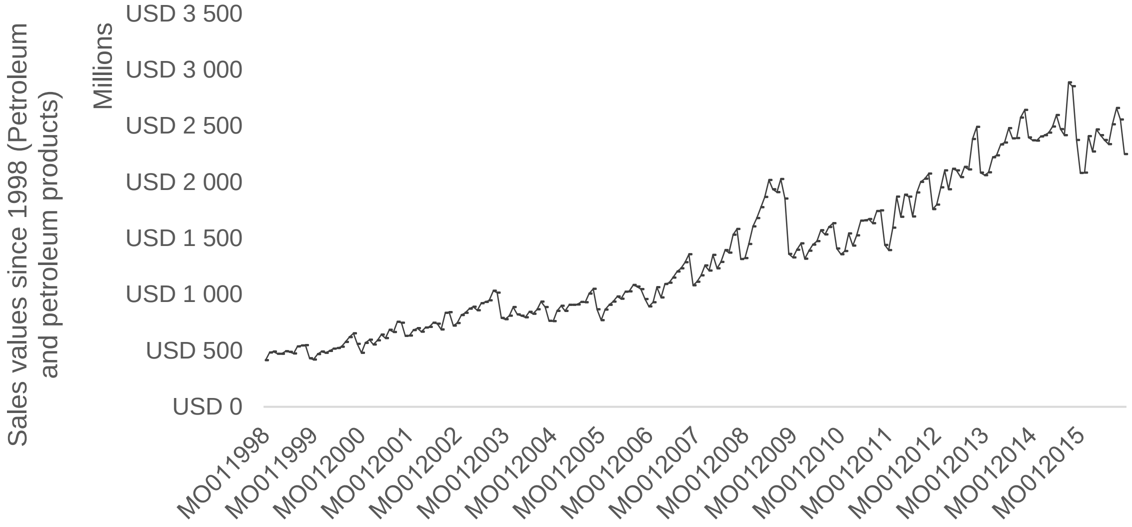


Figure 30: Historic sales values for the petroleum manufacturing sector in South Africa

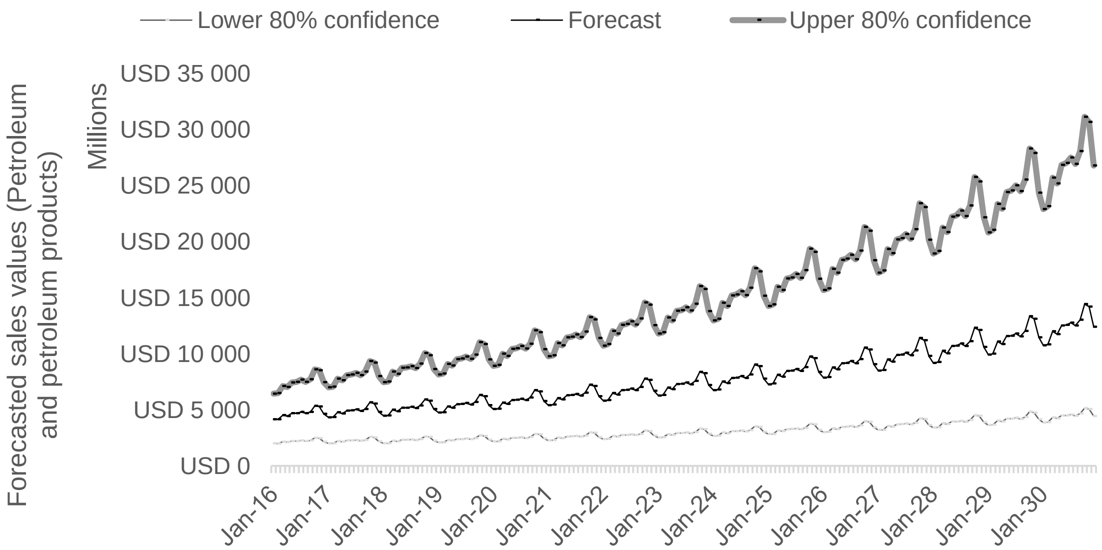


Figure 31: Forecast graphs for the petroleum industry from 2016 till 2030

***Plastics***

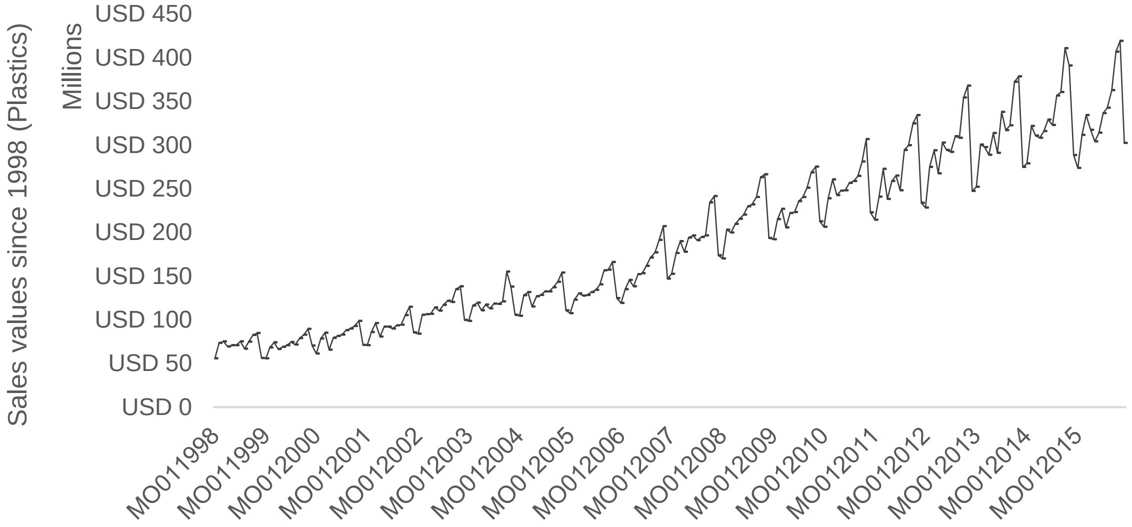


Figure 32: Historic sales values for the plastics' manufacturing sector in South Africa

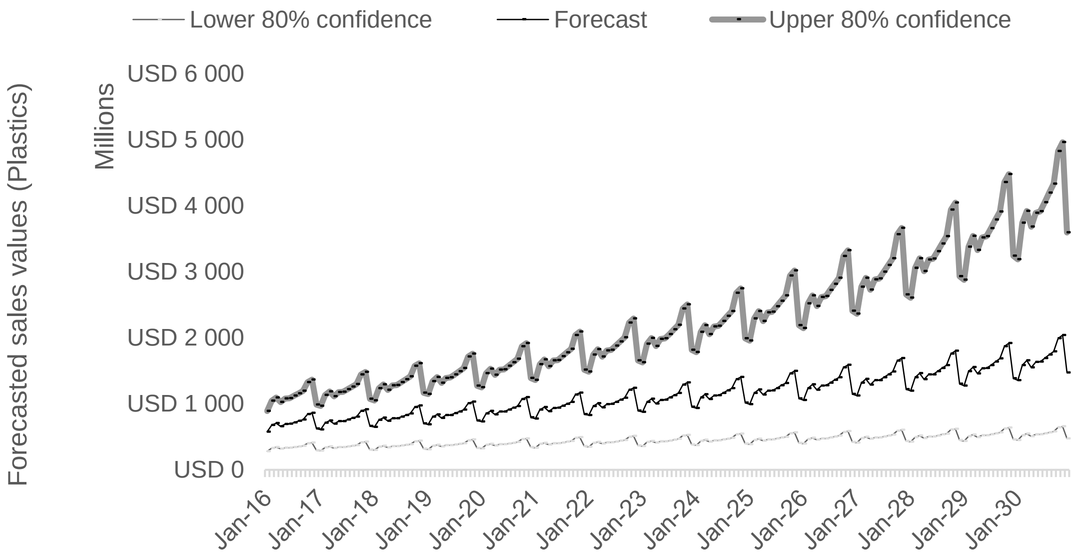


Figure 33: Forecast graphs for the plastics' industry from 2016 till 2030

***Rubber***

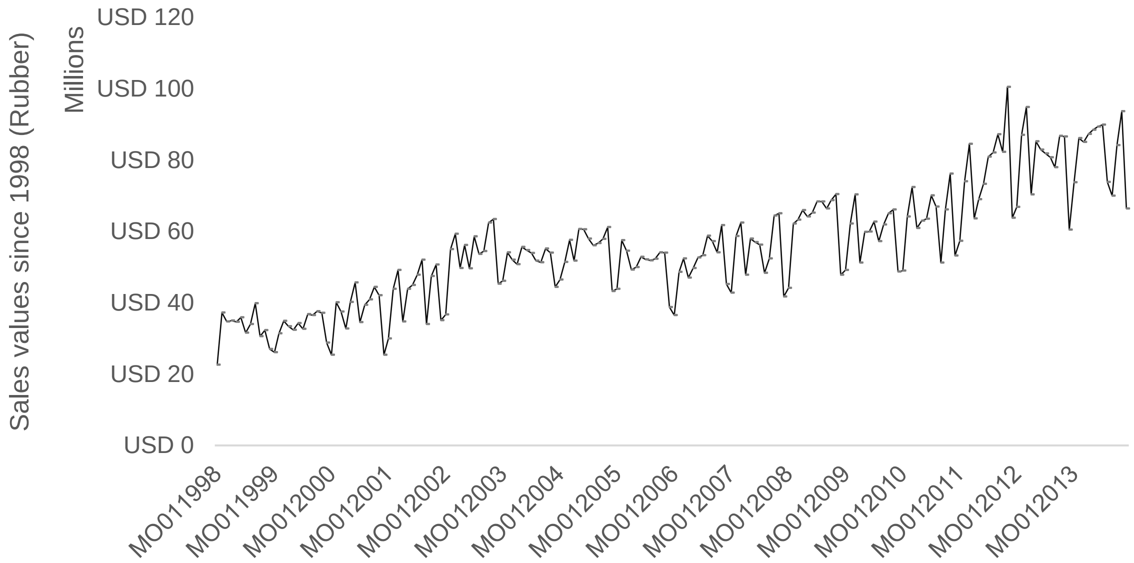


Figure 34: Historic sales values for the rubber and rubber products' manufacturing sector in South Africa

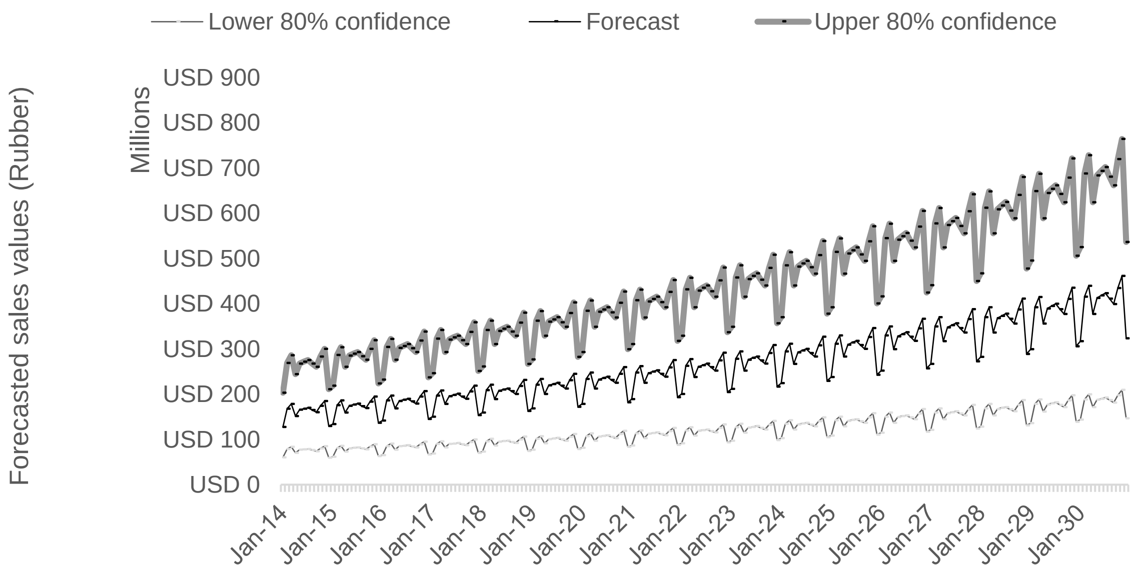


Figure 35: Forecast graphs for the rubber industry from 2014 till 2030

### *Motor vehicles*

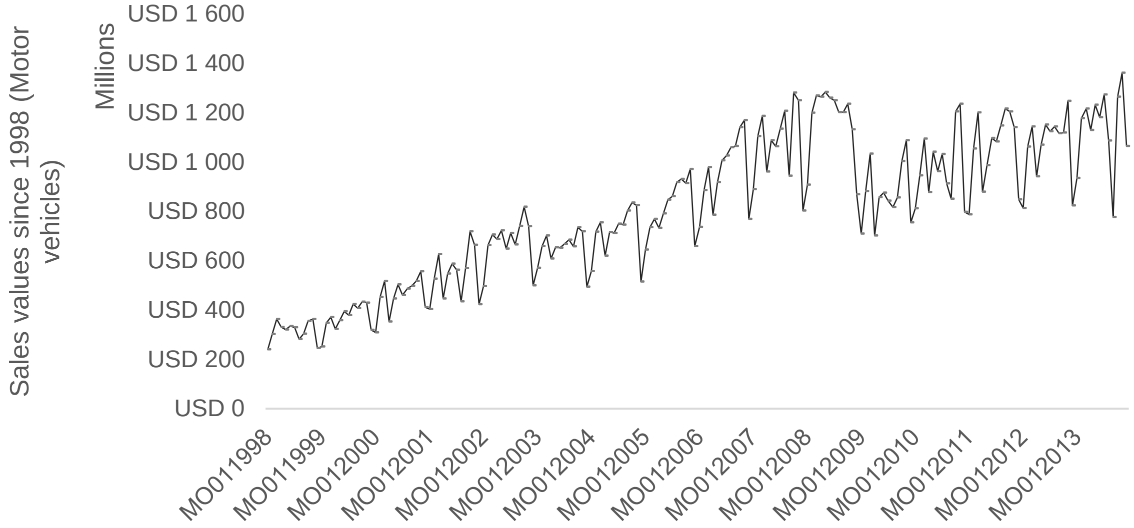


Figure 36: Historic sales values for the motor vehicles' manufacturing sector in South Africa

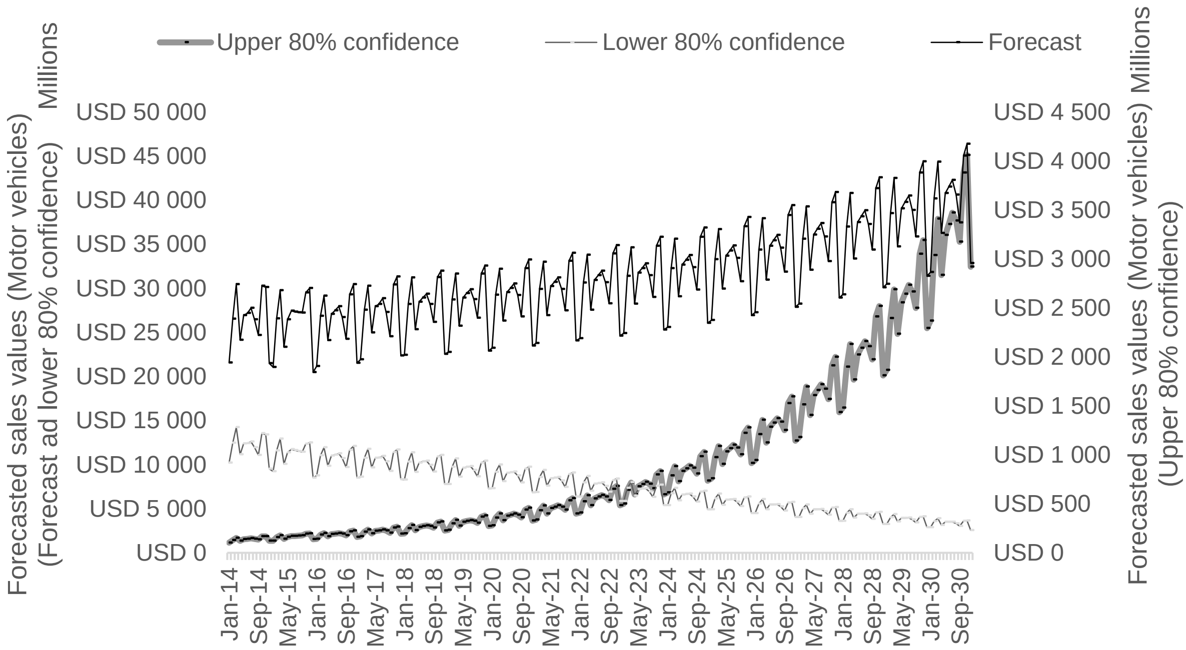


Figure 37: Forecasted sales values for the motor vehicles' sector in South Africa

***Textiles***

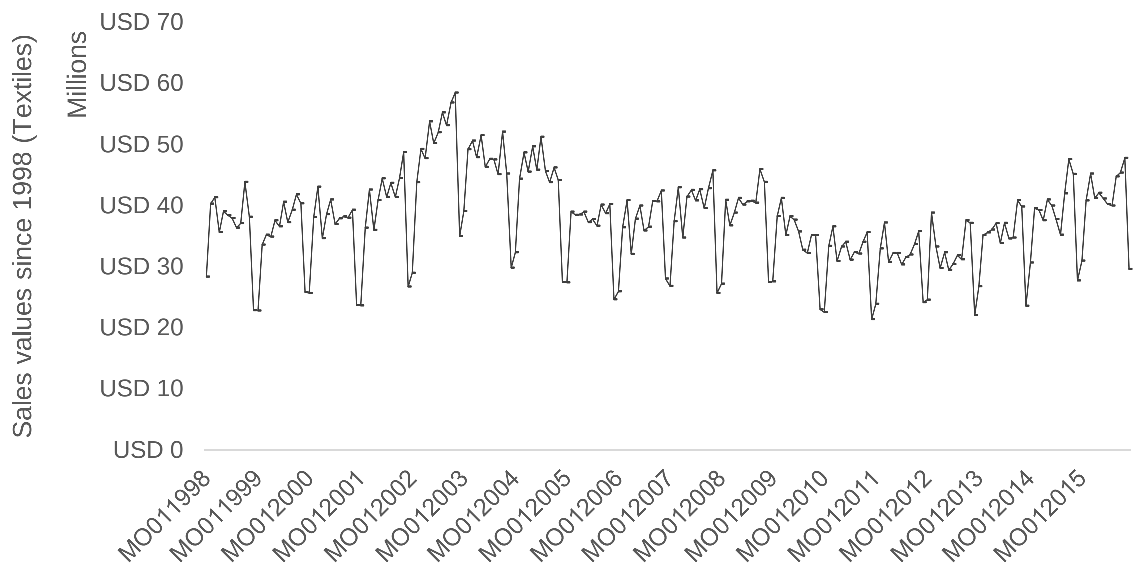


Figure 38: Historic sales values for the textiles' manufacturing sector in South Africa

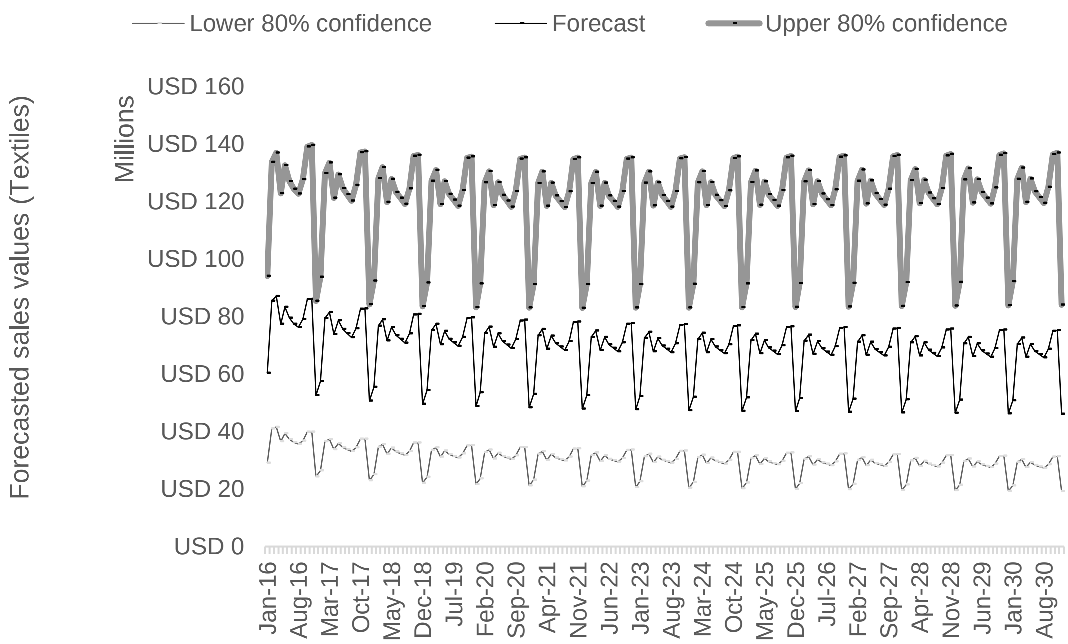


Figure 39: Forecast graphs for the textiles' industry from 2016 till 2030

# Appendix B: Simple moving average forecasts

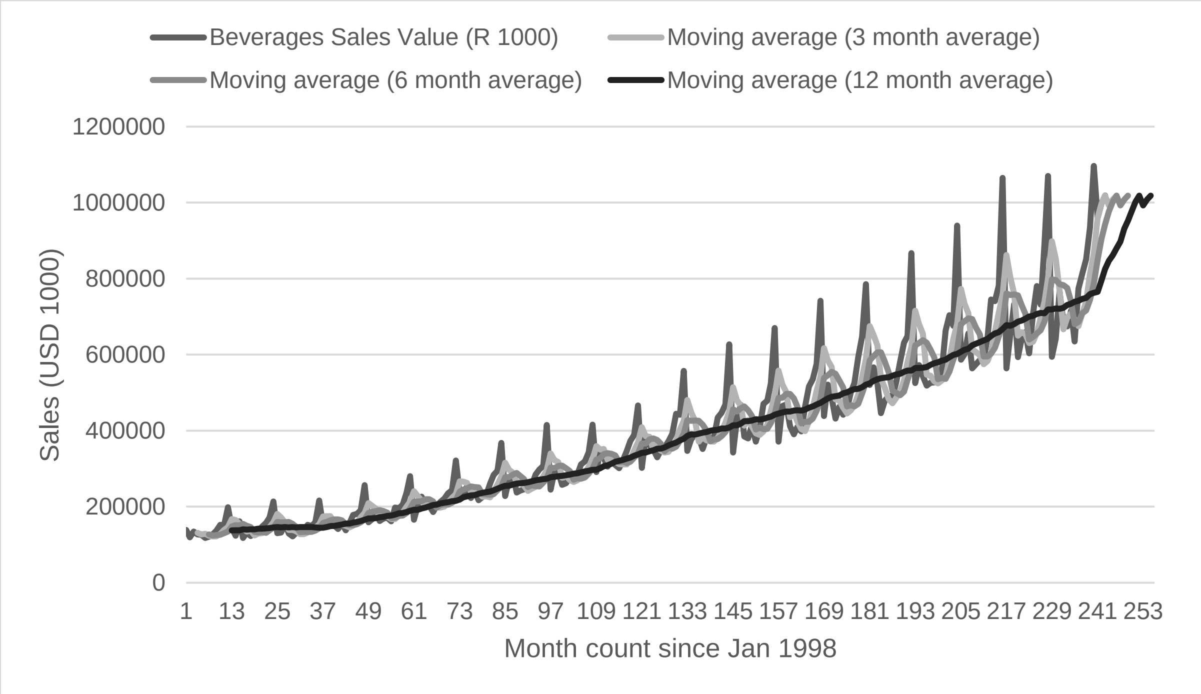


Figure 40: Forecast of beverages sales' data using simple moving averages

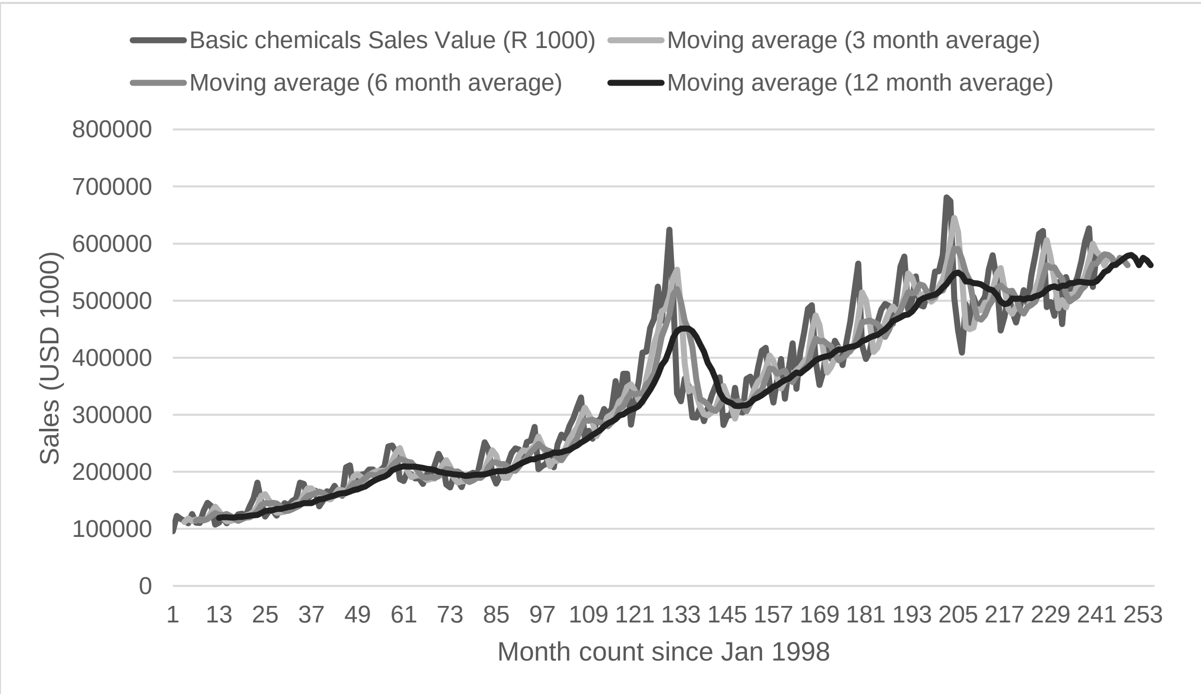


Figure 41: Forecast of basic chemicals sales' data using simple moving averages

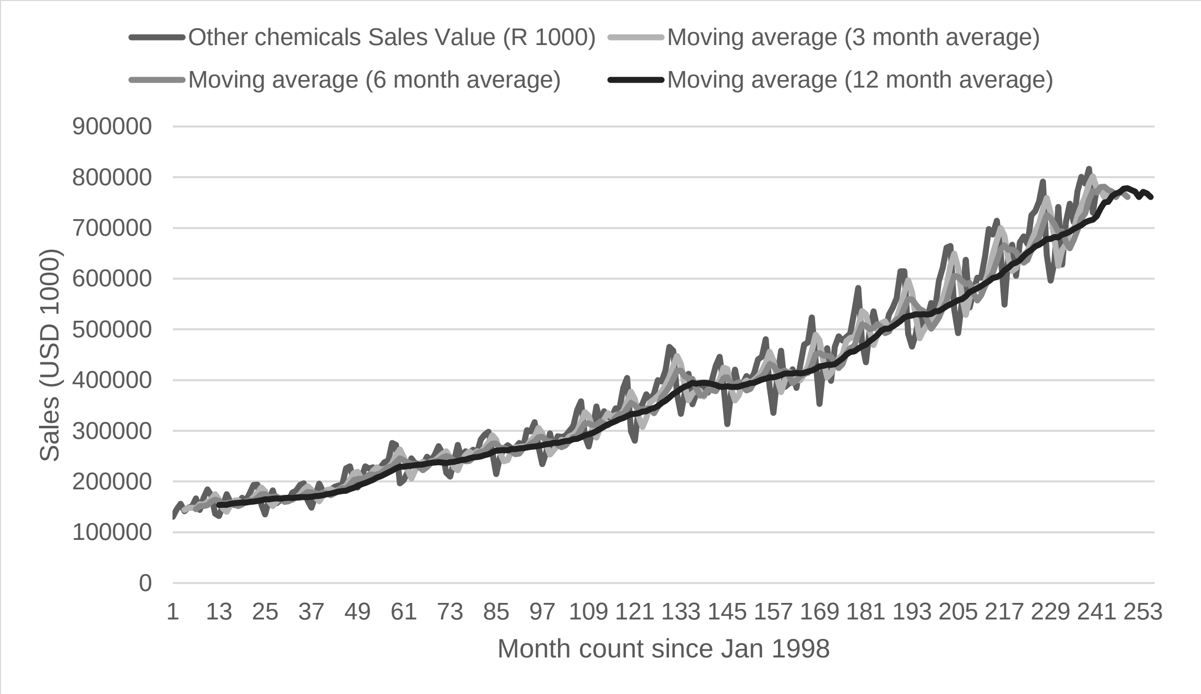


Figure 42: Forecast of other chemicals sales data using simple moving averages

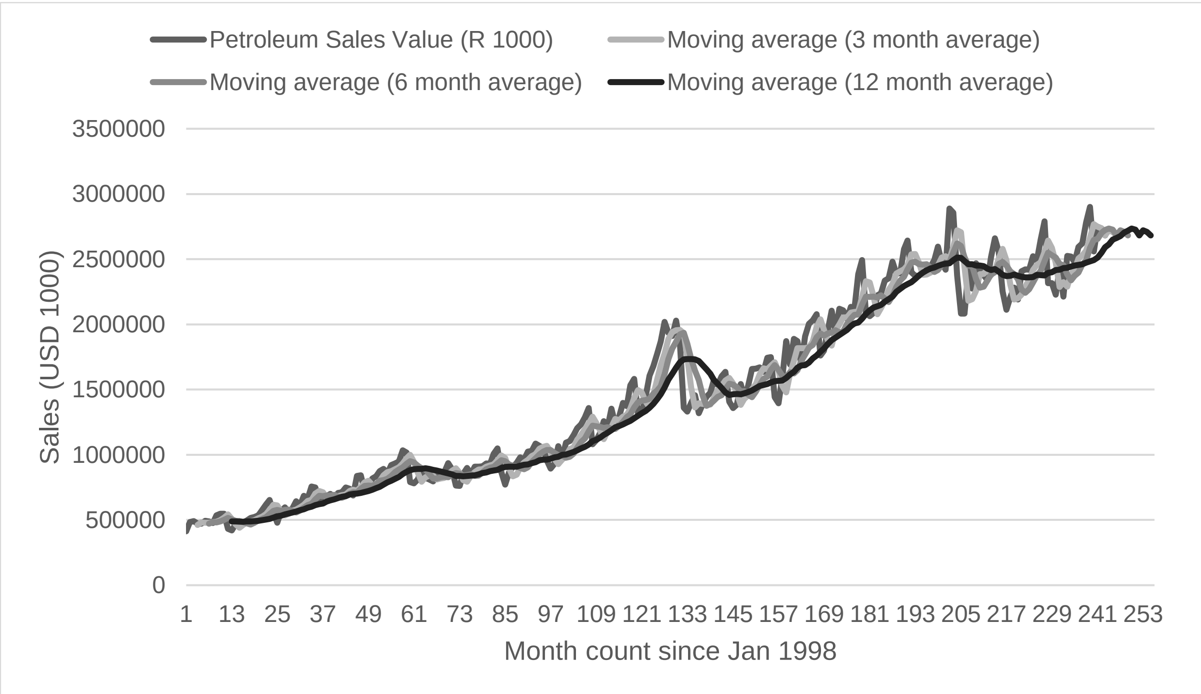


Figure 43: Forecast of petroleum sales' data using simple moving averages

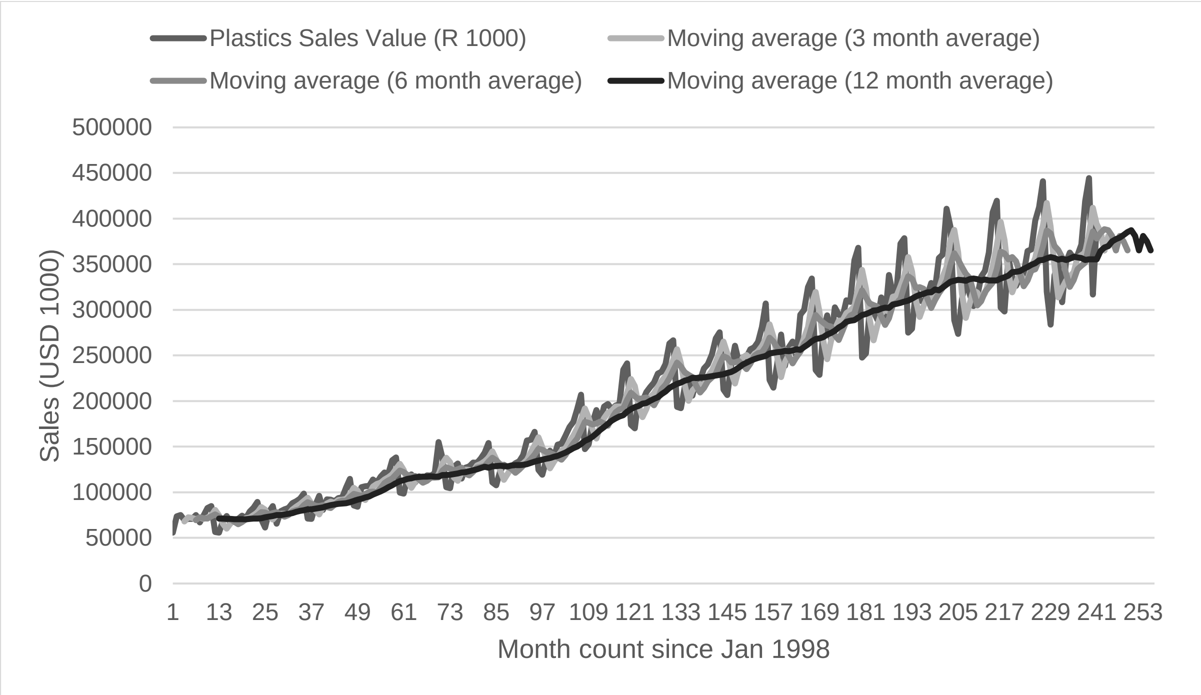


Figure 44: Forecast of plastics' sales data using simple moving averages

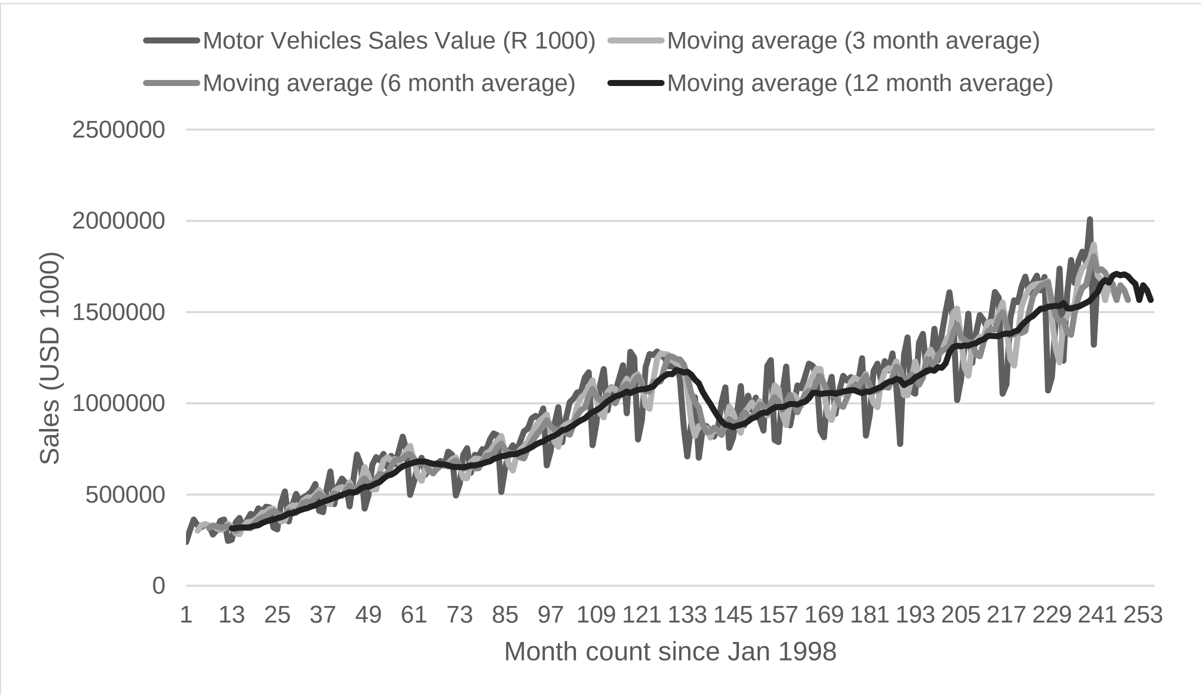


Figure 45: Forecast of motor vehicles' sales data using simple moving averages

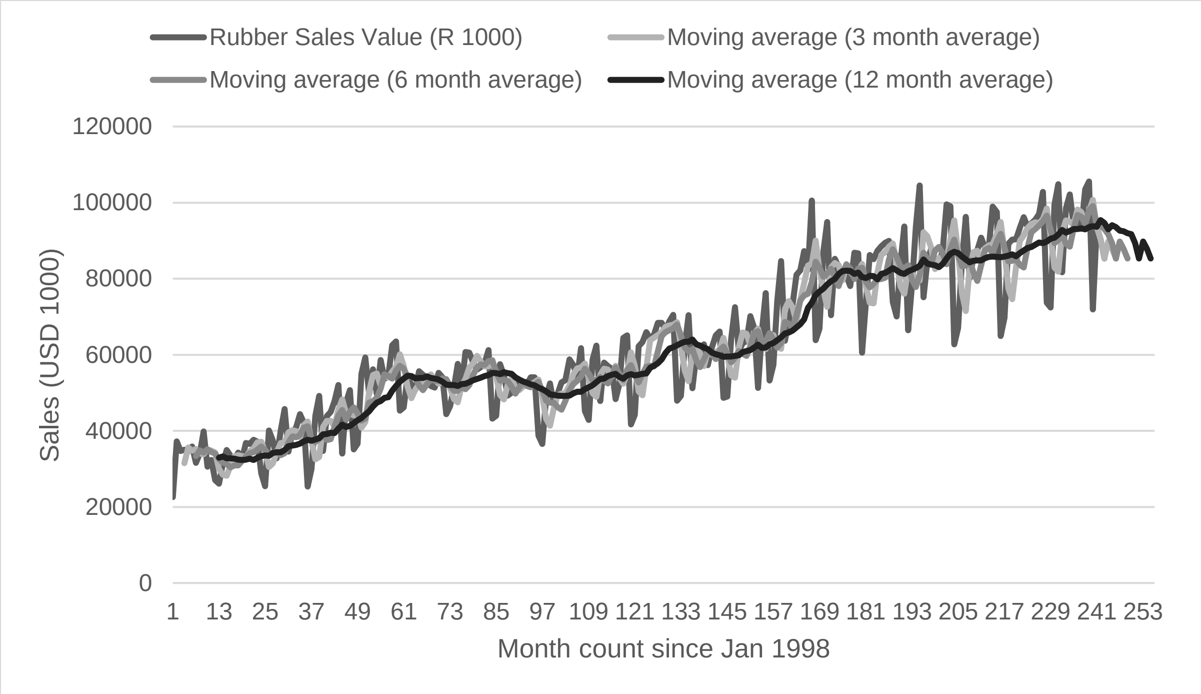


Figure 46: Forecast of rubber sales' data using simple moving averages

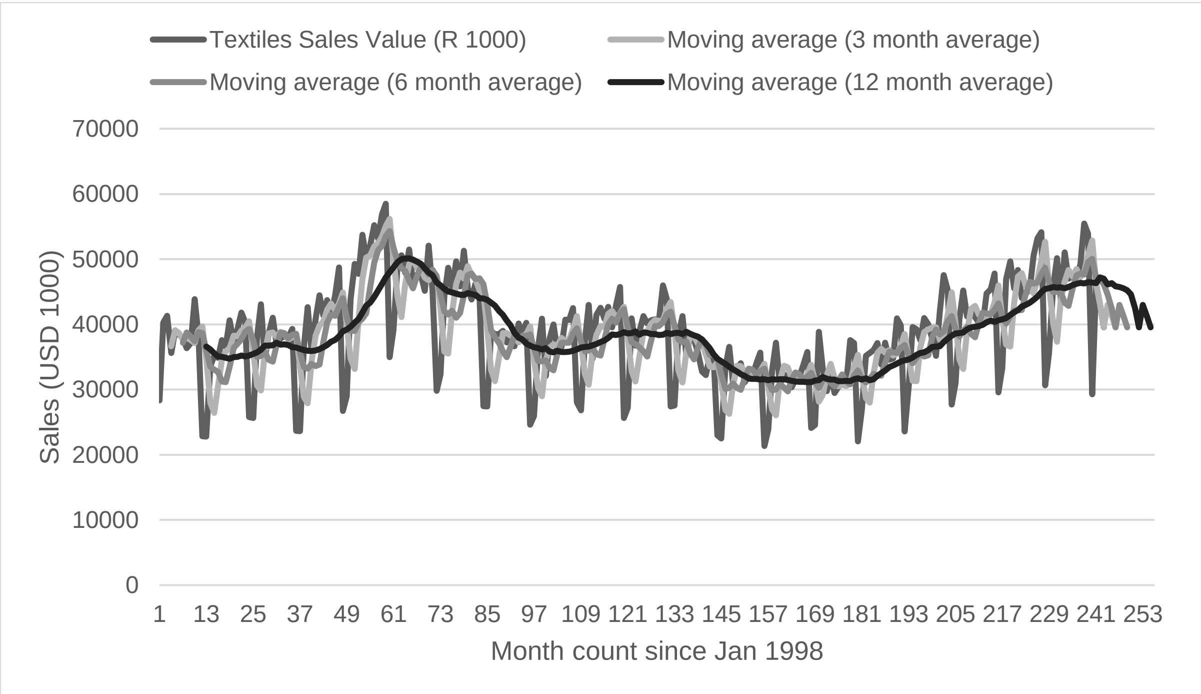


Figure 47: Forecast of textiles' sales data using simple moving averages

# Appendix C: Selection matrices

The selection matrices for all industries for the milestone year of 2022.

| **2022** | | | | | | |
|---|---|---|---|---|---|---|
| **Beverages** | **Growth Rate Factor** | | | | | |
| **Sales Value Factor** | **2022** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 94 |
| | 0.4 | | | | 88 | |
| | 0.5 | | | 85 | | |
| | 0.6 | | 82 | | | |
| | 0.8 | 76 | | | | |
| **Basic Chemicals** | **Growth Rate Factor** | | | | | |
| **Sales Value Factor** | **2022** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 32 |
| | 0.4 | | | | 34 | |
| | 0.5 | | | 35 | | |
| | 0.6 | | 36 | | | |
| | 0.8 | 38 | | | | |
| **Other Chemicals** | **Growth Rate Factor** | | | | | |
| **Sales Value Factor** | **2022** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 84 |
| | 0.4 | | | | 78 | |
| | 0.5 | | | 75 | | |
| | 0.6 | | 72 | | | |
| | 0.8 | 66 | | | | |
| **Plastics** | **Growth Rate Factor** | | | | | |
| **Sales Value Factor** | **2022** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 82 |
| | 0.4 | | | | 74 | |
| | 0.5 | | | 70 | | |
| | 0.6 | | 66 | | | |
| | 0.8 | 58 | | | | |

| Rubber | Growth Rate Factor | | | | | |
|---|---|---|---|---|---|---|
| Sales Value Factor | **2022** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 62 |
| | 0.4 | | | | 54 | |
| | 0.5 | | | 50 | | |
| | 0.6 | | 46 | | | |
| | 0.8 | 38 | | | | |
| **Motor Vehicles** | **Growth Rate Factor** | | | | | |
| Sales Value Factor | **2022** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 76 |
| | 0.4 | | | | 82 | |
| | 0.5 | | | 85 | | |
| | 0.6 | | 88 | | | |
| | 0.8 | 94 | | | | |
| **Textiles** | **Growth Rate Factor** | | | | | |
| Sales Value Factor | **2022** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 20 |
| | 0.4 | | | | 20 | |
| | 0.5 | | | 20 | | |
| | 0.6 | | 20 | | | |
| | 0.8 | 20 | | | | |

The selection matrices for all industries for the milestone year of 2025.

| **2025** | | | | | | |
|---|---|---|---|---|---|---|
| **Beverages** | **Growth Rate Factor** | | | | | |
| **Sales Value Factor** | **2025** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 98 |
| | 0.4 | | | | 96 | |
| | 0.5 | | | 95 | | |
| | 0.6 | | 94 | | | |
| | 0.8 | 92 | | | | |
| **Basic Chemicals** | **Growth Rate Factor** | | | | | |
| **Sales Value Factor** | **2025** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 32 |
| | 0.4 | | | | 34 | |
| | 0.5 | | | 35 | | |
| | 0.6 | | 36 | | | |
| | 0.8 | 38 | | | | |
| **Other Chemicals** | **Growth Rate Factor** | | | | | |
| **Sales Value Factor** | **2025** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 80 |
| | 0.4 | | | | 80 | |
| | 0.5 | | | 80 | | |
| | 0.6 | | 80 | | | |
| | 0.8 | 80 | | | | |
| **Plastics** | **Growth Rate Factor** | | | | | |
| **Sales Value Factor** | **2025** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 74 |
| | 0.4 | | | | 68 | |
| | 0.5 | | | 65 | | |
| | 0.6 | | 62 | | | |
| | 0.8 | 56 | | | | |
| **Rubber** | **Growth Rate Factor** | | | | | |

| | | | | | | |
|---|---|---|---|---|---|---|
| **Sales Value Factor** | **2025** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 62 |
| | 0.4 | | | | 54 | |
| | 0.5 | | | 50 | | |
| | 0.6 | | 46 | | | |
| | 0.8 | 38 | | | | |
| **Motor Vehicles** | **Growth Rate Factor** | | | | | |
| **Sales Value Factor** | **2025** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 76 |
| | 0.4 | | | | 82 | |
| | 0.5 | | | 85 | | |
| | 0.6 | | 88 | | | |
| | 0.8 | 94 | | | | |
| **Textiles** | **Growth Rate Factor** | | | | | |
| **Sales Value Factor** | **2025** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 20 |
| | 0.4 | | | | 20 | |
| | 0.5 | | | 20 | | |
| | 0.6 | | 20 | | | |
| | 0.8 | 20 | | | | |

The selection matrices for all industries for the milestone year of 2030.

| **2030** | | | | | | |
|---|---|---|---|---|---|---|
| **Beverages** | **Growth Rate Factor** | | | | | |
| **Sales Value Factor** | **2030** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 98 |
| | 0.4 | | | | 96 | |
| | 0.5 | | | 95 | | |
| | 0.6 | | 94 | | | |
| | 0.8 | 92 | | | | |
| **Basic Chemicals** | **Growth Rate Factor** | | | | | |
| **Sales Value Factor** | **2030** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 22 |
| | 0.4 | | | | 24 | |
| | 0.5 | | | 25 | | |
| | 0.6 | | 26 | | | |
| | 0.8 | 28 | | | | |
| **Other Chemicals** | **Growth Rate Factor** | | | | | |
| **Sales Value Factor** | **2030** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 76 |
| | 0.4 | | | | 72 | |
| | 0.5 | | | 70 | | |
| | 0.6 | | 68 | | | |
| | 0.8 | 64 | | | | |
| **Plastics** | **Growth Rate Factor** | | | | | |
| **Sales Value Factor** | **2030** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 74 |
| | 0.4 | | | | 68 | |
| | 0.5 | | | 65 | | |
| | 0.6 | | 62 | | | |
| | 0.8 | 56 | | | | |
| **Rubber** | **Growth Rate Factor** | | | | | |

| | | | | | | |
|---|---|---|---|---|---|---|
| **Sales Value Factor** | **2030** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 44 |
| | 0.4 | | | | 38 | |
| | 0.5 | | | 35 | | |
| | 0.6 | | 32 | | | |
| | 0.8 | 26 | | | | |
| **Motor Vehicles** | **Growth Rate Factor** | | | | | |
| **Sales Value Factor** | **2030** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 60 |
| | 0.4 | | | | 70 | |
| | 0.5 | | | 75 | | |
| | 0.6 | | 80 | | | |
| | 0.8 | 90 | | | | |
| **Textiles** | **Growth Rate Factor** | | | | | |
| **Sales Value Factor** | **2030** | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 |
| | 0.2 | | | | | 10 |
| | 0.4 | | | | 10 | |
| | 0.5 | | | 10 | | |
| | 0.6 | | 10 | | | |
| | 0.8 | 10 | | | | |

# Appendix D: Assumptions for the simulation

The following tables summarize the assumptions made in SuperPro Designer (Academic License) V9.5, Build 3 with the production of sucralose.

| **Equipment** | **Assumption/Decision** |
|---|---|
| **Reactor 1: Transesterification** | Assumed catalyst would be charged prior to the reaction and would be completely washed and recycled between batches. No mass loss assumed |
| | Did not include catalyst washing and recycling |
| | Assumed all product were transferred out after the reaction was complete, except for Ethyl Acetate and Ethanol which are in vapour phase |
| | Assumed only Ethanol would liquidize and be transferred after the reactor was cooled to 78°C |
| | Assumed only Ethyl Acetate would liquidize and be transferred out after the reactor was further cooled to 25°C |
| | Assumed both Ethanol and Ethyl Acetate are in pure and saleable condition |
| | Set the reactor to operate at 80°C |
| | Assumed only standard agitation was needed |
| | Assumed a set up time of 1 hour |
| | Assumed the turnaround time was included in the set-up time |

| | |
|---|---|
| | Assumed a maximum vessel working volume: vessel volume of 90% |
| | Assumed a minimum vessel working volume: vessel volume of 15% |
| | Assumed the transfer in time of feed material to be 5 minutes with no set up time |
| | Nitrogen and oxygen were evacuated from the reactor prior to the transfer in of the feed material |
| | Assumed no set up time for material transfer out |
| | Assumed 5 minutes for material transfer out |
| | Assumed a design pressure of 2 bar and no pressure drop |
| | Assumed no standby units |

| **Equipment** | Assumption/Decision |
|---|---|
| **Heater 1: Feed to Reactor 2** | Assumed set up time of 0 minutes |
| | Assumed process time of 5 minutes |
| | Assumed to use steam |
| | Assumed a heat transfer coefficient of 1500 Watt/m2-K |
| | Assumed 100% heat transfer efficiency |
| | Exit temperature set to be 85°C |

| **Equipment** | **Assumption/Decision** |
|---|---|
| **Reactor 2: Chlorination** | Nitrogen and oxygen were evacuated from the reactor prior to the transfer in of the feed material |
| | Assumed a design pressure of 2 bar and no pressure drop |
| | Assumed the reaction to take place at atmospheric pressure |
| | Assumed no standby units |

| | |
|---|---|
| | Assumed 15 minutes set up time for phosgene charge |
| | Assumed a 15-minute transfer in time for material from heat exchanger |
| | Assumed 5 minute set up time for the reactor heating |
| | Assumed 15-minute time to heat the reactor to 85°C using steam |
| | Assumed only standard agitation was needed |
| | Assumed a set up time of 1 hour |
| | Assumed the turnaround time was included in the set-up time |
| | Assumed a maximum vessel working volume: vessel volume of 90% |
| | Assumed a minimum vessel working volume: vessel volume of 15% |
| | Assumed the material would remain in the vessel and be heated to 125°C to convert all intermediates to sucralose-6-acetate |
| | Assumed the vessel contents would remain in the vessel for 2 hours at 125°C to complete intermediate conversion |
| | Assumed the vessel contents would be cooled to 50°C after the 2-hour holding time |
| | Assumed the reactor would be cooled with chilled water with an inlet temperature of 4°C and an outlet temperature of 10°C |
| | Assumed a cooling set up time of 5 minutes |
| | Assumed a cooling time of 5 minutes |
| | Assumed all vessel contents are transferred out as liquid except for phosgene which remains a gas within the vessel |

| | |
|---|---|
| | Assumed phosgene was evacuated using a gas sweep after other vessel contents were transferred out |
| | Assumed a gas sweep setting up time of 5 minutes |
| | Assumed the gas sweep to take 2 minutes |
| | Assumed nitrogen gas was used as a sweeping agent |

| **Equipment** | **Assumption/Decision** |
|---|---|
| **Coolers 1 & 2: Feed to Reactor 3** | Exit temperature assumed to be 15°C |
| | Process time assumed to be 240 minutes |
| | Assumed to use chilled water |
| | Heat transfer coefficient of 1500 Watt/m2-K assumed |
| | 100% heat transfer efficiency assumed |

| **Equipment** | Assumption/Decision |
|---|---|
| **Reactor 3: De-acylation** | Nitrogen and oxygen were evacuated from the reactor prior to the transfer in of the feed material |
| | Assumed a design pressure of 2 bar and no pressure drop |
| | Assumed the reaction to take place at atmospheric pressure |
| | Assumed no standby units |
| | Assumed a 15-minute transfer in time for material from heat exchanger |
| | Assumed 5 minute set up time material transfer in from heat exchanger |
| | Set up reactor to cool vessel contents to 15°C before reaction starts. Assumed no reaction took place before completely cooled |

| | |
|---|---|
| | Assumed chilled water used to cool vessel contents |
| | Assumed a reaction set up time of 5 minutes |
| | Assumed a reaction time of 4.5 hours |
| | Assumed a maximum vessel working volume: vessel volume of 90% |
| | Assumed a minimum vessel working volume: vessel volume of 15% |
| | Assumed only standard agitation was needed |
| | Assumed three reactions ran in parallel |
| | Assumed a yield of 70% based on sucralose-6-acetate |
| | Assumed 100% of $CO_2HCL$ produced in previous reaction vessel reacts with sodium hydroxide to produce sodium chlorocarbonate and water |
| | Assumed 100% of $CO_3H_2$ produced in previous reaction vessel reacts with sodium hydroxide to produce sodium carbonate and water |
| | Assumed a set up time of 15 minutes for material transfer out of all vessel contents |
| | Assumed 5 minutes for entire vessel to be transferred out |

| **Equipment** | Assumption/Decision |
|---|---|
| **Heater 2: Water feed to Stripper 1** | Assumed a set up time of 0 minutes |
| | Assumed a process time of 5 minutes |
| | Heat transfer coefficient of 1500 Watt/m2-K assumed |
| | 100% heat transfer efficiency assumed |
| | Exit temperature set to be 150°C |

| Equipment | Assumption/Decision |
|---|---|
| **Heater 3: Water feed to Stripper 2** | Assumed a set up time of 0 minutes |
| | Assumed a process time of 240 minutes |
| | Heat transfer coefficient of 1500 Watt/m2-K assumed |
| | 100% heat transfer efficiency assumed |
| | Exit temperature set to be 150°C |

| Equipment | Assumption/Decision |
|---|---|
| **Stripper 1** | Design component set to dimethylformamide (DMF) |
| | Diffusivity in gas phase set to 0.004052 x 10^-3 m2/s |
| | Diffusivity in liquid phase set to 0.000015 m2/s |
| | Only DMF assumed to be stripped |
| | 90% of DMF assumed to be stripped |
| | Total specific area assumed to be SuperPro Designer default value of 250 m2/m3 |
| | Packing constant assumed to remain at SuperPro Designer default value of 155 |
| | Nominal diameter assumed to remain at SuperPro Designer default value of 1m |
| | Critical surface tension assumed to remain at SuperPro Designer default value of 40 dyn/cm |
| | Stripping time assumed to be 240 minutes |
| | Assumed a set up time of 0 minutes |
| | Assumed a turnaround time of 0 minutes |
| | Water set to enter the stripper at a temperature of 150°C in gaseous form |

| Equipment | Assumption/Decision |
|---|---|
| **Stripper 2** | Design component set to dimethylformamide (DMF) |
| | Diffusivity in gas phase set to 0.004052 x 10^-3 m2/s |
| | Diffusivity in liquid phase set to 0.000015 m2/s |

| | |
|---|---|
| | 90% of DMF assumed to be stripped |
| | 99% of sodium hydroxide assumed to be stripped as well |
| | Total specific area assumed to be SuperPro Designer default value of 250 m2/m3 |
| | Packing constant assumed to remain at SuperPro Designer default value of 155 |
| | Nominal diameter assumed to remain at SuperPro Designer default value of 1m |
| | Critical surface tension assumed to remain at SuperPro Designer default value of 40 dyn/cm |
| | Stripping time assumed to be 240 minutes |
| | Assumed a set up time of 0 minutes |
| | Assumed a turnaround time of 0 minutes |
| | Water set to enter the stripper at a temperature of 150°C in gaseous form |

| **Equipment** | **Assumption/Decision** |
|---|---|
| **Liquid-Liquid Exchanger** | Temperature set to 90°C |
| | Heat transfer agent set as chilled water |
| | Specific mass transfer area set as default SuperPro Designer value of 200 m2/m3 |
| | Sucralose set as the product component |
| | Recovery yield assumed to be 100% |
| | Mass transfer coefficient set as 0.72 cm/h |
| | Extracted from heavy phase |
| | Operating pressure set as 1.013 bar |

| | |
|---|---|
| | Light phase set as ethyl acetate |
| | Solubility of ethyl acetate in heavy phase set as default SuperPro Designer value of 0.001 g/L |
| | Solubility of water in light phase set as default SuperPro Designer value of 0.001 g/L |
| | Partition coefficient of sucralose set as 0.8 |
| | Partition coefficients of all other components set as 0 |
| | Assumed set up time of 0 minutes |
| | Assumed turnaround time of 0 minutes |
| | Assumed process time of 360 minutes |
| | Assumed only ethyl acetate, sucralose and some water leaves to the crystallizer. Everything else assumed to leave for further processing downstream (not modelled) |

| **Equipment** | Assumption/Decision |
|---|---|
| **Crystallizer** | Assumed to only use standard power |
| | Specific power assumed to be default SuperPro Designer value of 0.1 KW/m3 |
| | Residency time assumed to be 2 hours |
| | Working to vessel volume ratio set as 90% |
| | Evaporation temperature set as 100°C |
| | Evaporation heat set as 539.5 kcal/kg |
| | Reference component set as water |

| | |
|---|---|
| | Heating agent set to be steam |
| | Sucralose set to be the only crystallizable component |
| | Crystallization yield set to be 90% |
| | Crystallization temperature set to be 25°C |
| | Cooling agent set to be chilled water |
| | Set up time of 5 minutes assumed |
| | Turnaround time assumed to be 0 minutes |

| **Equipment** | Assumption/Decision |
|---|---|
| **Hydro cyclone** | Pressure drop of 0.5 bar assumed |
| | Standard power consumption assumed |
| | 100% efficiency assumed |
| | Power dissipation to heat assumed to be 0% |
| | Only sucralose crystals assumed to be removed |
| | 100% removal of sucralose crystals assumed |
| | Particle mass % in underflow set to be 99% |
| | Process time assumed to be 2 hours |
| | Set up time assumed to be 0 minutes |
| | Turnaround time assumed to be 0 minutes |

| **Equipment** | Assumption/Decision |
|---|---|
| **Washing belt** | Sucralose crystals assumed to be the only component in wash out stream |
| | 100% recovery of sucralose crystals assumed |
| | Product steam temperature set to 25°C |
| | Set up time assumed to be 0 minutes |
| | Process time set to be 1 hour |

| **Equipment** | Assumption/Decision |
|---|---|
| **Splitter to freeze dryers** | Assumed to split washed crystal stream three ways |

| | |
|---|---|
| | Assumed to split incoming stream in a ratio of 33:33:34 |
| **Equipment** | Assumption/Decision |
| **Freeze dryers** | All three freeze dryers set to the same conditions |
| | Water set to be the only volatile component |
| | Drying time set to 900 minutes |
| | Set up time assumed to be 0 minutes |
| | Standard power consumption assumed |
| | Steam chosen as the heating agent |
| | Specific amount of 2 kg/kg evaporated assumed |
| | Turnaround time assumed to be 0 minutes |

# Appendix E: Summary of assumptions made during plant costing

| Section | Costing Decisions |
|---|---|
| Annual Product Requirement | Sucralose production calculated based on the sugar content in Coca Cola |
| | Assumed that the sugar in Coca Cola is purely sucrose |
| | Allocated sugar in Coca Cola a sweetness index of 1 |
| | Allocated sucralose a sweetness index of 600 (based on literature) |
| | Assumed that sucralose represents all sweeteners as a replacement to the sugar in Coca Cola |
| | Assumed that of the annual sweetener requirements, sucralose fulfils 33%. The remaining 66% is assumed to be fulfilled by other sweeteners. |
| | Assumed that sucralose will represent 33% of the sweetener requirements in 2030 |
| | Assumed the percentage of forecasted beverage sales in 2030 will comprise of 50% drinks using only artificial sweeteners in place of sugar |
| | Assumed 20% of total sucralose market capture in the first year of operation |
| | Assumed 5% inflation rate |
| **Section** | Costing Decisions |
| Feedstocks and Product Costs | Assumed that the price of sucrose feedstock is equivalent to the average retail price of sugar |
| | Assumed that the revenue streams which could be used in another batch would be purified downstream and re-used. This was not included as part of the current design |

| | |
|---|---|
| | Assumed that the catalyst is recovered completely after every batch |
| | Assumed that the catalyst lifetime is 4 months (i.e. replaced 3 times annually) |
| | Assumed that when used in all three reactors, the catalyst requirement triples |
| | Feedstocks of ACS reagent quality were chosen as appropriate for food production |
| | Assumed a DMF: Sucrose ratio between 8 and 9 on a mass ratio |
| **Section** | Costing Decisions |
| **Equipment Costing** | Used 79% yield and a residence time of 6 hours in transesterification reactor based on US 2008/0103295A1 |
| | Assumed 70% yield and a residence time of 6 hours in the chlorination reactor |
| | Assumed 70% yield and a residence time of 4.5 hours in the deacylation reactor |
| | Where the simulated equipment size was below the range allowed by the costing equation, the size was assumed to be the minimum size in the range for the costing equation |
| | Assumed a shaft power of 1 KW shaft power for the pumps. This was the lowest power range of the pump costing equation |
| | Selected a material conversion factor 1.8 where the costing equation referenced carbon steel and the required material was stainless steel |
| | Assumed the use of stainless for all equipment as a food product is involved |

| | | |
|---|---|---|
| | | Assumed a pump was present to transfer all liquid streams to the next vessel and between heat exchanges and the next vessel. Pumps were not allocated to streams containing solids |
| **Section** | Costing Decisions | |
| **Production Costing** | Production costing was done based on the heuristics described by Seider et al (2010) | |
| | 3 operators assigned to each process section | |
| | 5 process sections assumed (3 reactors, 1 stripping and LLE, 1 final purification stages) | |

| **Section** | **Costing Decisions** |
|---|---|
| **Profitability** | Cost of equipment including delivery set to be 1.05 x purchase cost of equipment |
| | Lang Factor of 5.03 chosen for a solids-fluids processing plant |
| | Total capital investment including working capital = (Lang Factor x Cost including delivery) |
| | ROI = (After tax earnings)/ (Total capital investment including working capital) |
| | Depreciation assumed to be 10% of cost of equipment including delivery |
| | Corporate income tax rate set as 28% (referenced from South African Revenue Services |
| | Only the material balances, cost of raw materials and products as well as the total construction cost calculated using Lang factors were used to calculate profitability. Energy was not considered. |

# Appendix F: Purchase and selling prices used in the costing

| Reference Prices | | | | |
|---|---|---|---|---|
| **Feedstocks** | **Unit** | **Unit purchase cost** | **Reference** | **Comments** |
| Sucrose | kg | USD 1.14 | USDA Agriculture 2019 Report | Average retail price of white sugar |
| DMF | L | USD 61.63 | Sigma-Aldrich | ACS Reagent 99% |
| Ethyl acetate | L | USD 59.56 | Sigma-Aldrich | ACS Reagent >99.5% |
| Phosgene (2007 price inflated to 2019) | kg | USD 2.07 | Independent Commodity Intelligence Services (ICIS) | ACS Reagents >98% pellets |
| Sodium Hydroxide | kg | USD 37.57 | Sigma-Aldrich | |
| Water | m3 | USD 0.20000 | Seider | High purity process water |
| Catalyst | kg | USD 36.18 | Sigma-Aldrich | 1:50 ratio of catalyst: sucrose. Price reference of TiO2 |
| **Utilities** | **Unit** | **Unit purchase cost** | | |
| Electricity | KW-hr | USD 0.06 | Seider | |
| Steam 50 psig/3.44 bar | kg | USD 0.01 | Seider | |
| Cooling water | m3 | USD 0.02 | Seider | |
| Chilled water 4°C | kg | USD 0.000084 | Seider | 5.02 kcal/kg (SuperPro default setting). Based on Seider's $4/GJ |
| **Products** | **Unit** | **Unit selling price** | | |
| Sucralose | kg | USD 481.95 | Sigma-Aldrich | Sucralose powder |
| Ethanol | L | USD 175.62 | Sigma-Aldrich | Ethanol absolute, >99.8% liquid |
| Ethyl acetate | L | USD 63.62 | Sigma-Aldrich | Ethyl acetate anhydrous, 99.8% |
| DMF | m3 | USD 61.63 | Sigma-Aldrich | ACS Reagent 99% |

# Appendix G: Bases for evaluating profitability

Below is a summary of the assumptions and bases used to evaluate plant profitability.

| Reference | Assumption |
|---|---|
| Land purchase value | USD 5 million. Land assumed to be purchased at time 0 |
| Construction period | 2 years |
| Fixed Capital | Taken to be the cost of equipment plus delivery. Distributed as 60% in first year of construction and 40% in the second |
| Project Lifetime | 10 years |
| Salvage | No salvage value |
| Working capital | Equal to the value of (Cost of equipment plus delivery x Lang Factor of 5.03 for solids/liquids) – (Cost of equipment plus delivery). Invested in second year of construction |
| Depreciation | MACRS 5-year basis used |
| Taxation Rate | 28% corporate tax as per South African regulations |
| Discount Rate | 10% |
| First year cost of production | 55% of total cost of production when plant at full capacity |
| Second year cost of production | 75% of total cost of production when plant at full capacity |
| Subsequent cost of production | 100% of total cost of production when plant at full capacity |
| Revenue in first year | 50% of total revenue of when plant at full capacity |
| Revenue in second year | 75% of total revenue of when plant at full capacity |
| Subsequent revenue | 100% of total revenue of when plant at full capacity |

Raw material costs and revenue streams for the base case

| **Base Case** | | | | | |
|---|---|---|---|---|---|
| **Feedstocks/Utilities** | **Unit** | **Requirement/batch** | **Batches/year** | **Requirement/year** | **Cost/year** |
| Sucrose | kg | 1 129.02 | 533 | 601 767.66 | USD 683 006.29 |
| DMF | L | 9 533.90 | 533 | 5 081 567.80 | USD 313 154 577.74 |
| Ethyl acetate | L | 111 973.39 | 533 | 59 681 818.18 | USD 3 554 666 585.91 |
| Phosgene | kg | 1 000.00 | 533 | 533 000.00 | USD 1 103 049.16 |
| Sodium Hydroxide | kg | 750.00 | 533 | 399 750.00 | USD 15 020 586.28 |
| Catalyst | kg | 22.58 | 3 | 67.74 | USD 2 450.60 |
| Water | kg | 34 379.00 | 533 | 18324007.00 | USD 3 664 801.40 |
| Electricity | KW-hr | 117.23 | 533 | 62483.59 | USD 3 749.02 |
| Steam 50 psig/3.44 bar | kg | 15 473.80 | 533 | 8 247 535.40 | USD 54 433.73 |
| Cooling water | m3 | - | 533 | - | USD 0.00 |
| Chilled water 4°C | kg | 530 544.91 | 533 | 282 780 437.03 | USD 23 783.56 |
| **TOTAL RAW MATERIALS & UTILITIES** | | | | | USD 3 888 377 023.69 |
| **Products** | **Unit** | **Production/batch** | **Batches/year** | **Production/year** | **Revenue/year** |
| Sucralose | kg | 456.93 | 533.00 | 243 543.69 | USD 117 374 753.73 |
| Ethanol | L | 120.04 | 533.00 | 63 981.32 | USD 11 236 159.86 |
| Ethyl acetate | L | 100 770.00 | 533.00 | 53 710 410.00 | USD 3 417 284 580.28 |
| Sucrose | kg | 237.09 | 533 | 126368.97 | USD 143 428.78 |
| DMF | kg | 9 533.90 | 533.00 | 5 081 567.80 | USD 313 154 577.74 |
| **TOTAL PRODUCTION STREAMS** | | | | | USD 3 859 193 500.39 |

Raw material costs and revenue streams for the case of a lower ethyl acetate/increased sucrose flowrate

| Optimization: Lower ethyl acetate flowrate, increased sucrose | | | | | |
|---|---|---|---|---|---|
| **Feedstocks/Utilities** | **Unit** | **Requirement/batch** | **Batches/year** | **Requirement/year** | **Cost/year** |
| Sucrose | kg | 1 151.88 | 533 | 613 952.04 | USD 696 835.57 |
| DMF | L | 9 533.90 | 533 | 5 081 567.80 | USD 313 154 577.74 |
| Ethyl acetate | L | 34 368.07 | 533 | 18 318 181.82 | USD 1 091 036 278.84 |
| Phosgene | kg | 1 000.00 | 533 | 533 000.00 | USD 1 103 049.16 |
| Sodium Hydroxide | kg | 750.00 | 533 | 399 750.00 | USD 15 020 586.28 |
| Catalyst in one reactor | kg | 23.04 | 3 | 69.11 | USD 2 500.22 |
| Water | kg | 34 401.88 | 533 | 18336202.04 | USD 3 667 240.41 |
| Electricity | KW-hr | 117.28 | 533 | 62510.24 | USD 3 750.61 |
| Steam 50 psig/3.44 bar | kg | 14 990.24 | 533 | 7 989 797.92 | USD 52 732.67 |
| Cooling water | m3 | - | 533 | - | USD 0.00 |
| Chilled water 4°C | kg | 373 280.87 | 533 | 198 958 703.71 | USD 16 733.64 |
| **TOTAL RAW MATERIALS & UTILITIES** | | | | | USD 1 424 754 285.14 |
| **Products** | **Unit** | **Production/batch** | **Batches/year** | **Production/year** | **Revenue/year** |
| Sucralose | kg | 456.93 | 533 | 243 543.69 | USD 117 374 753.73 |
| Ethanol | L | 122.47 | 533 | 65 276.51 | USD 11 463 616.28 |
| Ethyl acetate | L | 30 765.78 | 533 | 16 398 160.74 | USD 1 043 320 686.66 |
| Sucrose | kg | 241.89 | 533 | 128927.37 | USD 146 332.56 |
| DMF | kg | 9 533.90 | 533 | 5 081 567.80 | USD 313 154 577.74 |
| **TOTAL PRODUCTION STREAMS** | | | | | USD 1 485 459 966.97 |

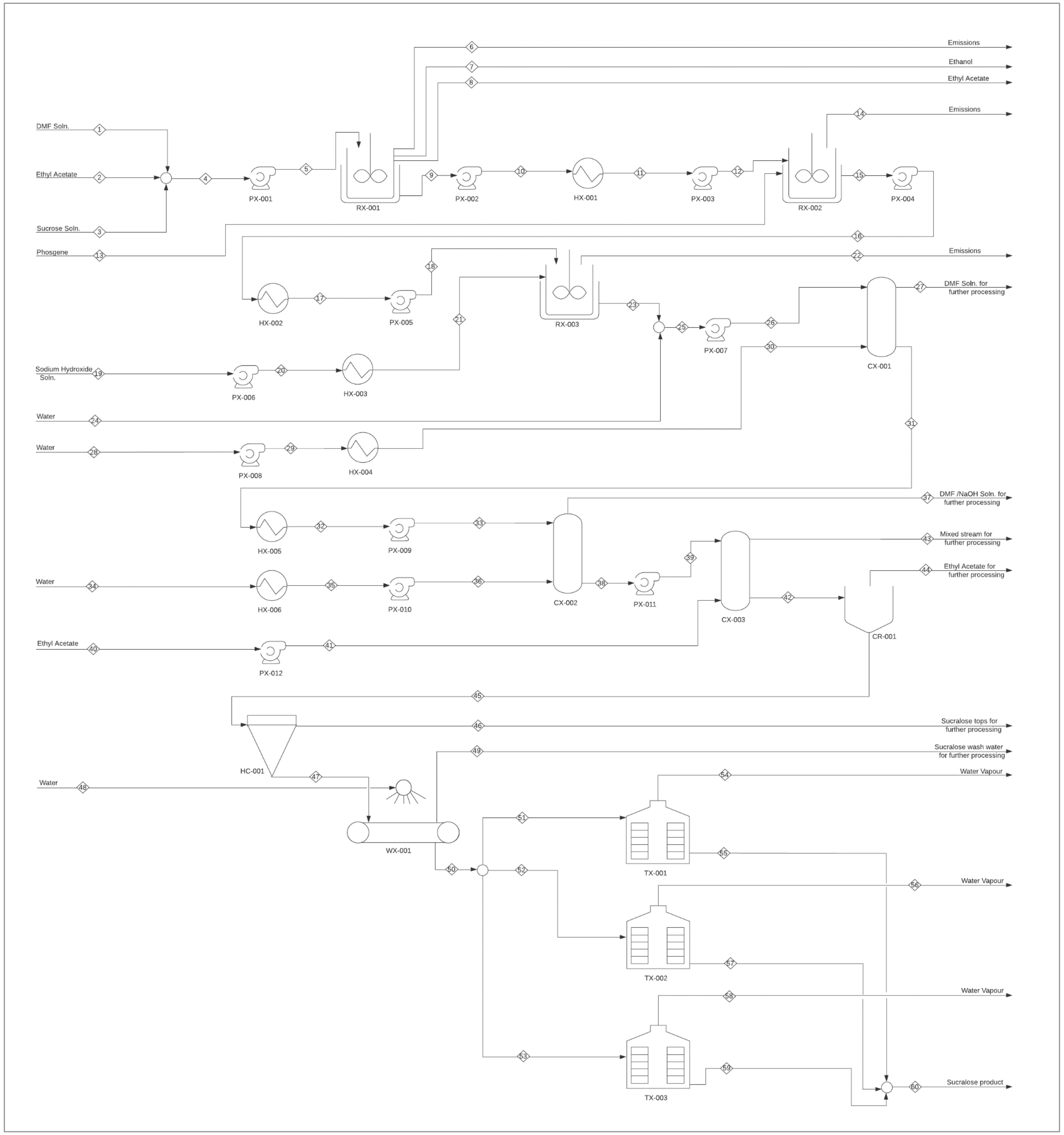


Figure 48: Process flow diagram

# Appendix H: Stream table and process flow diagram (Base case only)

| **Batch Process Stream Number** | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|---|
| **Description** | | DMF Soln. | Ethyl Acetate Soln. | Sucrose Soln. | Feed to PX -001 | Feed to RX-001 | RX-001 Emission | Ethanol Product | Ethyl Acetate Product |
| **Total Flow** | kg | 12 000.00 | 1 000.00 | 2 258.05 | 15 258.05 | 15 258.05 | 0.27 | 120.04 | 770.42 |
| **Temperature** | °C | 25.00 | 25.00 | 25.00 | 25.00 | 25.00 | 25.00 | 78.00 | 25.00 |
| **Pressure** | bar | 1.0 | 1.0 | 1.0 | 0.5 | 1.0 | 1.0 | 16.1 | 1.1 |
| **Vapour Fraction** | | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 1.0 | 0.0 | 0.0 |
| **Total Contents** | kg | 12 000.00 | 1 000.00 | 2 258.05 | 15 258.05 | 15 258.05 | 0.27 | 120.04 | 770.42 |
| Water | | 3 000.00 | - | 1 129.02 | 4 129.02 | 4 129.02 | - | - | - |
| Sucrose | | - | - | 1 129.02 | 1 129.02 | 1 129.02 | - | - | - |
| Sucrose-6-acetate | | - | - | - | - | - | - | - | - |
| Sucralose-6-acetate | | - | - | - | - | - | - | - | - |
| Sucralose (Crystallized) | | - | - | - | - | - | - | - | - |
| Sucralose | | - | - | - | - | - | - | - | - |
| Sodium Hydroxide | | - | - | - | - | - | - | - | - |
| Sodium Chloroformate | | - | - | - | - | - | - | - | - |
| Sodium Carbonate | | - | - | - | - | - | - | - | - |
| Sodium Acetate | | - | - | - | - | - | - | - | - |
| Phosgene | | - | - | - | - | - | - | - | - |
| Oxygen | | - | - | - | - | - | 0.06 | - | - |
| Nitrogen | | - | - | - | - | - | 0.20 | - | - |
| Ethyl Alcohol | | - | - | - | - | - | - | 120.04 | - |
| Ethyl Acetate | | - | 1 000.00 | - | 1 000.00 | 1 000.00 | - | - | 770.42 |
| DMF | | 9 000.00 | - | - | 9 000.00 | 9 000.00 | - | - | - |
| Chloroformic Acid | | - | - | - | - | - | - | - | - |
| Carbonic Acid | | - | - | - | - | - | - | - | - |

| Stream Number | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 |
|---|---|---|---|---|---|---|---|---|---|
| **Description** | Feed to PX -002 | Feed to HX-001 | Feed to PX-003 | Feed to RX-002 | Phosgene Feed | RX-200 Emission | Product to PX - 004 | Feed to HX-002 | Feed to PX-005 |
| **Total Flow** | 14 367.57 | 14 367.57 | 14 367.57 | 14 367.57 | 1 000.00 | 596.84 | 14 728.48 | 14 728.48 | 14 728.48 |
| **Temperature** | 80.00 | 80.00 | 85.00 | 85.00 | 25.00 | 49.26 | 50.00 | 50.00 | 15.00 |
| **Pressure** | 0.5 | 1.0 | 1.0 | 1.5 | 1.0 | 0.5 | 74.7 | 1.0 | 1.0 |
| **Vapour Fraction** | 0.0 | 0.0 | 0.0 | 0.0 | 1.0 | 1.0 | 0.0 | 0.0 | 0.0 |
| **Total Contents** | 14 367.57 | 14 367.57 | 14 367.57 | 14 367.57 | 1 000.00 | 596.84 | 14 728.48 | 14 728.48 | 14 728.48 |
| Water | 4 129.02 | 4 129.02 | 4 129.02 | 4 129.02 | - | - | 4 129.02 | 4 129.02 | 4 129.02 |
| Sucrose | 237.09 | 237.09 | 237.09 | 237.09 | - | - | 237.09 | 237.09 | 237.09 |
| Sucrose-6-acetate | 1 001.45 | 1 001.45 | 1 001.45 | 1 001.45 | - | - | 300.43 | 300.43 | 300.43 |
| Sucralose-6-acetate | - | - | - | - | - | - | 802.01 | 802.01 | 802.01 |
| Sucralose (Crystallized) | - | - | - | - | - | - | - | - | - |
| Sucralose | - | - | - | - | - | - | - | - | - |
| Sodium Hydroxide | - | - | - | - | - | - | - | - | - |
| Sodium Chloroformate | - | - | - | - | - | - | - | - | - |
| Sodium Carbonate | - | - | - | - | - | - | - | - | - |
| Sodium Acetate | - | - | - | - | - | - | - | - | - |
| Phosgene | - | - | - | - | 1 000.00 | 577.14 | - | - | - |
| Oxygen | - | - | - | - | - | 4.59 | - | - | - |
| Nitrogen | - | - | - | - | - | 15.11 | - | - | - |
| Ethyl Alcohol | - | - | - | - | - | - | - | - | - |
| Ethyl Acetate | - | - | - | - | - | - | - | - | - |
| DMF | 9 000.00 | 9 000.00 | 9 000.00 | 9 000.00 | - | - | 9 000.00 | 9 000.00 | 9 000.00 |
| Chloroformic Acid | - | - | - | - | - | - | 146.78 | 146.78 | 146.78 |
| Carbonic Acid | - | - | - | - | - | - | 113.14 | 113.14 | 113.14 |

| Stream Number | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 |
|---|---|---|---|---|---|---|---|---|---|
| **Description** | Feed to RX-003 | NaOH Solution | Feed to HX-003 | Feed to RX-003 | Emission from RX-003 | Product from RX-003 | Water | Mixed Feed to PX-007 | Feed to CX-001 |
| **Total Flow** | 14 728.48 | 1 500.00 | 1 500.00 | 1 500.00 | 10.50 | 16 228.44 | 20 000.00 | 36 228.44 | 36 228.44 |
| **Temperature** | 15.00 | 25.00 | 26.59 | 15.00 | 25.00 | 15.00 | 25.00 | 21.62 | 21.62 |
| **Pressure** | 1.0 | 1.0 | 2.0 | 2.0 | 0.5 | 4.6 | 1.0 | 1.0 | 1.5 |
| **Vapour Fraction** | 0.0 | 0.0 | 0.0 | 0.0 | 1.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| **Total Contents** | 14 728.48 | 1 500.00 | 1 500.00 | 1 500.00 | 10.50 | 16 228.44 | 20 000.00 | 36 228.44 | 36 228.44 |
| Water | 4 129.02 | 750.00 | 750.00 | 750.00 | - | 4 977.60 | 20 000.00 | 24 977.60 | 24 977.60 |
| Sucrose | 237.09 | - | - | - | - | 237.09 | - | 237.09 | 237.09 |
| Sucrose-6-acetate | 300.43 | - | - | - | - | 300.43 | - | 300.43 | 300.43 |
| Sucralose-6-acetate | 802.01 | - | - | - | - | 240.60 | - | 240.60 | 240.60 |
| Sucralose (Crystallized) | - | - | - | - | - | - | - | - | - |
| Sucralose | - | - | - | - | - | 507.70 | - | 507.70 | 507.70 |
| Sodium Hydroxide | - | 750.00 | 750.00 | 750.00 | - | 480.07 | - | 480.07 | 480.07 |
| Sodium Chloroformate | - | - | - | - | - | 186.87 | - | 186.87 | 186.87 |
| Sodium Carbonate | - | - | - | - | - | 193.32 | - | 193.32 | 193.32 |
| Sodium Acetate | - | - | - | - | - | 104.74 | - | 104.74 | 104.74 |
| Phosgene | - | - | - | - | - | - | - | - | - |
| Oxygen | - | - | - | - | 2.45 | - | - | - | - |
| Nitrogen | - | - | - | - | 8.06 | - | - | - | - |
| Ethyl Alcohol | - | - | - | - | - | - | | - | - |
| Ethyl Acetate | - | - | - | - | - | - | - | - | - |
| DMF | 9 000.00 | - | - | - | - | 9 000.00 | - | 9 000.00 | 9 000.00 |
| Chloroformic Acid | 146.78 | - | - | - | - | - | - | - | - |
| Carbonic Acid | 113.14 | - | - | - | - | - | - | - | - |

| Stream Number | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|---|---|---|---|
| **Description** | DMF Product | Water | Feed to HX-004 | Feed to CX-001 | Feed to HX-005 | Feed to PX-009 | Feed to CX-002 | Feed to HX-006 | Feed to PX-010 | Steam to CX-002 |
| **Total Flow** | 13 100.00 | 5 000.00 | 5 000.00 | 5 000.00 | 28 128.44 | 28 128.44 | 28 128.44 | 4 000.00 | 4 000.00 | 4 000.00 |
| **Temperature** | 100.00 | 25.00 | 26.86 | 150.00 | 100.00 | 100.00 | 100.00 | 25.00 | 150.00 | 150.00 |
| **Pressure** | 2.0 | 1.0 | 2.0 | 2.0 | 1.0 | 1.0 | 1.5 | 1.0 | 1.0 | 1.0 |
| **Vapour Fraction** | 0.0 | 0.0 | 0.0 | 1.0 | 0.0 | 0.0 | 0.0 | 0.0 | 1.0 | 1.0 |
| **Total Contents** | 13 100.00 | 5 000.00 | 5 000.00 | 5 000.00 | 28 128.44 | 28 128.44 | 28 128.44 | 4 000.00 | 4 000.00 | 4 000.00 |
| Water | 5 000.00 | 5 000.00 | 5 000.00 | 5 000.00 | 24 977.60 | 24 977.60 | 24 977.60 | 4 000.00 | 4 000.00 | 4 000.00 |
| Sucrose | - | - | - | - | 237.09 | 237.09 | 237.09 | - | - | - |
| Sucrose-6-acetate | - | - | - | - | 300.43 | 300.43 | 300.43 | - | - | - |
| Sucralose-6-acetate | - | - | - | - | 240.60 | 240.60 | 240.60 | - | - | - |
| Sucralose (Crystallized) | - | - | - | - | - | - | - | - | - | - |
| Sucralose | - | - | - | - | 507.70 | 507.70 | 507.70 | - | - | - |
| Sodium Hydroxide | - | - | - | - | 480.07 | 480.07 | 480.07 | - | - | - |
| Sodium Chloroformate | - | - | - | - | 186.87 | 186.87 | 186.87 | - | - | - |
| Sodium Carbonate | - | - | - | - | 193.32 | 193.32 | 193.32 | - | - | - |
| Sodium Acetate | - | - | - | - | 104.74 | 104.74 | 104.74 | - | - | - |
| Phosgene | - | - | - | - | - | - | - | - | - | - |
| Oxygen | - | - | - | - | - | - | - | - | - | - |
| Nitrogen | - | - | - | - | - | - | - | - | - | - |
| Ethyl Alcohol | - | - | - | - | - | - | - | - | - | - |
| Ethyl Acetate | - | - | - | - | - | - | - | - | - | - |
| DMF | 8 100.00 | - | - | - | 900.00 | 900.00 | 900.00 | - | - | - |
| Chloroformic Acid | - | - | - | - | - | - | - | - | - | - |
| Carbonic Acid | - | - | - | - | - | - | - | - | - | - |

| Stream Number | 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 |
|---|---|---|---|---|---|---|---|---|---|
| **Description** | Tops from CX-002 | Feed to PX-011 | Feed to CX-003 | Ethyl Acetate Feed | Ethyl Acetate to CX-003 | Feed to CR-001 | Mixed Product Stream | Ethyl Acetate | Feed to HC-001 |
| **Total Flow** | 5 285.27 | 26 843.17 | 26 843.17 | 100 000.00 | 100 000.00 | 100 507.79 | 26 335.38 | 99 999.97 | 507.81 |
| **Temperature** | 100.00 | 100.00 | 100.00 | 25.00 | 25.00 | 90.00 | 90.00 | -273.15 | 25.00 |
| **Pressure** | 1.0 | 1.0 | 1.5 | 1.0 | 1.5 | 1.0 | 1.0 | 1.0 | 1.0 |
| **Vapour Fraction** | 0.8 | 0.0 | 0.0 | 0.0 | 0.0 | 1.0 | 0.0 | 1.0 | 0.0 |
| **Total Contents** | 5 285.27 | 26 843.17 | 26 843.17 | 100 000.00 | 100 000.00 | 100 507.79 | 26 335.38 | 99 999.97 | 507.81 |
| Water | 4 000.00 | 24 977.60 | 24 977.60 | - | - | 0.11 | 24 977.49 | - | 0.11 |
| Sucrose | - | 237.09 | 237.09 | - | - | - | 237.09 | - | - |
| Sucrose-6-acetate | - | 300.43 | 300.43 | - | - | - | 300.43 | - | - |
| Sucralose-6-acetate | - | 240.60 | 240.60 | - | - | - | 240.60 | - | - |
| Sucralose (Crystallized) | - | - | - | - | - | - | - | - | 456.93 |
| Sucralose | - | 507.70 | 507.70 | - | - | 507.70 | - | - | 50.77 |
| Sodium Hydroxide | 475.27 | 4.80 | 4.80 | - | - | - | 4.80 | - | - |
| Sodium Chloroformate | - | 186.87 | 186.87 | - | - | - | 186.87 | - | - |
| Sodium Carbonate | - | 193.32 | 193.32 | - | - | - | 193.32 | - | - |
| Sodium Acetate | - | 104.74 | 104.74 | - | - | - | 104.74 | - | - |
| Phosgene | - | - | - | - | - | - | - | - | - |
| Oxygen | - | - | - | - | - | - | - | - | - |
| Nitrogen | - | - | - | - | - | - | - | - | - |
| Ethyl Alcohol | - | - | - | - | - | - | - | - | - |
| Ethyl Acetate | - | - | - | 100 000.00 | 100 000.00 | 99 999.97 | 0.03 | 99 999.97 | - |
| DMF | 810.00 | 90.00 | 90.00 | - | - | - | 90.00 | - | - |
| Chloroformic Acid | - | - | - | - | - | - | - | - | - |
| Carbonic Acid | - | - | - | - | - | - | - | - | - |

| Stream Number | 46 | 47 | 48 | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|---|---|---|
| **Description** | Mixed Sucralose Product | Feed to WSH-001 | Water | Sucralose Wash Water | Washed Sucralose Crystals | Feed to TX-001 | Feed to TX-002 | Feed to TX-003 | Water Vapour |
| **Total Flow** | 46.27 | 461.55 | 500.00 | 4.62 | 956.93 | 315.79 | 315.79 | 325.36 | 157.06 |
| **Temperature** | 25.00 | 25.00 | 5.00 | 25.00 | 8.79 | 8.79 | 8.79 | 8.79 | 25.01 |
| **Pressure** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| **Vapour Fraction** | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 1.0 |
| **Total Contents** | 46.27 | 461.55 | 500.00 | 4.62 | 956.93 | 315.79 | 315.79 | 325.36 | 157.06 |
| Water | 0.10 | 0.01 | 500.00 | 0.01 | 500.00 | 165.00 | 165.00 | 170.00 | 157.06 |
| Sucrose | - | - | - | - | - | - | - | - | - |
| Sucrose-6-acetate | - | - | - | - | - | - | - | - | - |
| Sucralose-6-acetate | - | - | - | - | - | - | - | - | - |
| Sucralose (Crystallized) | - | 456.93 | - | - | 456.93 | 150.79 | 150.79 | 155.36 | - |
| Sucralose | 46.16 | 4.61 | - | 4.61 | - | - | - | - | - |
| Sodium Hydroxide | - | - | - | - | - | - | - | - | - |
| Sodium Chloroformate | - | - | - | - | - | - | - | - | - |
| Sodium Carbonate | - | - | - | - | - | - | - | - | - |
| Sodium Acetate | - | - | - | - | - | - | - | - | - |
| Phosgene | - | - | - | - | - | - | - | - | - |
| Oxygen | - | - | - | - | - | - | - | - | - |
| Nitrogen | - | - | - | - | - | - | - | - | - |
| Ethyl Alcohol | - | - | - | - | - | - | - | - | - |
| Ethyl Acetate | - | - | - | - | - | - | - | - | - |
| DMF | - | - | - | - | - | - | - | - | - |
| Chloroformic Acid | - | - | - | - | - | - | - | - | - |
| Carbonic Acid | - | - | - | - | - | - | - | - | - |

| Stream Number | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| **Description** | TX-001 Crystals | Water Vapour | TX-002 Crystals | Water Vapour | TX-003 Crystals | Sucralose Crystal Product |
| **Total Flow** | 158.72 | 157.06 | 158.72 | 161.82 | 163.53 | 480.98 |
| **Temperature** | 25.00 | 25.01 | 25.00 | 25.01 | 25.00 | 25.00 |
| **Pressure** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| **Vapour Fraction** | 0.0 | 1.0 | 0.0 | 1.0 | 0.0 | 0.0 |
| **Total Contents** | 158.72 | 157.06 | 158.72 | 161.82 | 163.53 | 480.98 |
| Water | 7.94 | 157.06 | 7.94 | 161.82 | 8.18 | 24.05 |
| Sucrose | - | - | - | - | - | - |
| Sucrose-6-acetate | - | - | - | - | - | - |
| Sucralose-6-acetate | - | - | - | - | - | - |
| Sucralose (Crystallized) | 150.79 | - | 150.79 | - | 155.36 | 456.93 |
| Sucralose | - | - | - | - | - | - |
| Sodium Hydroxide | - | - | - | - | - | - |
| Sodium Chloroformate | - | - | - | - | - | - |
| Sodium Carbonate | - | - | - | - | - | - |
| Sodium Acetate | - | - | - | - | - | - |
| Phosgene | - | - | - | - | - | - |
| Oxygen | - | - | - | - | - | - |
| Nitrogen | - | - | - | - | - | - |
| Ethyl Alcohol | - | - | - | - | - | - |
| Ethyl Acetate | - | - | - | - | - | - |
| DMF | - | - | - | - | - | - |
| Chloroformic Acid | - | - | - | - | - | - |
| Carbonic Acid | - | - | - | - | - | - |

# Appendix I: Dataset Links

Raw data, training, test, model validation data
SuperPro simulation files
Model code
Profitability analysis