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Process design and economic analysis of a biorefinery co-producing itaconic acid and electricity from sugarcane bagasse and trash lignocelluloses

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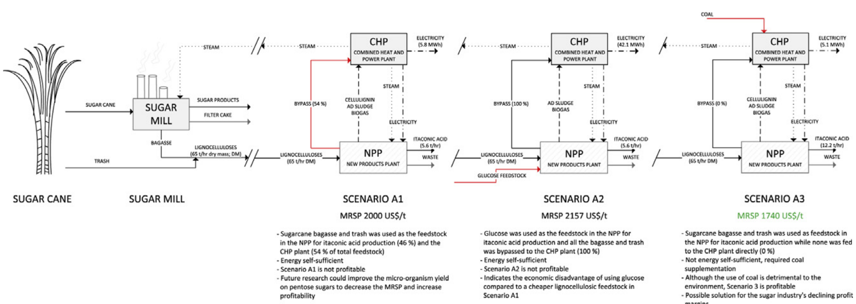
GRAPHICAL ABSTRACT



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ABSTRACT

Itaconic acid has economic potential as a commodity biochemical for the sugar industry, but its production is limited due to high production costs. Using cheaper and alternative lignocellulosic feedstocks together with achieving higher product titres have been identified as potential strategies for viable IA production. Consequently the use of sugarcane bagasse and trash for the production of itaconic acid (IA) and electricity have been investigated for an integrated biorefinery, where the production facility is annexed to an existing sugar mill and new combined heat and power (CHP) plant. Three IA biorefinery scenarios were designed and simulated in Aspen Plus®. Subsequent economic analyses indicated that cheaper feedstocks reduced the IA production cost from 1565.5 US$/t for glucose to 616.5 US$/t, but coal supplementation was required to sufficiently lower the production cost to 604.3 US$/t for a competitive IA selling price of 1740 US$/t, compared to the market price of 1800 US$/t.

1. Introduction

The drive towards sustainable manufacturing and decreasing our fossil fuel dependency has led to the investigation of green- or bio-chemicals (Koutinas et al., 2014). These biochemicals are produced from renewable biomass and can replace their fossil based equivalents. One such a biochemical is itaconic acid. Itaconic acid (IA) has potential as a commodity biochemical due to its wide range of applications in the agricultural, pharmaceutical and medical fields (Kuenz et al., 2012; Okabe et al., 2009). This organic acid is used as a co-monomer for the production of detergent builders, thermoplastics, surfactants, polymers and polyester resins (Okabe et al., 2009; Weastra, 2011). It was first discovered by Baup in 1836 as a product of citric acid distillation (Klement and Büchs, 2013; Okabe et al., 2009; Weastra, 2011), but is commercially produced through submerged fermentation with the fungi *Aspergillus terreus* (Klement and Büchs, 2013; Kuenz et al., 2012). However, it is currently seen as a niche chemical with low industrial relevance (Shekhawat et al., 2006) due to its high production cost and

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selling price (Okabe et al., 2009).

To promote IA from a niche chemical to a commercially produced biochemical, the price of IA should be competitive with end-use fossil based equivalent chemicals such as acrylic acid and maleic anhydride (Weastra, 2011). This could lead to an almost ten-fold expansion of the current IA market from 41 400 tonnes (2011) to 407 790 tonnes in 2020 (Weastra, 2011), ultimately building towards sustainable development and environmental conservation (Huang et al., 2014; Okabe et al., 2009; Werpy and Petersen, 2004). Factors contributing to the high cost of production are high feedstock costs of glucose and molasses, and the fermentation challenges of low titre and productivity seen for *A. terreus* (Klement and Büchs, 2013; Krull et al., 2017; Shekhawat et al., 2006).

Early fermentation improvements focused on achieving a higher IA yield from glucose (Yahiro et al., 1995), with recent studies focusing more on improving productivity and titre, aiming to achieve titres similar to that of citric acid production at 360 g/L (Hevekerl et al., 2014; Klement and Büchs, 2013; Krull et al., 2017; Kuenz et al., 2012). A reproducible and consistent titre of 86.2 g/L, though at a low productivity of 0.51 g/L/h, was obtained by Kuenz et al. (2012) using optimised nutrient media. The nutrient media conditions were further improved for the highest reported productivity to date of 1.15 g/L/h (Hevekerl et al., 2014). Furthermore, the IA titre was improved to 129 g/L (Hevekerl et al., 2014) and 160 g/L using a pH shift and control during fermentation (Krull et al., 2017). Although the IA titres obtained to date are not as high as that of citric acid, the improved IA titres together with a cheaper, alternative feedstock, could result in a viable commercial IA process. Alternative feedstocks such as hydrolysate (wheat bran, wood or corn syrup), corn starch (Okabe et al., 2009; Wu et al., 2017), and horticulture waste (Reddy and Singh, 2002) can replace glucose and molasses as feedstock (Mondala, 2015; Willke and Vorlop, 2001). Molasses is cheaper than glucose, at 100 US$/t compared to 580 US$/t (Humbird, 2011; Vieira et al., 2016), but no significant advances have been made for the fermentation parameters (Hashizume et al., 1966; Sumanjali et al., 2010). Sugarcane molasses contains 18.9% water, 31.8% sucrose, 17.11% invert sugars (i.e. glucose and fructose) with 32.3% constituents such as minerals and ash (Hashizume et al., 1966). The IA yield on sucrose is low, at 38.7% molar yield, compared to 80% molar yield for glucose (Sumanjali et al., 2010). Consequently, the titre achieved is also low at 27 g/L IA, compared to 160 g/L for glucose (Krull et al., 2017; Sumanjali et al., 2010). Glucose, together with other fermentable sugars can be obtained from cheaper lignocellulosic feedstocks (Benjamin, 2014).

Sugarcane bagasse is a cheap and abundant lignocellulosic feedstock. In 2013, 17.3 million tonnes of South African sugarcane were harvested, yielding 5.9 million tonnes of bagasse as by-product (Mbohwa, 2013). Sugarcane bagasse is the milled and crushed cane fibre residue after sugar juice extraction and contains 35–50% cellulose, 26.2–41% hemicellulose, 11.4–25.2% lignin and 2.9–1% other components, including 1.4% ash, which can be converted into simple sugars through pre-treatment and enzymatic hydrolysis (Benjamin, 2014; Borges and Pereira, 2011; Nanda et al., 2014; Xi et al., 2013). Currently the bagasse is burned in low efficiency boilers to produce steam and electricity for the sugar mill (Mbohwa, 2013). However, surplus bagasse and trash can be obtained by the introduction of green harvesting methods and high efficiency boilers (Ali Mandegari et al., 2017; Venkatesh and Roy, 2011). This excess bagasse and trash can be valorised as feedstock for biochemical production and co-generation of steam and electricity in a combined heat and power (CHP) plant.

To this end, an IA facility can be integrated with a CHP plant and annexed to an existing sugar mill to form a biorefinery complex (Ali Mandegari et al., 2017). The available lignocellulosic feedstock can therefore be split between the IA facility and CHP. If the IA facility is energy intensive, more of the available feedstock would have to be used in the CHP for energy generation. Alternatively the CHP can be supplemented with coal, allowing more of the biomass to be used as feedstock. However, this is not desirable due to the detrimental environmental impact of greenhouse gases and the contribution to human toxicity caused by burning coal (Ali Mandegari et al., 2017). Using an energy efficient CHP can also result in the production of excess electricity. By selling the excess electricity together with the IA biochemical, additional revenue can be generated from a viable biorefinery. This can assist in extending the sugar industry's sustainability, which is vital to its 430 000 employees and approximately 1 million dependants (Sugar Milling Research Institute NPC, 2016).

The aim of this study is to investigate whether the recent IA production improvements, namely higher titres and the use of a cheaper carbon feedstock (Okabe et al., 2009; Willke and Vorlop, 2001), such as sugarcane bagasse, will sufficiently decrease the cost of IA production in order to result in a commercially viable IA biorefinery. Alternative substrates to glucose, such as xylose, starch, molasses and lignocellulosic feedstocks have been used for IA production at laboratory scale (Klement and Büchs, 2013; Magalhães et al., 2017; Mondala, 2015; Willke and Vorlop, 2001). However, to the authors' knowledge, this study will be the first to design and simulate the process flow sheets for IA production from lignocellulosic biomass, followed by an economic analysis to determine and compare the viability of using an alternative substrate for IA production, to glucose. To this end, the first objective is to develop and describe the process for producing IA from sugarcane lignocellulose. The second objective is to determine if a lignocellulosic feed provides a better financial outcome than glucose, considering the capital and operational expenditures associated with pre-treating the lignocellulose to obtain fermentable sugars. The final objective is to determine if titre is the best process parameter to improve within the context of a biorefinery to further decrease the cost of IA production.

2. Process design and economic methods

2.1. Process design

2.1.1. Process simulation

Aspen Plus® version 8.8 was used to simulate the IA biorefinery. It was assumed that reported laboratory scale data will be applicable to an industrial process. Therefore the results are adequate for a conceptual level of study, and could be verified and optimised using a pilot plant prior to implementation. The waste water treatment (WWT) and combined heat and power (CHP) plant simulation and physical properties for the feedstock components are based on work developed previously (Ali Mandegari et al., 2017; Humbird, 2011; Leibbrandt, 2010; van der Merwe, 2010). The base property method is the electrolyte Non-Random Two Liquid (ELECNRTL) property method (Ali Mandegari et al., 2017; Gorgens et al., 2016). However, the equation of state (EOS) is adapted for single units, where required, such as the NRTL-HOC (Hayden-O'Connell) property method for IA recovery in the downstream process (DSP), or steam property IAPWS-95 for the boiler and condensing extraction turbine (CEST).

Stoichiometric reactor blocks are used for the pretreatment reactor, enzymatic hydrolysis reactor, and fermentation tanks. A separator block is used for the granular activated carbon (GAC) adsorption column, based on the furfural and hydroxymethylfurfural (HMF) removal rates reported (Hodge et al., 2009) and a water recovery yield of 90 wt% for the reverse osmosis (RO) membrane (McFall et al., 2008). The aerobic digestion, clarifier and dewatering steps are modelled as a single centrifuge block with a 10% solids loss to the liquid fraction (Gorgens et al., 2016) and all centrifuge blocks solid outlet streams are specified for a moisture content of 50%. Pumps are specified for an assumed discharge pressure of 2 atm with a pump efficiency of 75% and a mechanical efficiency of 95%. For cellulignin washing, a water to solid ratio of 2:1 is used.

2.1.2. Process scenarios

The IA production facility and CHP is annexed to an existing sugar