Multi-objective Optimization of Succinic Acid Production from Empty Fruit Bunch

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Empty Fruit Bunch (EFB) produced in plantation mill activities in Malaysia creates a major disposal problem. On the other hand, sustainability issues have driven industries to overcome the depletion of fossil fuels and reduction of greenhouse gases emissions. Therefore, as a renewable source, EFB can be an attractive option to address the above problems by converting it into fuels and chemicals. Succinic acid, one of 12 chemical building blocks identified by DOE to be used in synthesis of high-value materials, can be produced from biochemical conversion of the EFB. The present study evaluates succinic acid production process using EFB as the raw material from the perspective of three pillars of sustainability, namely economic, environment, and safety. Flowsheet modeling and techno-economic analysis methods are applied, followed by a multi-objective optimization using genetic algorithm method that simultaneously accounts for maximization of Net Present Value (NPV) and minimization of both Global Warming Potential (GWP) and Toxicity Damage Index (TDI). The pareto frontier reveals a trade-off among all objectives that the maximum NPV is 1,619 MMSD at the maximum EFB of 71,900 kg/hour. Meanwhile, the minimum GWP (12.4 kg CO_2-eq/kg succinic acid) and TDI (4.5) are acquired at the minimum EFB of 50,000 kg/hour.

Keywords: empty fruit bunch, multi-objective optimization, succinic acid, genetic algorithm

INTRODUCTION

The increasing of greenhouse gas (GHG) emissions and fossil fuel depletion have become major growing interests to be addressed. Substitution of fossil fuels with lignocellulosic biomass is hoped to resolve the problem of GHG emissions and energy scarcity because it is available abundantly and considered as a sustainable and renewable source (Özdenkçi et al. 2017). In Malaysia, the palm oil production facilities generate 45 million tonnes of biomass waste annually. The palm oil empty fruit bunch (EFB) waste accounts for around 43% of the total biomass waste or about 19.35 million tonnes (Chang 2014).

The US Department of Energy (DOE) has identified twelve chemicals as potential chemical building blocks that can be generated from biomass (Werpy 2004). Succinic acid is of a particular interest for its growing market and its potentials as one of the C4 building blocks in industrial organic chemistries.

Economically feasible, safer process, and environmentally-focus process are three main of sustainability aspects that should be considered during the design and operation of any chemical plants (Hurme and Rahman 2005). In previous studies of sustainability assessment for succinic acid, most of the works focused solely on economic performance or environmental impact. Pinazo et al. (2015) presented the sustainability assessment of succinic acid via fermentative synthesis and the petrochemical route with consideration of total production cost and energy efficiency. Liebal, Blank, and Ebert (2018) evaluated the economic performance of the microbial conversion of CO_2 to succinic acid. The economic assessment of integration of succinic acid process and a sugarcane-based biorefinery was conducted by Klein et al. (2017). In the context of multi-objective optimization problem, the combined economic and environmental criteria are mostly used for decision making in process design development of biorefinery (Tuazon and Gnansounou 2017). Furtado Júnior et al. (2019) developed a multi-type biomass-based biorefinery by using computerized-model experiment to identify the scenario with optimum economic and environmental performance. Akbari and Barton (2019)

proposed a computational framework of an algal biorefinery optimization by performing techno-economic analysis (TEA) and life cycle assessment (LCA). Sy et al. (2018) introduced a novel multi-objective target-oriented robust optimization (MOTORO) framework for the design of an integrated biorefinery with consideration of both economic and environmental performance. However, the challenges exist to hinder the sustainability of process such as the complexity of the process, severe operating conditions, toxic and flammable materials handling, and treatment hazardous materials (Ahmad, Hashim, and Hassim 2016). Meanwhile, many accidents within chemical processes occurred because of the overlooked hazards potentials at early stages in process design. Thus, the activity for understanding the hazard at initial design can be invaluable to eliminate and reduce the hazard in order to build an inherently safer chemical processes (Song, Yoon, and Jang 2018).

To be aligned with the above-mentioned sustainability aspects, this study aims to perform a sustainability assessment of succinic acid production from EFB by considering simultaneously economic, environment, and safety aspects at an early design stage. To quantify the economic feasibility, the net present value (NPV) will be calculated, the life cycle assessment (LCA) is performed to quantify the global warming potential (GWP) and hazard identification and ranking (HIRA) is determined to evaluate the safety level of the biorefinery. Moreover, the multi-objective

optimization is performed using the combination of Pareto optimal frontier and a well-known Genetic Algorithm (GA) method.

MATERIALS AND METHOD

In this regard, empty fruit bunch (EFB) is identified as the feedstock to produce succinic acids. The processing route of EFB utilization is divided into 4 stages of processing steps namely (1) pretreatment, (2) enzyme production, (3) saccharification, and (4) succinic acid production. The process overview of succinic acid production from EFB is depicted in Fig. 1. The process design and simulation are carried out using Aspen Plus V10 and the process design criteria associated to operation conditions, equipment consideration, conversion, pre-treatment method, and assumption are primarily based on Humbird (2011) and Lee, Song, and Lee (2006).

Pretreatment

The pre-treatment process is performed to remove lignin and to convert the cellulose into hexose. Lignin is removed and separated from the cellulose and hemicellulose through sulfuric acid pre-treatment process at elevated temperatures (158-200°C). An on-site enzyme production process is required to produce cellulase for conversion of cellulose in EFB into hexose sugars via the saccharification process at 90% conversion. Processes are then sent to conversion process to produce the succinic acid. The hexose sugars produced in these processes are then sent to conversion process to produce succinic acid.

Production of succinic acid

The hexose sugars are fermented to produce succinic acid. The fermentation of C6 sugars are performed at 39°C and 1 atm for approximately 29 hours with the presence of *Escherichia coli* as a microorganism.

Model Formulation

Objective function of the multi-objective optimization problem considers simultaneous maximization of economic performance and minimization of both environmental impact and inherent safety. Then, the simplification of succinic acid production is made through RSM to simplify the complex model. The multi-objective optimization problem is then performed using Genetic Algorithm (GA).

Techno-economic analysis

The economic objective function is formulated in terms of the net present value (NPV). The NPV is calculated as the summation of the discounted cash flows (DCF) generated in each of the time periods, as stated in Eq. 1.

$$NPV = -TCI + \sum_t \frac{CFt}{(1+i)^t} \qquad (1)$$

Where *TCI* is the total capital investment including the capital cost and annual production cost and i corresponds to interest rates. The *CFt* is obtained from after-tax-cash flow calculation.

The cash flow for the year t is calculated using Eq. 2.

$$CyFt = (R - COMd - d)(1 - \Theta) + d \quad (2)$$

Where R is revenue of product, COM_d is the annual manufacturing cost, Θ is the tax rate, and d is the depreciation.

Life cycle assessment

Life cycle assessment (LCA) method is described in the ISO 14000 series of standards (ISO 2006) and is the most used worldwide methodology for the environmental assessment of products and processes, including bioenergy production systems (Klein et al. 2018). The goal of this study is to evaluate environmental impact of the process of converting EFB to succinic acid and the system boundary is limited to the above-mentioned four processes.

The collection of inventory data quantifies the inputs and outputs of energy and materials associated to the above-mentioned four processes which are further translated into emissions released and waste generated. In this case, all the environmental emissions are expressed as function of process emission, heat, steam, and electricity consumed in the system. The direct emissions of process under study is available from simulation. While, the environmental data associated with grid electricity and heat generation can be acquired in commercial LCA databases such as Ecoinvent 3.4 and SimaPro 8.5.2. The total life cycle inventory (LCI) can be expressed as a function of the emission process, the electricity, heat, and steam consumption, as given in Eq. 3.

$$LCI_{tot} = LCI^{process} + LCI^{electricity}$$
$$+ LCI^{heat} + LCI^{steam} \qquad (3)$$
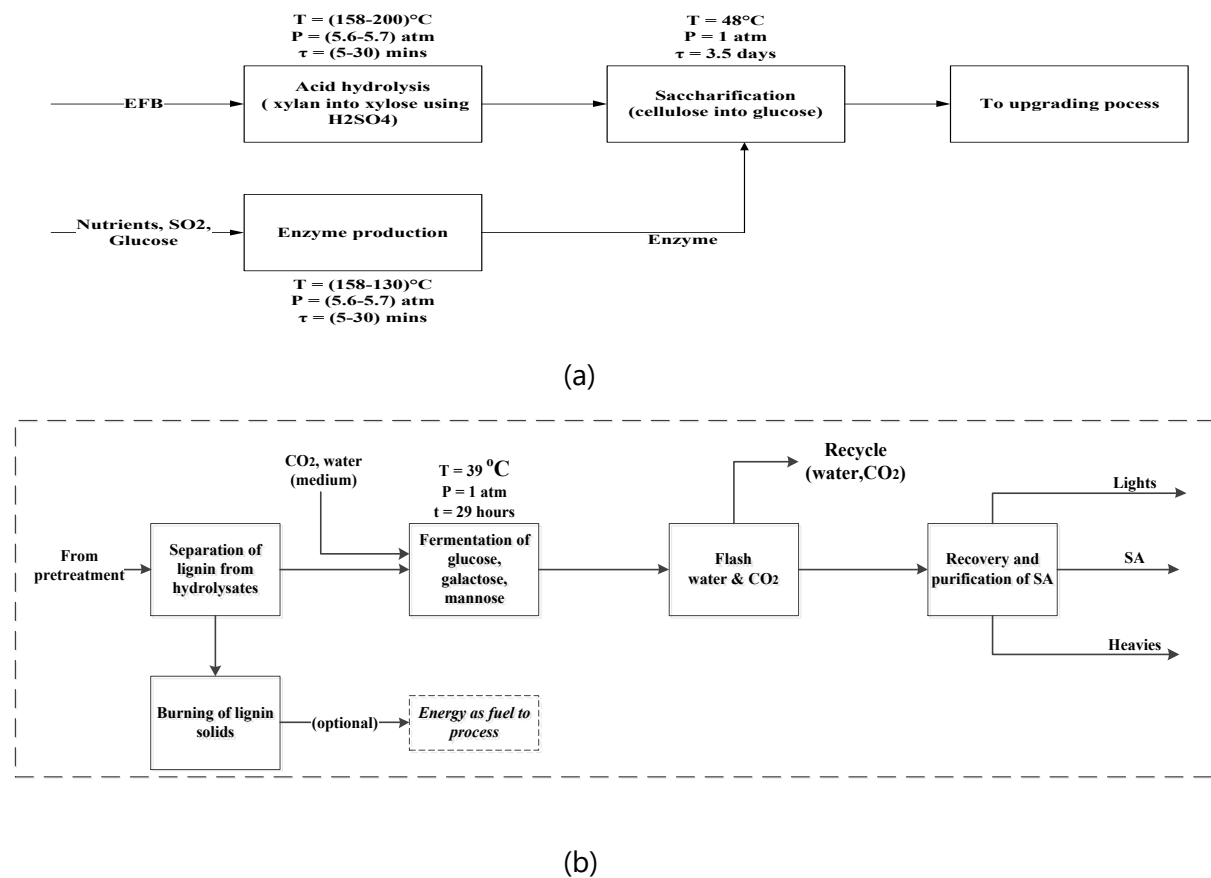

(a)

(b)

Fig. 1: The process flow diagram: (a) pretreatment process and (b) succinic acid production

The life cycle inventory is then converted into the corresponding environmental impacts. In this work, the climate change impact category is measured in kg CO_2-eq. The GWP is calculated as the total of the GWP from each emission as shown in Eq. (4).

$$GWP = \sum_i LCI_{tot} \; x \; m_i \qquad (4)$$

In this equation, *GWP* denotes the global warming potential caused in impact category while m_i is the damage factor that accounts for each greenhouse emissions are retrieved from (Guinée 2002).

Inherent safety

The inherently safer approach or index-based approach is a suitable approach for hazard identification as it does not consume time, simple approach, easy interpretation, it provides net scores that can be used for hazard comparison to help decision-making activities, and it does not require high level of expertise (Jafari et al. 2018; Khan and Abbasi 1998). One of the index-based approach is hazard identification and ranking (HIRA) from Khan and Abbasi (1998). HIRA is a systematic and comprehensive approach that is easy to implement, gives a reliable result sand provides the penalties which are quantified using empirical model and hazard ranking procedures (Zainal Abidin et al. 2016).

In this work, toxicity damage index (TDI) will be used for safety measurement. Penalties for locations of the nearest hazardous unit and space occupied by the unit is not accounted due to the data unavailability. The TDI formulation can be seen in Eqs. (5) and (6).

$$G = A \; x \; M \qquad (5)$$

$$TDI = a \; (G \; x \; Pn_1 x \; Pn_2 \; x \; Pn_3 \; x \; Pn_4)^b \qquad (6)$$

TDI involves a *G* factor and several penalties. *G* factor is obtained from *A* (the release condition) and *M* is the anticipated release rate in kg/s. The conditions of *A* and all penalties of each parameter can be found in (Khan and Abbasi 1998).

The availability of the empty fruit bunch

Even though the empty fruit bunch biomass waste is abundantly available, it is limited to the geographical location. Transporting all the EFB across the states of Malaysia to a centralized location is costly. Thus, a location for biorefinery is predetermined. The upper and lower bound of EFB availability is determined based on the EFB availability in that location. It is stated as follows:

$$EFB_{min} \; \leq EFB \; \leq EFB_{max}$$

Yield constraint

Another constraint of optimization problem considers yield of glucose to succinic acid.

$$\propto_{min} \leq \; \propto \; \leq \; \propto_{max}$$

Succinic acid demand constraint

The constraint of product demand helps to prevent an excessive production. Current global demand of succinic acid reaches up to 710,000 ton/year (Pateraki

et al. 2016). Due to the limitation of EFB availability, the process is designed to meet up 20% of the succinic acid global demand.

$Product \leq demand$

Model simplification of Succinic acid production

The developed succinic acid process in Aspen Plus is used to evaluate the three criteria of NPV, GWP, and TDI simultaneously. Then, the simplification model of succinic acid production is performed to shorten the consuming time for optimization. Therefore, it is modelled through the central composite design (CCD) of the response surface methodology (RSM) in JMP software, which used for developing, improving, and optimizing process (Khuri and Mukhopadhyay 2010). The values of (-1), (0), and (1) correspond to the minimum, base, and maximum values, respectively. Nine simulations run are simulated to see the correlation of two variables: the empty fruit bunch input rate (X_1) and the succinic acid yield (X_2), as shown in Table 1.

The empirical model was generated to see a correlation the response variable to the two process variables, which can be modelled using a second-degree polynomial shown in Eq. (7).

$$Y = \beta_0 + \sum_{i=1}^{n} \beta_i X_i + \sum_{i=1}^{n} \beta_{ii} X_{ii}$$
$$+ \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \beta_{ij} X_i X_j \tag{7}$$

Where Y is response variable, β_0 is a constant coefficient, β_i is a linear coefficient, β_{ii} is the quadratic coefficient, β_{ij} is an interaction coefficient, and X_i and X_j are the input variables.

ANOVA analysis with F-test is performed to examine the goodness of fit of the model, each term of model is tested statistically which confirmed the significance of F-values with $p \leq 0.05$. The values of R_2, adjusted R_2, and predicted R_2, predictive models are obtained to check the quality of the suggested polynomial, as shown in Table 2.

Table 1. Experimental design matrix of succinic acid

Coded Factor		Actual factor		NPV ($million)	GWP (kgCO$_2$-eq)	TDI
X1	X2	X1 (ton/hour)	X2 (%)	Observed response	Observed response	Observed response
-1	-1	50	76	984	141822	4.42
-1	1	50	82	1102	147691	4.57
0	0	75	81	1664	208790	5.41
0	1	75	82	1694	210881	5.43
1	1	100	82	2223	286382	6.14
0	-1	75	76	1530	196973	5.25
1	-1	100	76	1975	283636	5.94
-1	0	50	81	1076	146830	4.55
1	0	100	81	2187	286168	6.11

Table 2. Model summary statistics

Model		R square	adjusted R square	F-values	P-values
Succinic Acid (Y)	NPV	0.9998	0.9997	18655.14	<0.0001
	GWP	0.9985	0.9980	1998.45	<0.0001
	TDI	0.9999	0.9999	37007.46	<0.0001
	Product	0.9999	0.9999	681131	<0.0001

The quadratic models are shown in Eqs. (8)-(11).

Net Present Value
$$Y = -344.70 + 0.391X_1X_2 - 0.0065X_1^2 \quad (8)$$

Global Warming Potential
$$Y = -1338.89 + 18.633X_1^2 + 1263.92X_2 \quad (9)$$

Toxicity Damage Index
$$Y = 0.9692 + 0.036X_1 + 0.0175X_2 + 0.00016X_1X_2 - 0.00012X_2^2 \quad (10)$$

Succinic Acid Production Rate
$$Z = -40.5203 - 0.0221X_1 + 1.0399X_2 + 0.0033X_1X_2 - 0.0067X_2^2 \quad (11)$$

These simplified models of the developed process become the multi-objective functions for the following optimization.

Multi-objective optimization formulation

The model formulation of multi-objective optimization can be illustrated in Fig. 2.

Objective function
$$Max\ NPV = F(X_1, X_2)$$
$$Min\ GWP\ \&\ TDI = F(X_1, X_2)$$

Subject to
$$h(x) = 0\ (mass\ and\ energy\ balance,$$
$$techno - economic\ analysis,$$
$$life\ cycle\ assessment, and\ inherent\ safety\ )$$

$$g(x) \leq 0\ (\ demand\ of\ succinc\ acid)$$
$$x^l \leq x_1 \leq x^u\ (EFB\ supply)$$
$$x^l \leq x_2 \leq x^u\ (succinic\ acid\ yield)$$
$$x_1, x_2\ > 0$$

The equality constraints are mass and energy balance, economic performance calculation that includes Eqs. (1) and (2), life cycle assessment that includes Eqs. (3)- and (4) and hazard potential measurement that includes Eqs. (5)-(6). The inequality constraint for global demand is Eq. (11). The objective function that includes Eqs. (8)-(10). The upper and lower bounds of EFB are based on the availability of EFB in Malaysia, which are 50 and 100 ton/hr.

RESULTS AND DISCUSSION

The Pareto frontier best solution was generated through genetic algorithm in Matlab, as shown in Fig. 3. The Pareto resulted in 28 solutions, which are represented as the dotted point, it corresponded to specific EFB and succinic acid yield. As shown in Fig. 3, it revealed an obvious a trade-off among all objectives. While all solutions on the Pareto frontier were optimal, solutions on the left emphasized more on higher NPV scenarios and solutions on the right tend to achieve more GWP and TDI. As an example, point S1 in Fig. 3 corresponded to the best economic solution with
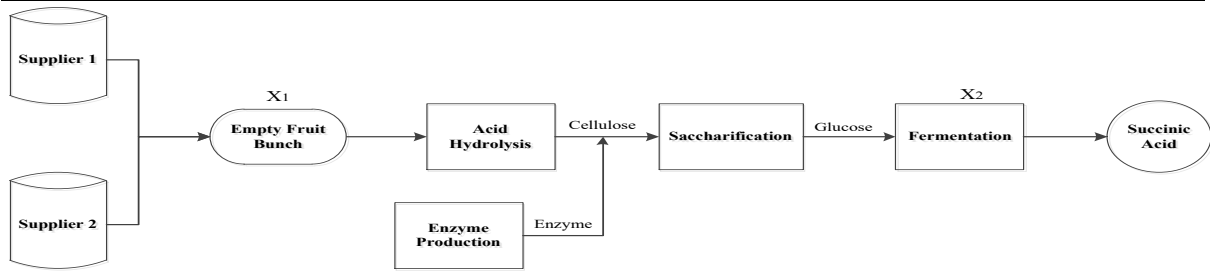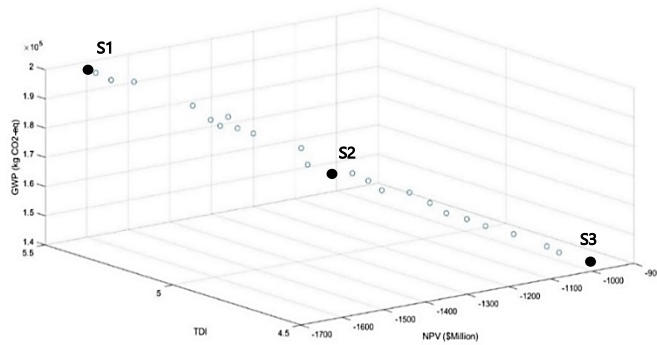
Fig. 2: Scheme of succinic acid production

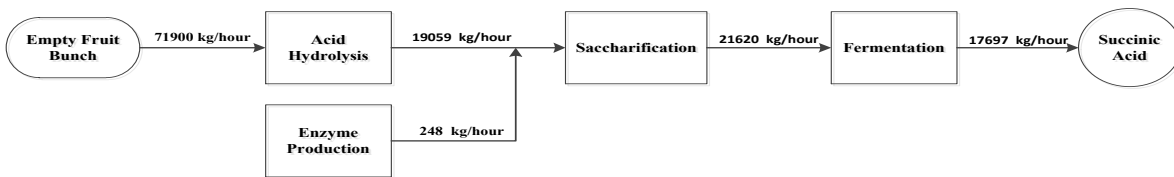

Fig. 3: Pareto frontier best solution

Fig. 4: The configuration of succinic acid production for maximum NPV
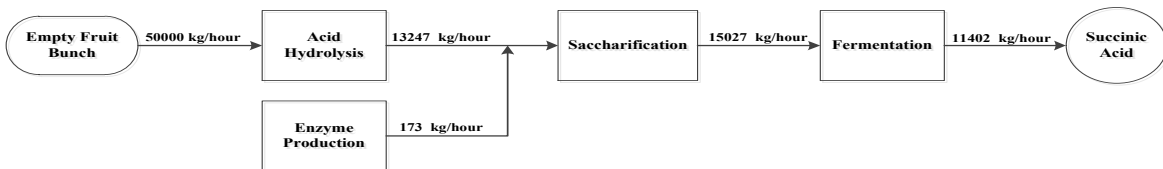

Fig. 5: The configuration of succinic acid production for minimum GWP and TDI

maximum NPV but it had worse performance for both GWP and TDI. The optimal solution had NPV of 1619 MMSD, whereas the GWP and TDI were 198.6-ton CO_2-eq/hour and 5.46. The maximum EFB which required on succinic acid production was 71900 kg/hour where it could satisfy 20% of global demand.

The amount of succinic acid produced was found to be 17697 kg/hr with 83% of succinic acid yield from glucose, as can be seen in Fig. 4.

Point S3 was the scenario with the lowest values of both GWP and TDI, whereas it acquired the minimum NPV. This point had GWP and TDI scores of about 141-ton CO2-eq and 4.5. These numbers are lower by 15.41% and 8.62% from point S1 for the GWP and TDI. Its NPV was the smallest by 979 MMSD. For

the minimum GWP and TDI, it required 50 ton/hour of EFB to produce 11402 kg/hour of succinic acid where it fulfilled 13% of global demand, as can be illustrated in Fig. 5. Another point, S2, represented a trade-off between point S1 and S3 where it has neither the highest economic performance, nor the worst environmental and safety issues.

CONCLUSION

This paper performs multi-objective optimization of succinic acid production from empty fruit bunch covering net present value, global warming potential, and toxicity damage index. The simplification model of succinic acid is made using the central composite design through JMP software. The constraints are made up of the supply of empty fruit bunch, succinic acid yield, and global demand. The solution of the optimization determines the optimal EFB required and succinic acid yield is solved using a well-known genetic algorithm method. The generated pareto allows decision makers to select the most acceptable solution based on their preferences. The analysis of the pareto-optimal solutions revealed trade-off among all objectives.

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