Sustainability assessment of xylitol production from empty fruit bunch

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Abstract. Empty fruit bunch (EFB), one of the wastes from palm oil production, can be utilized into fuels and chemicals. The aim of this paper is to find the optimum capacity to produce xylitol from EFB. The optimum capacity was found by simultaneously considering its profitability, hazard potential and environmental performances. The process was developed and simulated using Aspen Plus to analyze its technical challenges and economic performances, covering net present values, internal rate of returns and payback period. On the other hand, hazard identification and ranking (HIRA) was used to evaluate its safety performances, while Simapro V.8.5.2 was used to assess the environmental impact via a life cycle assessment (LCA). The results show that the high consumption of steam in chemical hydrogenation causes the main contribution of Global Warming Potential (GWP) by 62%. This acid pre-treatment is also considered the most toxic part of the process while the hydrogenation of xylitol is the most hazardous part based on fire and explosion perspectives. Then, multi-objective optimization using Genetic Algorithm (GA) was performed in Matlab to find the optimum capacity. The methodology and result of this work lay the foundation of future works in utilizing.

1 Introduction

Nowadays, the intensity uses of fossil feedstock to produce fuels and chemicals has caused repercussion to the level of CO\(_2\) in the atmosphere as well as the depletion of fossil fuel. For that reason, the utilization of agricultural residues as raw materials in a biorefinery is a promising alternative to fossil resources to produce fuels and chemicals, mitigating climate change and enhancing energy security [1].

The palm oil industry accounts for the largest biomass production in Malaysia, at a conservative estimate, for every ton of palm oil produced from a fresh fruit bunch, it was estimated that 22% of EFBs would be generated [2]. Xylose can be obtained by selective acid hydrolysis of the hemicellulosic fraction of EFB. This process also indirectly produces cellulose and lignin which in turn can be utilized as a source of glucose by enzymatic hydrolysis [3]. Xylitol can be obtained by the hydrogenation of xylose.

Currently, there is numerous pretreatment process of lignocellulosic biomass decomposition which had been developed by many researchers, to gain an efficient pretreatment of biomass [4]. In this paper, acid pretreatment is chosen because the advantages of dilute acid hydrolysis are the relatively low acid consumptions, limited problems associated with equipment corrosion and less energy demanding for acid recovery. Mostly xylitol production is conducted through chemical hydrogenation over a Raney-nickel catalyst under severe operating condition, but it offers high yield and conversion efficiency [5].

The sustainability assessment tool is the part of strategies to develop the most promising biorefinery processing paths with respect to specific design criteria, economic performance and environmental impact [6] presented techno-economic and life-cycle assessments of biorefineries based on palm empty fruit bunches in Brazil. Study of [7] reported the analysis of process design and techno-economic of an integrated mango processing waste biorefinery. The previous works of sustainability assessment are limited to process design, economic performance and an environmental problem only in determining the optimal route for a biorefinery. Whereas, hazards of chemical process are inherent in nature, caused primarily due to operating conditions, quantities of chemicals, characteristics of chemicals and design.

The aim of this study is to find an optimal capacity of xylitol production from EFB in terms of techno-economic, hazard potential and environmental performance. Since conflicting occurred in nature among them the genetic algorithm of multiobjective optimization is adapted in this work by maximizing NPV and minimum either environmental impact and hazard potential. The genetic algorithm is a powerful optimization techniques and is able to gain a global optimal solution in a complex multidimensional search space. The Pareto frontier of the best solution will be used to determine the optimum capacity of the process.

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2 Materials and methods

2.1 Process design description

Process routes for pretreating biomass and conversion of xylose into a xylitol were identified. The process flow and process conditions for these processes were based on [8] and [9] respectively. The simulation was conducted using Aspen plus (V9.0).

In the diluted acid pretreatment method, the EFB was diluted by water then the stream was heated in a preheater to a temperature of 100 °C. Sulfuric acid (5wt%) was then blended with EFB in pretreatment reactor operating at 158°C and 5.6 atm at 5 minutes of residence time. The pretreated EFB was then flashed to remove water, acetic acid and furfural. Then the bottom stream of flash was sent to the oligomer conversion reactor where the xylose oligomers were converted into monomers. The oligomer conversion reactor operates at 130°C and 5.7 atm and has a residence time of 20 to 30 minutes. The effluent of the reactor was sent to a second flash tank to remove water and some inhibitors. Then, the bottom of the flash column was diluted ammonia then pumped into the reactor operated at atm and 53°C. Ammonia was used for increasing the pH to 5. The pure xylose from the chromatography separator was then diluted with water. A diluted xylose was then fed along with hydrogen gas and raney-nickel catalyst into a bed reactor operates at 120°C and 5500 kPa for 120 minutes. The reactor temperature was maintained with the installed heating and cooling system. The reaction yields about 95% of xylitol. All products left the reactor and enter a pressure filter. Raney-nickel catalyst was assumed to recover from and recycled back into the reactor. The aqueous mixture was then sent into an evaporation tower to recover the xylitol at high purity. The main aim is to separate impurities from the xylitol. Then, purification is carried out by ion exchange and crystallization.

2.2 Techno-economic analysis

Techno-economic analysis (TEA) is used to calculate the feasibility of xylitol production from EFB. The key factors that affecting the economic feasibility of the biomass conversions were the plant capacity, feedstock cost, product yield, and process configuration [10]. Economic feasibility analysis starts from the estimation of the total capital investment (TCI) using the Peters and Timmerhaus factors seen in Table 1 [11].

Capital investment costs are estimated based on the purchased cost of each piece of operating equipment. The equipment pricing and sizing are performed in Aspen Process Economic Analyzer V.9.0 (APEA).

The financial scenario of xylitol production from EFB can be seen in Table 2. The operational expenditure (OPEX) comprises raw materials, utilities, and fixed costs (operating labor, maintenance, supervision, operating charges, plant overhead, and general and administrative costs). The profitability analysis is undertaken to estimate Net present value (NPV). Then, the NPV is selected as an economic objective.

| Parameter | Factor |
|-----------|--------|
| Total purchase equipment cost (TPEC) | 100% |
| Purchased equipment installation | 39% |
| Instrumentation and controls | 26% |
| Pipng | 10% |
| Electrical systems | 31% |
| Buildings (including services) | 29% |
| Yard improvements | 12% |
| Services facilities | 55% |
| Total direct cost (TDC) | 32% |
| Engineering | 32% |
| Construction | 34% |
| Total indirect cost (TIC) | |
| Total direct and indirect cost (TDIC) | TDC + TIC |
| Legal and contractors’ fees | 23% of TDIC |
| Contingency | 20% of TDIC |
| Fixed capital investment (FCI) | TDIC + contingency+ legal |
| Working capital (WC) | 30% of FCI |
| Land use | 6% of TPEC |
| Total capital investment (TCI) | FCI + WC + Land |

| Item | Assumption |
|------|------------|
| Plant life | 20 years |
| Equity | 100% |
| Construction period | 3 years |
| first year expenditure | 50% |
| second year expenditure | 30% |
| third year of expenditure | 20% |
| Income tax rate | 24% |
| Interest rate | 10% |
| Depreciation method | Straight-line depreciation |
| Depreciation time | 10 years |
| Operation time | 8000 hours |

2.3 Life cycle assessment

2.3.1 Goal and scope study

This goal of the study is to evaluate the environmental performance of xylitol production from EFB. The functional unit employed in this study is 1 kg xylitol.
produced. The system boundary includes two subsystems: acid hydrolysis and chemical hydrogenation. Then, gate to gate system boundary is applied to examine the potential environmental impacts. Mass and energy inventories are obtained from Aspen Plus results. The limitation and definition of the study as well as the components of the system boundaries which cover acid hydrolysis and chemical hydrogenation are illustrated in Fig. 1.

![Fig. 1. System boundary of xylitol production.](image)

### 2.3.2 Life cycle inventory (LCI)

In this work, the avoided products will be sent to waste treatment as waste. Although, it can be used for generating another valued product. The life cycle inventory data for xylitol process is presented in Table 3. This data based on mass and energy balance of process from Aspen plus.

### 2.3.3 Life cycle impact assessment (LCIA)

For life cycle impact assessment (LCIA) method CML-IA baseline method is used based on the emissions associated to either processing stage which specified in the system boundary and all inputs are entered the LCA software Simaprio V.8.5.2. The impact categories studied are abiotic depletion (AD), ozone layer depletion (ODP), global warming potential (GWP), acidification potential (AP), eutrophication potential (EP) and photochemical oxidation creation potential (POCP). Land use changes are not accounted for in the current study.

### 2.4 Inherent safety

Khan and Abbasi [12] introduced a systematic and comprehensive method of hazard identification what so-called the hazard identification and ranking system (HIRA). There are two essential indices of HIRA, the fire and explosion damage index (FEDI), and the toxicity damage index (TDI) [12].

The FEDI is estimated based on a thermodynamic model. In addition, the penalties can be chosen based on available information at preliminary design and FEDI already classified the various units of industry into five categories such as storage units, units involving physical operations, units involving chemical reactions, transportation units and other hazardous units. The energy factors are evaluated then given penalties is assigned based on operating range of process variables. The damage potential is obtained by multiplying energy factors and penalties. The scope of this work is restricted only the major reactor in acid hydrolysis and chemical hydrogenation process and the penalty for the location of the nearest hazardous unit and space occupied by the unit is neglected. FEDI will be used for objective in optimization represented as process safety objective.

The toxicity potential that contained in chemicals is considered to estimate by applying TDI. The lethal toxic load over an area is represented in TDI.

### Table 3. LCI of 1 kg xylitol production.

| Inputs                  | Outputs               |
|-------------------------|-----------------------|
| **Acid hydrolysis**     |                       |
| Delivered EFB           | 6.58 Kg/kg           |
| Steam                   | 3.85 Kg/kg           |
| H₂SO₄                   | 0.13 Kg/kg           |
| H₂O                     | 7.60 Kg/kg           |
| Electricity             | 0.033 kWh/kg         |
| NH₃                     | 0.067 Kg/kg          |
| H₂                      | 0.02 Kg/kg           |
| Raney-nickel            | 0.06 Kg/kg           |
| Heat                    | 18.75 MJ/kg          |
| **Chemical hydrogenation** |                      |
| Product                 |                       |
| Xylitol                 | 1 kg                 |

### Results and discussion

#### 3.1. Economic performance

The effect of plant capacity is investigated in this work. This is performed by varying the input mass flow rate of empty fruit bunch from 10 MT/hour to 100 MT/hour. The base case of the design is used 1 MT/hour of EFB. The capex of base case is $10 million and opex is $5 million/year. The total equipment cost of chemical hydrogenation is higher than acid hydroyysis process with $1 million and $0.3 million, respectively. Furthermore, the chemical hydrogenation is the most costly for raw material cost around $2 million/year. The raw material cost also contributes majorly approximately 43% to the total production cost.

The discounted cash flow rate of return (DFCROR) is used to determine NPV of xylitol production. For the base case capacity has NPV of $–13 million which means not financially attractive. As observed in Fig. 2, the NPV shows increase continually with regarding increased capacity.
3.2 Environmental impact

All the stages of the life cycle are covered in the results, from acid hydrolysis and chemical hydrogenation. Based on the result of simapro, it is estimated that for 1-kilogram xylitol produced, 3.83 kg of CO2 equivalent is emitted. The chemical hydrogenation is the major contribution of GWP by 95% due to heat consumption of purification process. The heat consumption is around 18 MJ/kg xylitol produced. Meanwhile, the acid hydrolysis only gives 38.4% contribution.

In order to identify the processes with the highest impact on the life-cycle performance of the system, the contributions to the individual impact categories can be seen in Fig. 5. Acid hydrolysis accounted for the highest contribution to abiotic depletion by 93% due to sulfuric acid consumption. Meanwhile, the heat consumption of xylitol production in chemical hydrogenation dominates majorly contribution for almost all impact categories. The natural gas which is used for generating heat makes up several emission that has certain impact such as POCP and acidification by 60% and 63%, respectively, due to sulfur dioxide. In addition, phosphate emission causes eutrophication with impact percentages 65% and methane, bromotrifluoro-, halon 1301 is responsible for ODP with impact percentages 64%.

The projection of plant capacity is conducted to examine the leverage of capacity over global warming potential. Reference flow is chosen based on the yield of xylitol in either capacity. Fig. 4 shows that the increased plant capacity will be aligned to increase of global warming potential.

3.3 Hazard potential

Table 4 shows that result of HIRA from the base case of xylitol production. It can conclude that acid hydrolysis which is represented by pretreatment reactor and ammonia reactor is relatively inherently safer than chemical hydrogenation as regard to fire & explosion damage index. The high FEDI is due to the severe operating condition of chemical hydrogenation. It is noted that a chemical property of hydrogen is categorized as highly flammable material.

Table 4. Fire, explosion and toxic damage index for different units.

| Units                  | Chemical      | Type of Hazard             | FEDI  | TDI  |
|-----------------------|---------------|----------------------------|-------|------|
| Pretreatment reactor  | Sulfuric acid | Fire & toxic release       | 34    | 12   |
| Ammonia reactor       | Ammonia       | Fire & toxic release       | 18    | 5    |
| Reactor hydrogenation | Hydrogen      | Fire & explosion           | 393   | 1    |

On the other hand, acid hydrolysis is more hazardous for toxicity damage index. It is caused by toxicity the chemical of sulfuric acid. The FEDI result of xylitol production is projected in various plant capacity. It can be seen in Fig. 5, the hazard potential of xylitol production increased continually with the elevated capacity. It evidences that the increased quantities of chemical will escalate the hazard potential of the chemical process.
3.4 Multiobjective optimization

Multi-objective optimization is implemented in this work over three objective functions, maximize NPV and minimize both GWP and FEDI. The genetic algorithm is used to find the optimum plant capacity that fulfill the objectives. Furthermore, pareto frontier of the best solution is generated. As all the algorithms in this work are designed for minimization problems. Thus, the maximization of NPV set to be minimizing (−NPV). The range capacity is set to be bound constraints where the lower and upper bound are \(10 \leq x \leq 100\).

As can be observed in Fig. 8, there is obvious trade-off among NPV, GWP and FEDI. Since, the increment of capacity resulted in high NPV as well as GWP and FEDI. The each point shown on the figure corresponds to feasible solutions. It can be seen that for solution S1, as 100 ton/hour of EFB capacity, has the highest NPV with $780 million and has either GWP of 7.5 x103 kg CO2 eq or FEDI of 920. Meanwhile, for the solution of S2 which has 50% of economy satisfaction, 55 ton/hour of EFB, has NPV $800 million with either GWP of 3.9x104 kg CO2 eq and FEDI of 1600. The optimum capacity along with maximum NPV and minimum both GWP and FEDI depends on the chosen perspective.

![Fig. 6. Pareto frontier of the best solution.](image)

4 Conclusion

A multiobjective optimization model is developed to find the optimum capacity in production process of xylitol. The model simultaneously takes maximizing NPV and minimizing both GWP and FEDI subject to capacity constraints. The multicriteria problem is solved with genetic algorithm method and resulting pareto-optimal reveals the tradeoff among the considered objectives. The proposed approach may a provide a very worthy and useful tool that helps decision maker to select optimum production capacity.

Future work, the model and result of sustainable assessment can be a foundation for utilizing wastes from palm oil production to valuable products.

The author gratefully acknowledges the financial support and facilities provided by Universiti Teknologi PETRONAS (UTP) upon completion of this project.

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