



## Software Integration of Life Cycle Assessment and Economic Analysis for Process Evaluation

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*Published in:*

Proceedings of the 6th International Conference on Process Systems Engineering (PSE ASIA)

*Publication date:*

2013

*Document Version*

Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

*Citation (APA):*

Kalakula, S., Malakula, P., Siemanonda, K., & Gani, R. (2013). Software Integration of Life Cycle Assessment and Economic Analysis for Process Evaluation. In Proceedings of the 6th International Conference on Process Systems Engineering (PSE ASIA) (pp. 917-922)

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## Sustainable Process Design of Biofuels : Bioethanol Production from Cassava rhizome

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### ABSTRACT

This study is focused on the sustainable process design of bioethanol production from cassava rhizome. The study includes: process simulation, sustainability analysis, economic evaluation and life cycle assessment (LCA). A steady state process simulation is performed to generate a base case design of the bioethanol conversion process using cassava rhizome as a feedstock. The sustainability analysis is performed to analyze the relevant indicators in sustainability metrics, to define design/retrofit targets for process improvements. Economic analysis is performed to evaluate the profitability of the process. Also, simultaneously with sustainability analysis, the life cycle impact on environment associated with bioethanol production is performed. Finally, candidate alternative designs are generated and compared with the base case design in terms of LCA, economics, waste, energy usage and environmental impact in order to identify the most sustainable design for the production of ethanol. The capacity for ethanol production from cassava rhizome is set to 150,000 liters/day, which is about 1.3 % of the total demand of ethanol in Thailand. LCA on the base case design pointed to large amounts of CO<sub>2</sub> and CO emissions (related to combustion engine from transportation), biowaste and waste water that are released from the distillation columns, which affect the terrestrial ecotoxicity. Sustainability analysis on the base case pointed to a large waste of the water and lignin, which were then targeted for potential improvement.

**Keywords:** Sustainable; Process design; Bioethanol; Cassava rhizome.

### 1. Introduction

Energy is an important factor in our daily lives, helping to improve the quality of life and playing a significant role in the country's economic development. In particular, energy demand in Thailand, where this study is conducted, has been increasing continuously together with the energy prices. Furthermore, Thailand has to face the environmental impacts caused by energy usage, particularly the impact on climate change resulting from, for example, global warming. Relevant international agreements have strict policies to reduce greenhouse gas emissions. These are driving factors for Thailand to push towards a low-carbon energy system. Thus, alternative and renewable energy need to be considered.

Biofuel is a type of alternative energy that is obtained from living or biological materials. Cassava rhizome is an attractive lignocellulosic material for bioethanol production, which mostly comes from agricultural residuals. More importantly, cassava rhizome is non-edible material. Production of cassava in Thailand is about 29 million tons per year and Thailand is ranked 1 as cassava producer in South-East Asia and 3 in the world. Furthermore, as every kilogram of cassava is accompanied by production of 0.06-0.09 kilogram of cassava rhizome, around 1.5–2.6 million tons of cassava rhizome is estimated to be produced per year and most of it is used as firewood while the rest goes to waste. Cassava rhizome has several characteristics that make it a highly desirable feedstock for ethanol production. It has high cellulose and hemicellulose content that can be readily hydrolyzed into fermentable sugars. However, cassava rhizome has also a high lignin content [Pattiya *et al*, 2007], which is a drawback to its use for ethanol production.

This work presents results from a systematic model based analysis of bioethanol production from potential lignocellulosic materials in Thailand in general and cassava rhizome in particular. First a base case design of a bioethanol conversion process from cassava rhizome as the raw material is analyzed. Next, more sustainable alternatives are generated and evaluated through life cycle

assessment and sustainability analysis in terms of reduced cost of production, waste, energy usage and environment impact. Well-known CAPE/PSE methods and tools for process simulation, economic analysis, process synthesis and sustainability-LCA analysis are used.

## 2. Methodology

### 2.1 Methods and tools

Process Simulation: To perform the process analysis, it is necessary to have information about the mass and energy balance for the process converting the raw materials to the desired products. In this work, only simulation results corresponding to the steady state of the process operation are considered. To perform the simulation, a process simulator is necessary, which requires information about the process flowsheet together with the design specifications of the unit operations present in the flowsheet as well as process constraints and material input. In this work, although the PRO/II simulator [PRO/II manual, 2006] is used, the methodology is independent of which simulator is used. An important issue, with respect to bioethanol production, is that the database of chemicals within the simulator includes all the chemicals present in the process under investigation and the models library contains the unit operations found in the flowsheet.

Sustainability analysis: In order to obtain more sustainable design alternatives, it is necessary to generate and compare feasible design alternatives according to an established set of performance criteria, for example, the sustainability metrics as defined by the IChemE [Azapagic *et al.*]. More sustainable design alternatives can be generated by first identifying operations in the process flowsheet that indicate bottlenecks in terms of waste or inefficiency and then revising the design/operation to overcome the bottlenecks. The SustainPro software [Carvalho *et al.*, 2008], which uses the steady state process simulation data to identify process bottlenecks, is used in this work to define targets for improvement and to estimate the sustainability metrics.

LCA: In order to verify that the environmental impacts of the proposed design alternatives are lower, it is necessary to generate and compare the feasible design alternatives according to an established set of performance criteria. Design alternatives can be generated by identifying and quantifying energy and materials used and wastes released to the environment in terms of GHG emissions and fossil resource depletion to acidification and toxicity. The SimaPro software [Mark *et al.*, 2010], which uses the steady state process simulation data to compare the full range of environmental effects assignable to products and services is used in this work.

Economic analysis: Since the implementation of the final design will most likely be based on economic factors, assuming all other issues have been found acceptable, every feasible and sustainable design alternative also needs an economic analysis. The objective is to find, in case of design/retrofit, how much would be the additional costs and how long would it take to recover the investment? The ECON software [Saengwirun, 2012], which is ideally suited for this type of analysis, is used in this work. Like the other analysis tools, it also uses the steady state simulation results to generate the capital and operating costs and from it, the economic analysis. A feature of ECON that helps in identifying retrofit (sustainable) design targets is the break-down of the cost items in terms of operations and materials. In this way, if the expensive operation also happens to be the operation that is inefficient or produces wastes, then obtaining a more sustainable alternatives is easily achieved by targeting this operation.

### 2.2 Procedure employed

Literature survey: The objective here is to define the sustainable design problem, taking into account, the available knowledge of the process.

- a. Study and review the background of bioethanol production including their environmental impact through the LCA and sustainability techniques.

- b. Study the feasibility of the potential of raw materials (cellulosic materials) in Thailand and select the best material for the process.
- c. Focus on the selected raw material (in this work, it is cassava rhizome), getting all the necessary information.

Process Simulation: The objective here is to obtain steady state mass and energy balance information for the process so that analysis related to cost, sustainability, LCA, etc., can be performed.

- a. Simulate the process at the established base case design for the process flow- diagram and the selected materials, using the selected process simulator.
- b. Verify that the necessary assumptions for the steady state simulation models to be used in process simulation are compatible with the actual process-operation scenario.
- c. Verify if the available data satisfy the data needed by the simulator.
- d. Generate the missing data through suitable model-based tools, for example, ICAS-tools (for missing property data, operation design, solvents, etc.).

Sustainability analysis: The objective here is to perform the sustainability analysis in order to compare the process alternatives.

- a. Collect of mass and energy balance data from simulation results.
- b. Identify all the mass and energy flow-paths in the process by decomposing the flow-diagram into open- and close-paths for each compound in the process.
- c. Determine the parameters (indicators) for the sensitivity analysis.
- d. Calculate of Sustainability Metric.
- e. Generate alternative designs based on operability, energy consumption, waste reduction, environmental impact, safety and cost. Verify the new designs through process simulation.

Life cycle assessment (LCA): The objective here is to perform the LCA in order to compare the process alternative.

- a. Define the functional unit for bioethanol production.
- b. Perform inventory analysis and collect data related to environmental and essential quantities for all relevant data and within the defined system boundary.
- c. Generate the life cycle impact assessment (LCIA) data with the selected software.
- d. Analyze and compare the impacts on human health and the environment burdens associated with raw material and energy inputs and environmental releases quantified by the inventory.

Economic evaluation: The objective here is to perform economic analysis in order to compare the generated sustainable design alternatives

- a. Select location of the bioethanol production plant.
- b. Collect stream and operational data of materials, unit operations and utilities from process simulation.
- c. Determine the indicators for the economic analysis with the selected software.
- d. Analyze and compare the cost requirements of each part of the process based on materials, equipment and utilities.

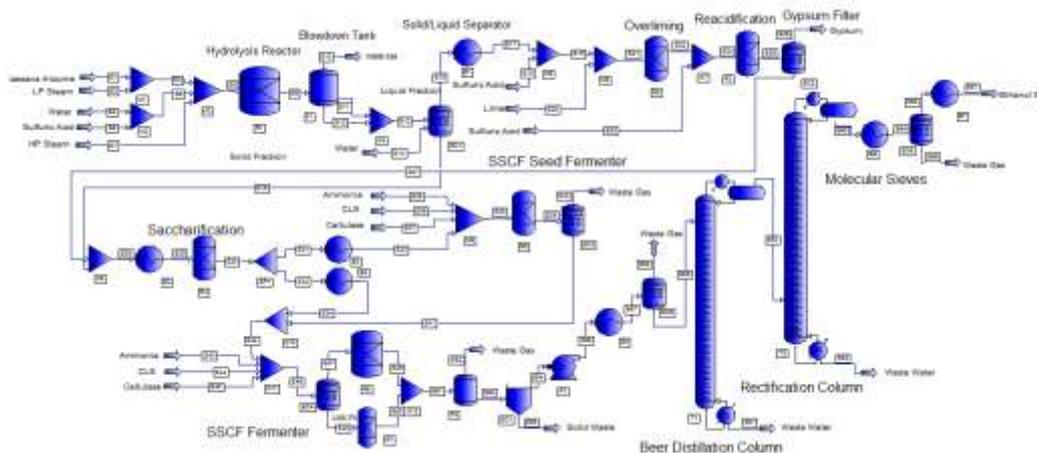
### 3. Results and Discussion

#### 3.1 Literature survey

Thailand has available, unused cassava rhizome of about 2.55 million tons/year. Theoretical ethanol production yield from cassava rhizome is about 0.16 L/kg dry (Chumnong *et al.*, 2011). According to the total demand of ethanol in Thailand (2011), which is about 11.50 million liters per day (DEDE, February 2012), Plant operate 330 days/year (Chumnong *et al.*, 2011), Price of cassava rhizome is about 500 Baht/ton (16.67 \$/ton), Price of ethanol is about 27 Baht/L (0.90\$/L). The capacity for ethanol production from cassava rhizome is selected to be 150,000 liters/day (average for operating plants in Thailand), which is about 1.30 % of the total demand of ethanol in Thailand. 940 tons/day or 310,000 tons/year of cassava rhizome is required for this production rate.

### 3.2 Process simulation – base case design

The process to convert cassava rhizome to ethanol is adopted from the process proposed by NREL [Morales-Alvarado et al. 2010]. Cassava rhizome is milled into small pieces and then sent to the pre-treatment area. After pre-treatment, concentrated sulfuric acid is added to the hydrolysis reactor to convert cellulose and Hemicellulose into C6 and C5 sugars. The hydrolyzate is sent for detoxification to remove contaminants such as furfural and HMF. Then, the detoxified hydrolyzate is split into two parts. 10% is used for yeast (seed) production and the rest is sent to the fermenter. The output of the fermenter is sent to the ethanol recovery section from which the dehydrated ethanol product is obtained. The final product is ethanol with 99.5 % purity. The complete process flowsheet is shown in Figure 1 and has been modeled and simulated through the selected process simulator. The process has 67 streams with 39 unit operations and the simulation reflects a rigorous steady state mass and energy balance.



**Figure 1.** Flowsheet of the bioethanol production process from cassava rhizome for base case design.

### 3.3 Sustainability analysis of base case design

SustainPro has been used to analyze the sustainability of the base case design as well as new design alternatives. The indicators in terms of open paths (OP), which are paths taken by the compounds present in the system as they enter and leave the process, are analyzed for a total of 333 OPs. The analysis shows that the OP 326 has the highest loss of material value (cellulase-enzyme). This is because the price of the enzyme is high and it is not recovered. Considering that the enzyme would rarely be recovered or recycled, the next most sensitive indicators are selected for improvement. Corn steep liquor (OP 322, 326) is the water with nutrients (a nutrient source in the seed train) and SSCF, so it is also not reasonable to separate and recycle. However, the indicators in OPs for water from several operations of the process also show loss of value because of their high flow-rates and levels of contaminations (sugars contained in some waste water can be recycled). Moreover, lignin (OP 15) is another target for potential improvement as there is a large amount (3653.45 kg/h) of it released after SSCF fermentation- it could be used as an energy source.

### 3.4 Life cycle assessment (LCA) of base case design

The results of sustainability analysis of base case. There were three main alternative process design ideas as follows:

- Rearrange the energy consumption in the process by using heat integration method.
- Install the membrane section into the process to treat water from S61 and S63, and recycle treated water into the process.
- Generate the energy by burn lignin and other solid wastes from SSCF fermenter (stream S55).

In addition, these alternatives could be mixed with another. For instance, after rearrange heat exchanger, the lignin combustion could be also installed in the process as well. Based on this approach, the total of seven alternative designs was generated from different combinations of these ideas as described in Table 1.

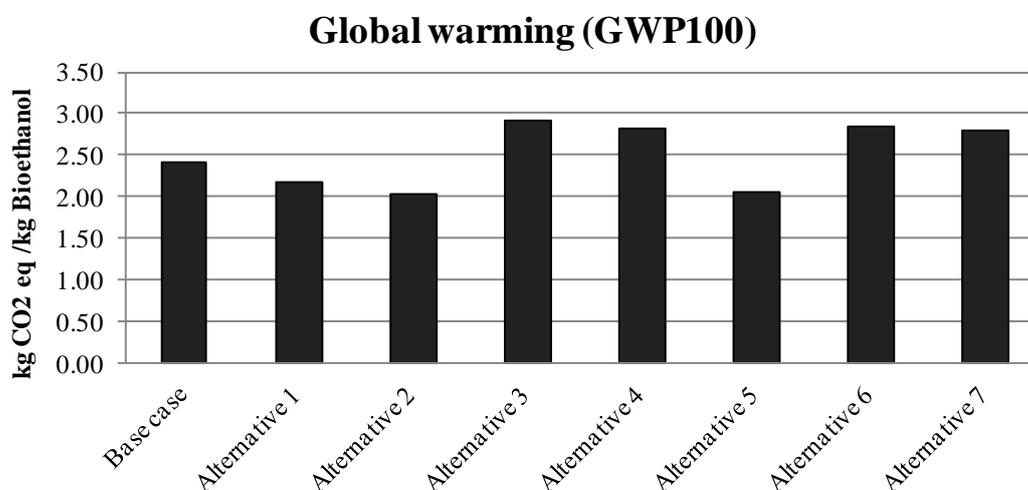
**Table 1** Overall alternative designs

Alternative	Description
1	Base Case with Heat Integration
2	Waste Water Recover by Membranes
3	Lignin Combustion
4	Waste Water Recover by Membranes + Lignin Combustion
5	Waste Water Recover by Membranes with Heat integrate
6	Lignin Combustion with Heat integrate
7	Waste Water Recover by Membranes + Lignin Combustion with Heat integrate

### 3.5 Life Cycle Assessment (LCA) Comparison

After performing the life cycle inventory analysis (bioethanol production process from cassava rhizome) by using SimaPro 7.1, the CML 2 baseline 2000 methods were then utilized to evaluate the environmental impacts in various categories. The impact assessment results comparison between new design alternatives and base case are shown in Figure 2.

Focusing on global warming potential (GWP as CO<sub>2</sub>-equivalent), alternatives 2 and 5 were shown to have lowest GWP impact. In particular, the wastewater recovery using membranes with heat integrate (alternative 5) was the best design in term of global warming point of view as it had lowest GHG emission. This is due to the facts that this design not only reduced GHG emissions, but also reduced energy usage in the process by rearrangement of heat exchanger.



**Figure 2.** Comparison of the greenhouse effect (kg CO<sub>2</sub>-equivalent) per kilogram of bioethanol for each design.

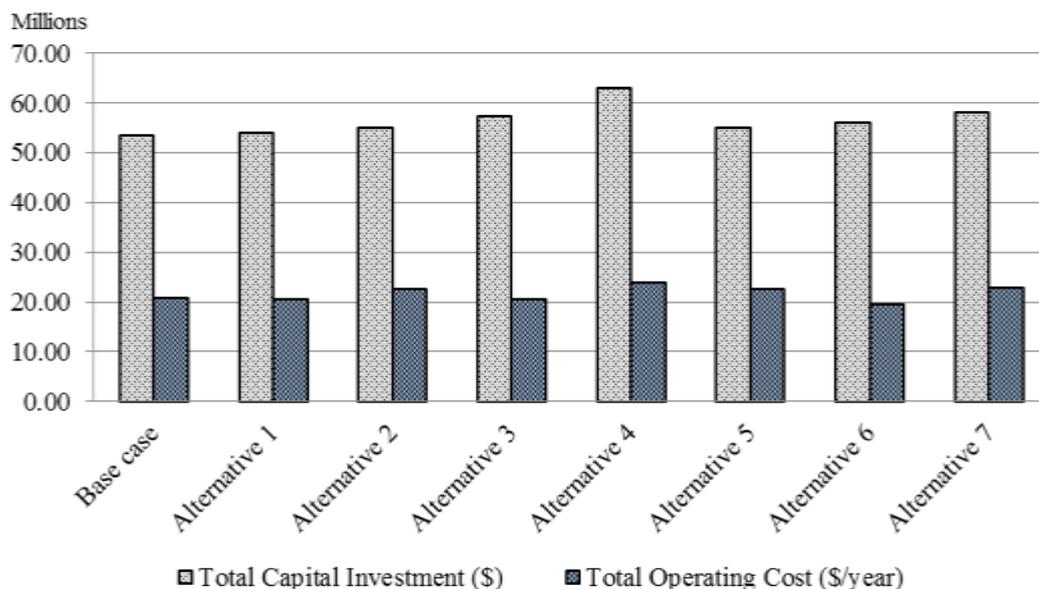
### 3.6 Economic Evaluation Comparison

The reasonable location for the plant should be placed close to the available raw material sources and also not too far from ethanol distributors or refineries. Based on the information available from the Office of Agricultural Economics (Ministry of Agriculture and Cooperatives, 2010), the most appropriate location for places bioethanol production from cassava rhizome plant for this work is Nakhonratchasima province.

As can be seen from Figure 3, heat integration designs (alternatives 1, 5, 6 and 7) required higher investment than general designs due to the addition of heat exchangers, but the operating cost was lowered because the reduction of energy consumption. Similarly, alternatives with membrane (alternatives 2, 4, 5 and 7), the capital cost of these designs was increased because more unit operations were installed. This could be compensated by lower operating cost of these designs as a result of recycle of water and some raw materials. For lignin combustion processes (alternatives 3, 4, 6 and 7), these designs led to a significant increase of the investment cost because the combustor and generator units were very expensive. However, because of the electricity and steam generators, the

designs with lignin combustion process can reduce the some amount of energy consumption so the operating cost was reduced.

In terms of profitability, alternatives 6 was shown to have the highest NPV (98.44 MM\$) and IRR (50.4 %) for 20 years life time, followed by alternative 1 with NPV of 94.1 MM\$ and IRR 50.2%.



**Figure 3** Comparison of capital cost and operating cost of each design.

#### 4. Conclusions

The application of CAPE/PSE methods and tools through the systematic methodology has been highlighted for the case of bioethanol production from cassava rhizome. Based on SustainPro results, five ideas of new design alternatives were generated for possible improvement. These new alternative designs were then compared with the base case design in both energy and environmental aspects in terms of global warming potential (GWP as CO<sub>2</sub> equivalent) and profitability of the design. Based on this approach, the results indicated that alternative 1, wastewater recovery using membranes and lignin combustion with heat integration, was shown to be the best design for bioethanol production from cassava rhizome because this design had the most water and energy saving and highest profit while maintaining environmentally friendly.

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