CHAPTER III

EXPERIMENTAL

3.1 Materials and Equipment

3.1.1 Equipment:

- Desktop computer (Pentium IV, RAM 1 GB, Window XP and Microsoft Office 2003)

3.1.2 Software:

- PRO/II version 8.2
- SustainPro program
- SimaPro version 7.0
- ICAS version 12

3.2 Procedures

3.2.1 Literature Survey

- Study the background of bioethanol production from molasses including their environmental impact through the LCA technique and gathering the available data
- Study the composition of molasses that is the raw material for bioethanol production and must be known for process simulation
- Minimize the waste that is released from the bioethanol production process such as amounts of waste water and solid waste.

3.2.2 Process Simulation

- Simulate the base case process design for process flow diagrams shown in Figure 3.1 using molasses as the raw material and using the PRO/II 8.2 software as the process simulator.

- Identify the functional units of bioethanol production. In this work, the ethanol production rate was set to 100 kilograms per hour.
- Collect the necessary data that needs to be specified.

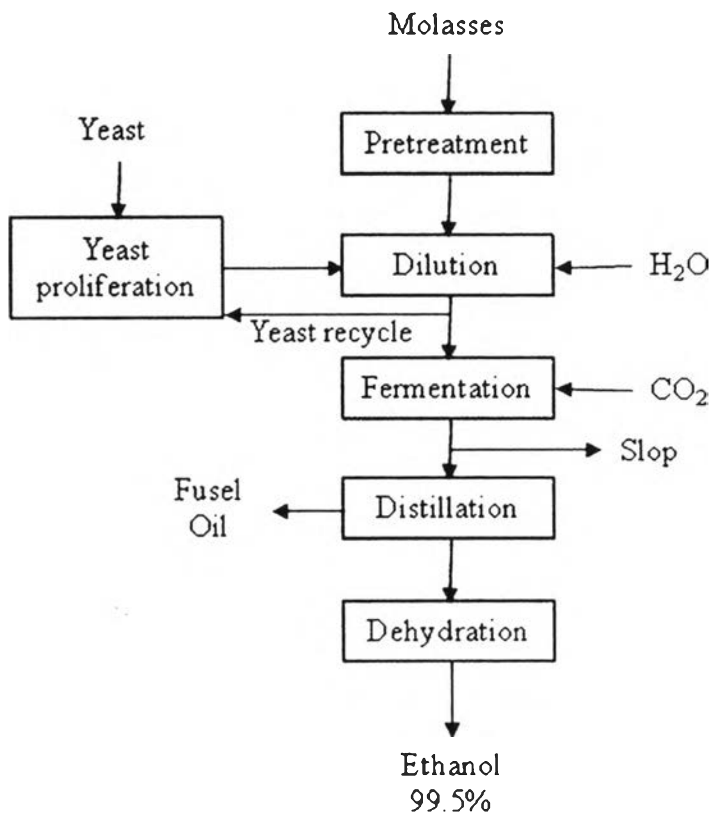

Figure 3.1 Bioethanol production process from molasses.

3.2.3 Sustainability Analysis

Perform sustainability analysis of base case design using SustainPro. This analysis is divided into five steps as follows:

3.2.3.1 Collection of Steady-state Data

This step involves the collection of mass and energy balance data from simulation results with PRO/II 8.2

3.2.3.2 Flowsheet Decomposition

The objective of this step is to identify all the mass and energy flow-paths in the process by decomposing into open-paths and close-paths for each compound in the process. An open-path consists of an entrance and an exit of a specific compound in the process. The closed-paths are the process recycles with respect to each compound in the process, in this report only illustrated in alternative 1.

3.2.3.3 Calculation of Indicator Sensitivity Analysis

The objective of this step is to determine the parameters (indicators) for the sensitivity analysis.

- Material-value Added (MVA) - This is calculated from the difference between the value of the component path flows outside the process boundaries and the costs in raw material consumption or feed cost. Negative values for MVA indicate value lost and show that there are potentials for improving the economic efficiency. MVA is calculated in cost units per year.

$$\mathbf{MVA = (mass)\ (sales\ price - raw\ material\ cost)}$$

For base case design, the solid waste and flue gas streams are released to the environment without treatment, the sales price is set to zero. For waste water streams that are used to generate electricity via biogas, the sales price is set to 0.00136 USD per kilogram of waste water (1 USD = 32 THAI BAHT) (http://www.thaibiogas.com)

- Energy and Waste Cost (EWC) - The EWC indicator consists of two parts: EC considers the energy costs and WC the process waste costs associated with a given path, by allocating the utility consumption and waste treatment costs. They indicate the maximum theoretical saving potential for a given path. High EWC values indicate high energy consumption and waste costs that could be reduced by decreasing the path flow or the duties. EWC is calculated in cost units per year.

$$\mathbf{EWC = EC + WC}$$

$$\mathbf{EC = (duty)\ (cost) \times \frac{Component\ mass \times characteristic\ physical\ property}{sum\ of\ all\ component\ (mass \times characteristic\ physical\ property)}}$$

WC = (mass) (waste treatment cost)

- Reaction Quality (RQ) - This indicator measures the effect a component path flow may have on the reactions that occur in its path. If the RQ value is positive, the path flow has a positive effect on the overall plant productivity. Negative values indicate an undesirably located component path flow in the process.

$$\mathbf{RQ} = \frac{\text{extent of reaction} \times \text{reaction parameter}}{\text{sum of desired products}}$$

- Accumulation Factor (AF) - AF provides a way of measuring the accumulative behavior of individual components in recycles. Note that the term ''accumulation'' is not used to mean inventory in this method. It indicates the amount of material being recycled relative to its input to the process and/or output from the process.

$$\mathbf{AF} = \frac{\text{mass of component in recycle}}{\text{sum of component mass leaving recycle}}$$

- Total Value Added (TVA) - This indicator describes the economic influence a component path flow may have on the variable process costs. Negative TVA values indicate improvement potentials in the process. Still, if a path flow has a high EWC value that was compensated by a high MVA value and gave a positive TVA value it could still be possible to reduce the energy cost. TVA is calculated in cost units per year.

TVA = MVA – EWC

- Energy Accumulation Factor (EAF) - The energy accumulation factor (EAF), calculates the accumulative behavior of energy in an energy cycle path flow. Since it is of interest to recycle or recover energy, these factors should be as large as possible in order to save energy. The energy accumulation factor could be calculated as:

$$\mathbf{EAF} = \frac{\text{energy recycled}}{\text{enery leaving the recycle}}$$

- Total Demand Cost (TDC) - This indicator is applied only to open-paths and traces the energy flows across the process. For each demand in the process the sum of all DC, which passes through it, are calculated. DC can be calculated using the following equation:

$$\mathbf{DC_{Su,d} = PE_{Su}\ EOP_{Su,d}}$$

Where, PE was the utility cost, in units of price/energy. The total cost for all the paths is expressed by:

$$\mathbf{TDC_d = \sum_{Su=1}^{SS} DC_{Su,d}}$$

Where, SS is the total number of supplies (Su) with significant energy contributions corresponding to their demands (d). High values of this indicator identify the demands that consume the largest values of energy, so these are the process parts, which are more adapted to heat integration.

3.2.3.4 Calculation of Sustainability Metric

The use of the sustainability metrics follow the simple rule that the lower the value of the metric the more effective (sustainable) the process. A lower value of the metric indicate that either the impact of the process is less or the output of the process is more. The metric calculated in this analysis are shown in Table 3.1, divided into different groups.

Table 3.1 The sustainability metrics considered in SustainPro

Group	Metrics
Energy	Total Net Primary Energy Usage rate (GJ/y)
	% Total Net Primary Energy sourced from renewable
	Total Net Primary Energy Usage per Kg product (kJ/kg)
	Total Net Primary Energy Usage per unit value added (kJ/$)
Material	Total raw materials used per kg product (kg/kg)
	Total raw materials used per unit value added
	Fraction of raw materials recycled within company
	Fraction of raw materials recycled from consumers
	Hazardous raw material per kg product
Water	Net water consumed per unit mass of product (kg/kg)
	Net water consumed per unit value added
Economic	Value added ($/yr)

The results report the energy used, raw material used, water consumption, and value added of this process. After new design alternative perform in SustainPro, this work would compare these new values with those of the base case design. Then, results are shown in terms of how much improvement is achieved by the new design.

3.2.3.5 New Alternative Design

Alternatives are created based on operability, energy consumption, waste reduction, environmental impact, safety and cost. The new design is simulated with Pro/II 8.2.

3.2.4 Life Cycle Assessment (LCA)

The assessment is carried out in four phases consisting of:

3.2.4.1 Goal and Scope Definition

- Identify functional unit of bioethanol production: In this work, two functional units are used: 1 kilogram of bioethanol of 99.5 wt% purity and 1 megajoule of bioethanol 99.5 wt% purity.
- Determine system boundaries of bioethanol production (what is and is not included in this research) based on the goal definition. In this

research, the selected system boundary of bioethanol production process is shown in Figure 3.2. For the life cycle assessment, the biogas and cogeneration stage was included in order to perform the whole life cycle of the bioethanol conversion stage.

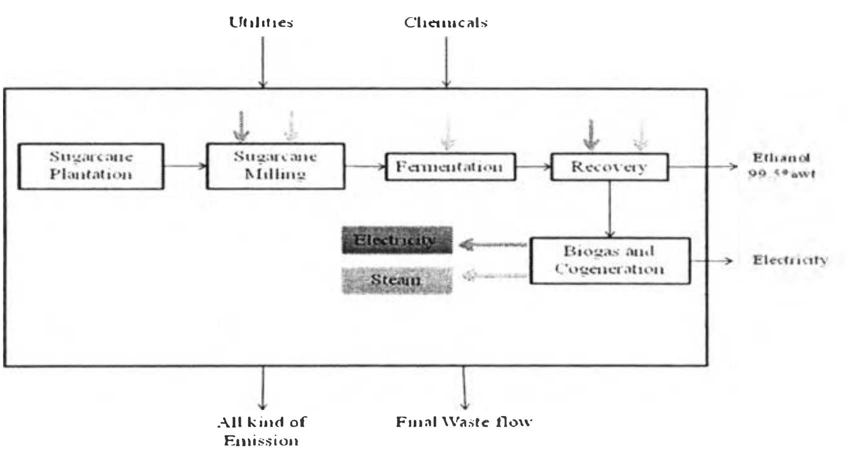

Figure 3.2 System boundary for bioethanol conversion process.

3.2.4.2 Inventory Analysis

• Collect data related to environment and technical quantities for all relevant assessment terms and within the boundaries, the unit processes, for example;

- Raw materials, utilities, and energy consumptions
- Air and water emissions
- Waste generations

The source of inventory data of bioethanol conversion process is given in Table 3.2.

Table 3.2 Sources of inventory data of bioethanol conversion process

Step	Type of data	Data source
Sugarcane farming and processing	2^{nd} Data	MTEC Research
Ethanol conversion	2^{nd} Data	Process Simulation
Waste water treatment	2^{nd} Data	TRE CDM project *

* Thai Roong Ruang Energy Co.,Ltd (TRE)

- Quantify how much energy and raw materials are used, and how much solid, liquid and gaseous wastes are generated, at each stage of the product's life.

3.2.4.3 Impact Assessment

- Calculate impact potentials based on the LCI results by using the SimaPro software (version 7.0—with CML 2 baseline 2000 methods).
- Analyze and compare the impacts on human health and the environment burdens associated with the raw material and energy inputs and environmental releases quantified by the inventory, for example Global warming and Energy Resources.

3.2.4.4 Interpretation

- Evaluate the net energy gain, net energy ratio and GHG emission per one kilogram of ethanol for the designed of bioethanol conversion process.
- Evaluate opportunities to reduce energy, material inputs, or environmental impacts at each stage of the product life-cycle.
- Analyze an improvement, in which recommendations are made based on the results of the inventory and impact stages.

3.2.5 <u>Re-modeling</u>

3.2.5.1 Generate New Design Alternative Using PRO/II and Consider the Results from Sustainability Analysis.

3.2.5.2 Perform Sustainability Analysis of New Design to Calculate Indicators, Sustainability Metrics, and Safety Indices. Examples of indicators are:

- Material-value added (MVA)
- Energy and waste cost (EWC)
- Total value added (TVA)

3.2.5.3 Perform Life Cycle Assessment of New Design to Evaluate EnvironmentalImpact.

3.2.6 Comparison between Base Case and New Design

Compare the results between base case and alternatives to determine the improvement achieved by the new designs. The results are given in terms of;

3.2.6.1. Indicators

3.2.6.2 Sustainability Metrics

3.2.6.3 Life Cycle Assessment