

## **pCHAPTER IV**

### **RESULTS AND DISSCUSSION**

The framework of this work consists of four main tools. The first three tools are dedicated to LCSOFT version 2.0 and the last tool is dedicated for software integration. The results of each tool and its application are presented. Furthermore, in order to test LCSOFT version 2.0, the validation was done and compared with the commercial LCA software, SimaPro.

#### **4.1 Tool 1: LCI knowledge management**

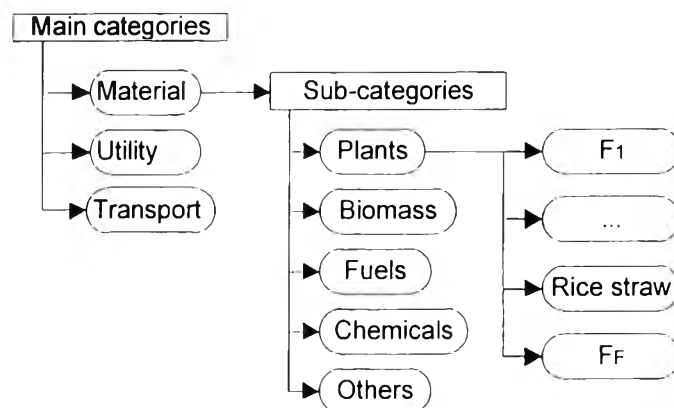
In order to extend the application range of LCSOFT that can calculate more LCA related terms, LCI data from several sources is passed throughout Tool 1. All datasets are clearly addressed and included all details in order to have a maximum of transparency in the database. LCI knowledge base (LCI KB) is generated for combination of LCI data from various single step processes in the most appropriate way, and to edit input and/or output values in the LCI for a better reflection of the product or process system under study.

LCSOFT originally has LCI data of 35 unit processes. In order to extend the application ranges of LCSOFT, LCI data from US LCI database and other literatures are passed through this tool and managed with the ontology models for easy maintenance, and quick retrieval for LCA calculations. The structure of LCI knowledge base (LCI KB) is divided into 2 parts; LCI KB for LCSOFT LCI database and extended LCI KB for added LCI database by users. Each KB can be divided into 2 levels; LCI KB's first level and second level (See Figure 4.2).

##### **4.1.1 LCI KB's first level**

This level divides input flows into 3 main types; material, utility, and transport. Material is divided into 5 sub-categories which are biomass, chemicals, fuels, plant, and others (LCI data added by users). Utility is divided into 5 sub-categories which are hot utility, cold utility, electricity by fuel, electricity by county, and others. Transport is divided into 2 sub-categories which are transport by mode of transport (air, pipeline, rail, road, and water), and transport by country. In each sub-

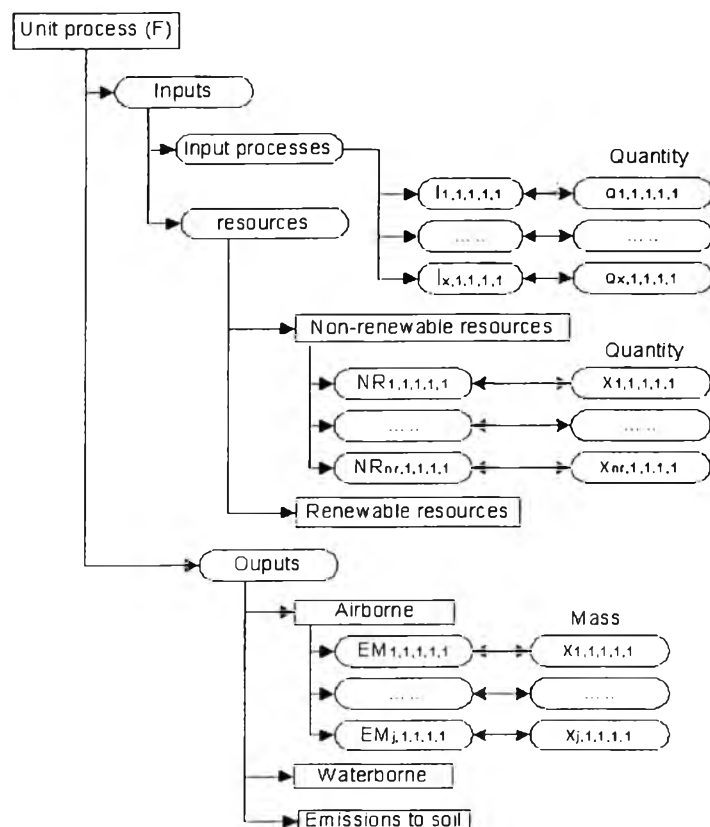
category, all the unit process's names in each category are listed from unit process  $F_1$  to unit process  $F_F$ . For example, hierarchies of rice straw production are material (main category), plant (sub-category), and rice straw (the unit process's name).



**Figure 4.1** Structure of LCI KB's first level.

#### 4.1.2 LCI KB's second level

The first category of LCI KB's second level is "Inputs" which accounts input processes (activities and materials required for a specific unit process), and resources (resources consumed in the unit process). For example, the unit process is rice straw production, activities and resources are listed as shown in Table 4.1 and Table 4.2, respectively. The second category of data in LCI KB's second level is "Outputs" which accounts emissions regarded to the compartments (airborne, waterborne, and emissions to soil). The names and amount of emitted substances are stored as shown in Table 4.3. LCI KB allows the user to examine inputs and outputs of the specific upstream process order to use LCI data with the correct data and avoid double counting. For example in order to produce 1 kg of rice straw the N-fertilizer is added as the input of the process to produce rice straw, it is not necessary to add N-fertilizer again.



**Figure 4.2** Structure of LCI KB's second level.

**Table 4.1** Input processes of rice straw production in LCI KB's second level

Input processes	Unit	Quantity
Dummy, Agrochemicals, at plant	kg	0.0007565
Dummy, Copper, at regional storage	kg	0.0001318
Diesel, combusted in industrial equipment	L	0.0399146
Electricity, at grid, US, 2000	kWh	0.0411174
Quicklime, at plant	kg	0.0056602
Liquefied petroleum gas, combusted in industrial boiler	L	0.0023236
Natural gas, combusted in industrial boiler	m <sup>3</sup>	0.0044122
Nitrogen fertilizer, production mix, at plant	kg	0.0195534
Dummy, Phosphorous Fertilizer (TSP as P <sub>2</sub> O <sub>5</sub> ), at plant	kg	0.0042452
Dummy, Potash Fertilizer (K <sub>2</sub> O), at plant	kg	0.0036791
Transport, train, diesel powered	tkm	0.0327841
Transport, single unit truck, diesel powered	tkm	0.0133957

**Table 4.2** Resources for rice straw production in LCI KB's second level

Resources	Type	Heating value (MJ/kg)	Sub-compartment	Unit	Quantity
Water, well	-	-	ground-	L	201.8062
Carbon dioxide	-	-	in air	kg	-1.04264
Oil, crude	non-renewable	42.7	ground-	kg	0.215757
Coal, bituminous	non-renewable	24.8	ground-	kg	0.014545
Uranium oxide (U3O8)	non-renewable	332000	ground-	kg	2.94E-07
Carbon dioxide, in air	-	-	in air	kg	0.000548
Gas, natural	non-renewable	49.8	ground-	m3	0.023547

**Table 4.3** Emitted substances of rice straw production in LCI KB's second level

Chemicals	Compartment	Sub-compartment	Unit	Amount
2,4-D	air	low population density	kg	7.81149E-06
Ammonia	air	low population density	kg	0.001175287
Bentazone	air	low population density	kg	2.02447E-06
Carbaryl	air	low population density	kg	1.31749E-06
Carbofuran	air	low population density	kg	4.50271E-06
Carbon monoxide	air	low population density	kg	0.005929639
Glyphosate	air	low population density	kg	3.89688E-06
Hydrocarbons, unspecified	air	low population density	kg	0.000453875
Malathion	air	low population density	kg	2.13383E-06
MCPA	air	low population density	kg	2.00312E-06
Methane	air	low population density	kg	0.03662069
Parathion, methyl	air	low population density	kg	3.22759E-06
Molinate	air	low population density	kg	5.81544E-05
Nitrogen oxides	air	low population density	kg	0.003498686
Dinitrogen monoxide	air	low population density	kg	0.000609926
Paraquat	air	low population density	kg	1.17406E-07

## 4.2 Tool 2: Calculation factor estimation

In order to characterize the emissions that occur in the life cycle of a product or process in terms of environmental impacts, substance-specific characterization factors (CFs) that represent the substance's potency of environmental damage are necessary. LCSofT version 1.0 obtains CFs for 8 impacts from literatures and 423 values for each impact by average, however, this has been improved by using the greater accurate method using group contribution<sup>+</sup> method

(GC)<sup>+</sup> since all of available experimental data of the property in the regression is possible to improve the predictive capability and application range of the property model.

#### 4.2.1 Database

This part of this work has been published within the study of "Estimation of Environment-Related Properties of Chemicals for Design of Sustainable Processes: Development of Group-Contribution<sup>+</sup> (GC<sup>+</sup>) Property Models and Uncertainty Analysis" (Hukkerikar *et al*, 2012). Using CFs (experimental values) of from the US Environmental Protection Agency (EPA), the predictive models for CFs of 8 impacts; human toxicity by ingestion (HTPI), human toxicity by exposure (HTPE), aquatic toxicity (ATP), Terrestrial toxicity (TTP), global warming (GWP), ozone depletion (ODP), photochemical oxidation (PCOP), and acidification (AP) have been developed. Furthermore, CFs obtained from USEtox<sup>TM</sup> database have been used to developed predictive models of CFs for 3 impacts; carcinogenics (HTC), non carcinogenics (HTNC), and fresh water ecotoxicity (ET) are estimated. Details are listed.

- Human toxicity by ingestion (HTPI, unit 1/LD<sub>50</sub>): Human toxicity from ingestion and inhalation is used to estimate toxicity potential because they considered all of the primary routes of exposure of a chemical. HTPI were calculated for a chemical if it existed as a liquid or solid at a temperature of 0°C and atmospheric pressure, and an exposure potential. The lethal dose that produced death in 50% of rats by oral ingestion (LD<sub>50</sub>) was used as an estimate for the HTPI. The value was chosen because of its prevalence in the literature and acceptance as a standard toxicity indicator. For those chemicals for which a rat-oral LD<sub>50</sub> value was not available, a value was estimated by molecular methods.

- Human toxicity by exposure (HTPE, unit 1/TWA): Human toxicity from dermal exposure used to estimate toxicity potential because they considered all of the primary routes of exposure of a chemical. To estimate the HTPE, time-weighted averages (TWA) of the threshold limit values (TLV) were used. These values were obtained from OSHA, ACGIH, NIOSH and represent occupational safety exposure limits. This was considered to be an adequate me

measuring stick for comparison of chemicals that would pose a more thorough and relevant human toxicity value. Once completed, those values will supplant the human toxicity values that are currently stored in the LCSoft database.

- Aquatic toxicity (ATP, unit 1/ LC<sub>50</sub>): The ATP was estimated by using toxicological data for a single, representative species of fish, *Pimephales promelas* (fathead minnows). This species was chosen again because of its acceptance as a universal aquatic indicator and its prevalence of data. The data for this assay comes in the form of a LC<sub>50</sub>, a lethal concentration which causes death in 50% of the test specimens.
- Terrestrial toxicity (TTP, unit 1/ LD<sub>50</sub>): For the time being the LD<sub>50</sub> values will be used to provide a relative toxicity comparison for both human and terrestrial entities.
- Global warming (GWP unit kg CO<sub>2</sub> eq. ): GWP is determined by comparing the extent to which a unit mass of a chemical absorbs infrared radiation over its atmospheric lifetime to the extent that CO<sub>2</sub> absorbs infrared radiation over its respective life-times. The half-lives of each of these chemicals was factored into the calculation for determining the GWP. Since, chemicals have different atmospheric half-lives the length of time over which the comparison is made will change the GWP of a chemical. For this database, 100 years was chosen as the base time frame.
- Ozone depletion (ODP, unit kg CFC-11 eq.): The ODP is determined by comparing the rate at which a unit mass of chemical reacts with ozone to form molecular oxygen to the rate at which a unit mass of CFC-11 (trichlorofluoromethane) reacts with ozone to form molecular oxygen. For a chemical to have ODP it must exist in the atmosphere long enough to reach the stratosphere, it, also, must contain a chlorine or bromine atom.
- Photochemical oxidation (PCOP, kg C<sub>2</sub>H<sub>2</sub> eq.): The PCOP or smog formation potential is determined by comparing the rate at which a unit mass of chemical reacts with a hydroxyl radical (OH•) to the rate at which a unit mass of ethylene reacts with OH•.

- Acidification (AP, unit H<sup>+</sup> eq.): The AP or acid rain potential is determined by comparing the rate of release of H<sup>+</sup> the atmosphere as promoted by a chemical to the rate of release of H<sup>+</sup> in the atmosphere as promoted by SO<sub>2</sub>.
- Carcinogenics (HTC, unit kg benzene eq.): The characterization factors for human toxicity (carcinogenic impacts) for chemical emissions to urban air, rural air, freshwater, sea water, agricultural soil and/or natural soil.
- Non carcinogenics (HTNC, unit kg toluene eq. ): The characterization factors for human toxicity (non carcinogenic impacts) for chemical emissions to urban air, rural air, freshwater, sea water, agricultural soil and/or natural soil.
- Fresh water ecotoxicity (ET, unit kg 2,4-D eq.): The characterization factors for ecotoxicological characterization factor of chemicals include impacts for emissions to urban air, rural air, freshwater and/or agricultural soil.

#### 4.2.2 Model performance statics

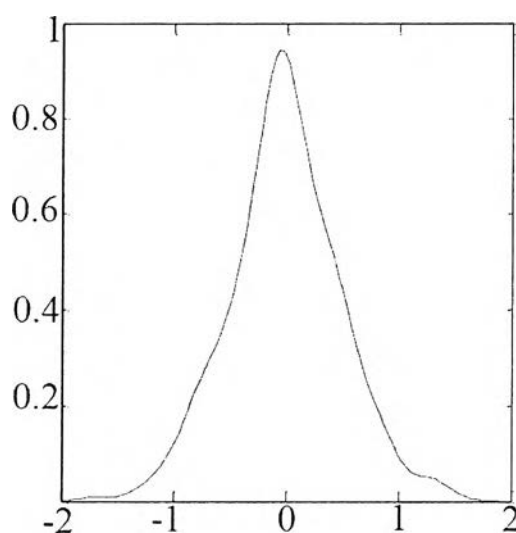
The model performance statics for property prediction using the simultaneous regression method are mentioned (Hukkerikar *et al*, 2012). This is illustrated for the case of characterization factor of non-carcinogenic emitted to urban air (HTNC<sub>EUA</sub>). After cross-validation has been perform, the property HTNC<sub>EUA</sub> can be modeled using a linear model as shown in equation 4.1.

$$-\log(\text{HTNC}_{\text{EUA}}) + A_{\text{HTNC}_{\text{EUA}}} = \sum_i N_i C_i + w \sum_j M_j D_j + z \sum_k E_k O_k \quad (4.1)$$

The model performance statistics for property models analyzed using simultaneous regression have been done. For the case of HTNC<sub>EUA</sub>, 341 data-points have been considered in the regression. The degree of freedom obtained by subtracting number of estimated model parameters from 341 data-points is 128. The percentage of the experimental data-points found within ± 1%, ± 5%, and ± 10% relative error ranges are 27.57, 60.70, and 84.46 respectively. The values of SD, AAE, ARE, and R<sup>2</sup> can be calculated using equation 2.2-2.5. The values for the case of HTNC<sub>EUA</sub> are 0.36,

0.26, and 4.87 respectively. The residuals calculated from the differences experimental values and predicted values are smaller than the estimation errors and followed a normal distribution curve (see Figure 4.3). These confirm the reliability of the method. Similar analyses have been performed to obtain a suitable predictive model for other characterization factor of environmental impacts with the objective of providing the accurate and reliable property estimation.

The molecular structures of environmental related chemical are passed through this tool with the specially predictive models, increasing CFs to 26,155 substances for all 11 environmental impacts. Therefore, LCSOFT version 2.0 has the potential to calculate environmental impacts for a very wide range of organic substances.



**Figure 4.3** Residual distribution plot of  $HTNC_{EUA}$  (Hukkerikar *et al*, 2012).

### 4.3 Tool 3: Calculation of LCA

This tool is for calculation of LCA related terms, modules in LCSOFT version 1.0 is improved and expanded as shown Figure 4.4. The gray area represents improvement of source codes in LCSOFT. There are 5 main steps in this tool as described below. Furthermore, additional features which are analysis and alternative comparison are added (see appendix A).



#### 4.3.1 Step 1: Check existence

After the user add LCA data to perform LCA, it is importance to check the existence of LCI data for the related products or processes. In this step the user will be noticed from the software that the selected product or process does not exist, enabling the user opportunity to add or modify LCI data and enable the complete LCA conduction.

#### 4.3.2 Step 2: Retrieve LCI data

The data are retrieved from LCI KB to be stored in the systematic worksheet and be calculated in the next step. The retrieved data are input processes, resource consumption, and emissions. The names and amount of input process, resource, and emissions are listed in the separated specific worksheet.

#### 4.3.3 Step 3: Calculate resource and energy consumption

Energy consumption is the amount of energy (MJ) consumed by the resources per functional unit of product (such as 1 kg of product, 1 L of product, or 1 MJ of product) over the life cycle. Resources used in production of raw material phase, energy production phase and manufacturing phase are converted to total energy consumption and % renewable energy. Calculation models are described below.

$$R_{\text{total}} = R_{\text{renew}} + R_{\text{non-renew}} \quad (4.2)$$

$$R_{\text{renew}} = (\sum_{r,i} m_i^{\text{PI}} \times x_{r,i} \times HV_r) / m_{\text{product}} \quad (4.3)$$

$$R_{\text{nonre}} = (\sum_{nr,i} m_i^{\text{PI}} \times x_{nr,i} \times HV_{nr}) / m_{\text{product}} \quad (4.4)$$

Where

$r$  = Renewable resource used to produce input  $i$

$nr$  = Non-renewable resource used to produce input  $i$

$x_{r,i}$  = Mass of renewable resource  $r$  used to produce 1 kg of input  $i$   
(kg)

$x_{nr,i}$  = Mass of non-renewable resource  $nr$  used to produce 1 kg of  
input  $i$  (kg)

$HV_r$  = Heating value of renewable resource r (MJ/kg<sub>r</sub>)

$HV_{nr}$  = Heating value of non-renewable resource nr (MJ/kg<sub>nr</sub>)

$R_{total}$  = Total energy from resource consumption per 1 kg of product  
(MJ/kg<sub>product</sub>)

$R_{renew}$  = Total energy from renewable resource consumption per 1  
kg of product (MJ/kg<sub>product</sub>)

$R_{nonre}$  = Total energy from non-renewable resource consumption per  
1 kg of product (MJ/kg<sub>product</sub>)

#### 4.3.4 Step 4: Calculate carbon footprint

Carbon footprint (CF) is the overall amount of carbon dioxide and other greenhouse gas emissions associated with one kilogram of product. The carbon footprint is quantified using indicators such as the global warming potential (GWP). GWP is an indicator that reflects the relative effect of a greenhouse gas in terms of climate change considering a fixed time period (100 years). Emissions of utility consumptions in the process are converted to carbon dioxide emissions (carbon dioxide equivalent) per functional unit of product (such as 1 kg of product, 1 l of product, or 1 MJ of product). This way will be easy to identify which equipment should be improved, the calculation models are described below. Carbon footprint is total carbon dioxide equivalent from the process per 1 kg of product

$$CO2_{eq} = (m_{GHG,air}^{PRO} \times CF_{GHG,air}^{GWP})/m_{product} \quad (4.5)$$

$$\text{Carbon footprint} = \sum CO2_{eq} \quad (4.6)$$

Where

GHG = Greenhouse gas emitted to air from process

$m_{GHG,air}^{PRO}$  = Mass flow rate of greenhouse gas (GHG) emitted to air  
from the process

$CF_{GHG,air}^{GWP}$  = Characterization factor for global warming of green-  
housegas (GHG)

$CO2_{eq}$  = Carbon dioxide equivalent per 1 kg of product

#### 4.3.5 Step 5: Assess impacts

Environmental impacts are calculated from mass of emitted substance multiply by its characterization factors for a specific compartment per functional unit of product (such as 1 kg of product, 1 L of product, or 1 MJ of product). In LCSOFT version 2.0, 11 impact categories are calculated. Calculation models are described below. The descriptions of each environmental impact are also described.

$$I^k = \sum_{t,c} EM_{t,c} \times CF_{t,c}^k \quad (4.7)$$

Where

- t = chemical emitted to compartment c
- k = impact category (see Table 4.4)
- $CF_{t,c}^k$  = The characterization factor of chemical n emitted to compartment c for impact category k
- $EM_{t,c}$  = Mass of chemical t emitted to compartment c per 1 kg of product
- $I^k$  = The potential environmental impact of chemical t for a specific impact category of concern k

**Table 4.4** Characterization factors and compartments of environmental impacts

Impact category ( $I^k$ )	Characterization factor ( $CF_{t,c}^k$ )	Compartment (c)
Human toxicity by ingestion	$CF_{t,c}^{HTPI}$	Air
Human toxicity by exposure	$CF_{t,c}^{HTPE}$	Air
Aquatic toxicity	$CF_{t,c}^{ATP}$	water
Terrestrial toxicity	$CF_{t,c}^{TTP}$	soil
Global warming	$CF_{t,c}^{GWP}$	Air
Ozone depletion	$CF_{t,c}^{ODP}$	Air
Photochemical oxidation	$CF_{t,c}^{PCOP}$	Air
Acidification	$CF_{t,c}^{AP}$	Air
Carcinogenics	$CF_{t,c}^{HTC}$	Air, water, soil
Non carcinogenics	$CF_{t,c}^{HTNC}$	Air, water, soil
Fresh water ecotoxicity	$CF_{t,c}^{ET}$	Air, water, soil

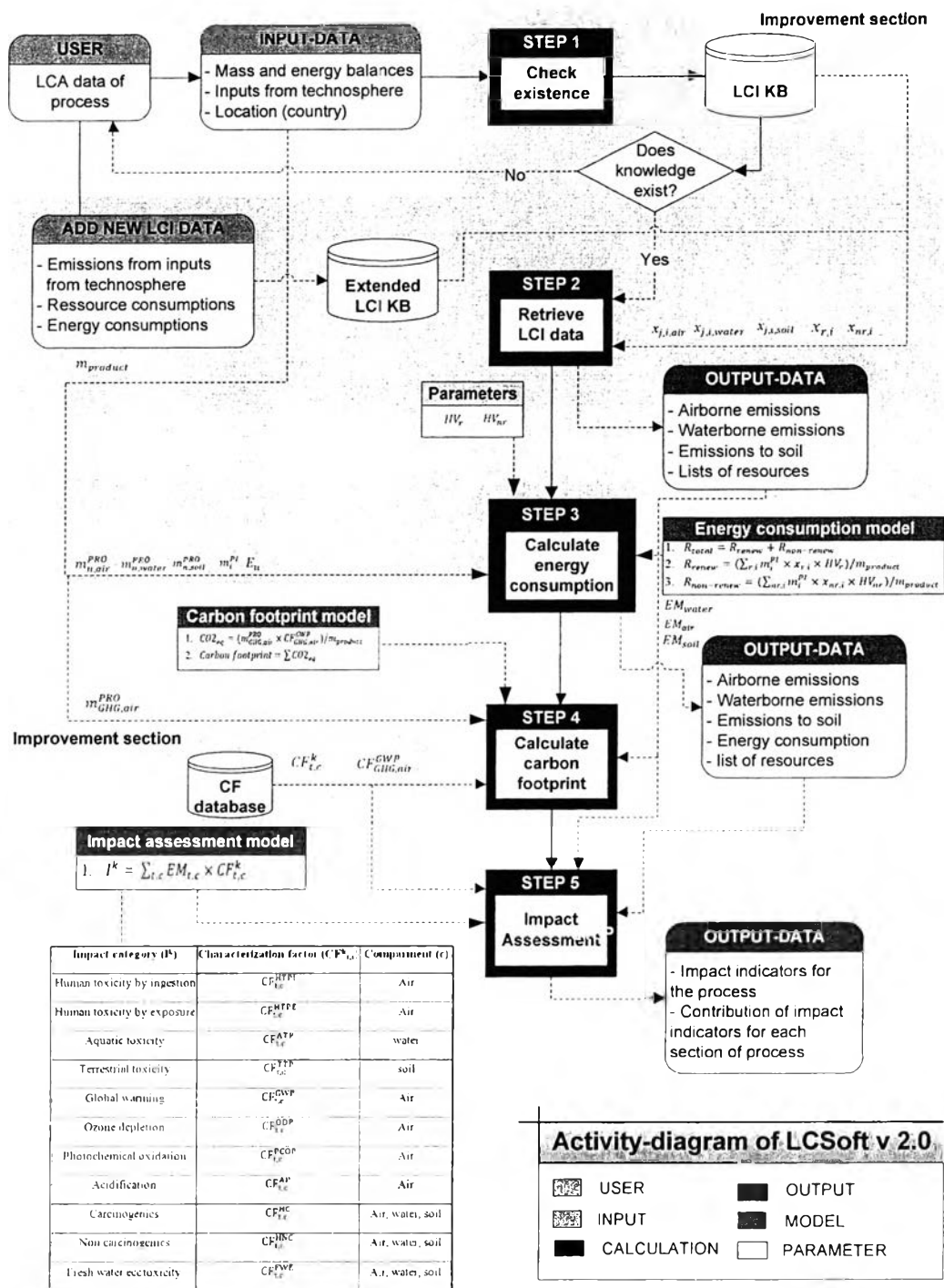


Figure 4.4 The structure of LCSoft version 2.0.

#### 4.3.6 Additional features

In order to be a complete process evaluation software for LCA, LCSoft is added the new features which are sensitivity analysis and alternative comparison. Sensitivity analysis is created for study the variation of raw material type, utility type, and transport type on environmental impacts or the variation of the amount of input processes in order to weight what is the main contribution of the design process and find the optimal solution in order to minimize environmental impacts. Alternative comparison is for selection the best design among the process based on the amount of environmental impacts contributed by the alternative processes.

#### 4.4 Tool 4: Integration of LCSoft, ECON and SustainPro

The objective of this tool is to create the interface that the user can easily enter necessary data for all software (SustainPro, ECON, and LCsoft). The advantage of this interface is to perform the robust multi objective optimization of the design process since the data is linked to software and each software separately performs calculation and the results from each software will be sent to the main interface. The structure for the interface is illustrated in Figure 4.5. Instructions for each step to perform process evaluation are mentioned in appendix B.

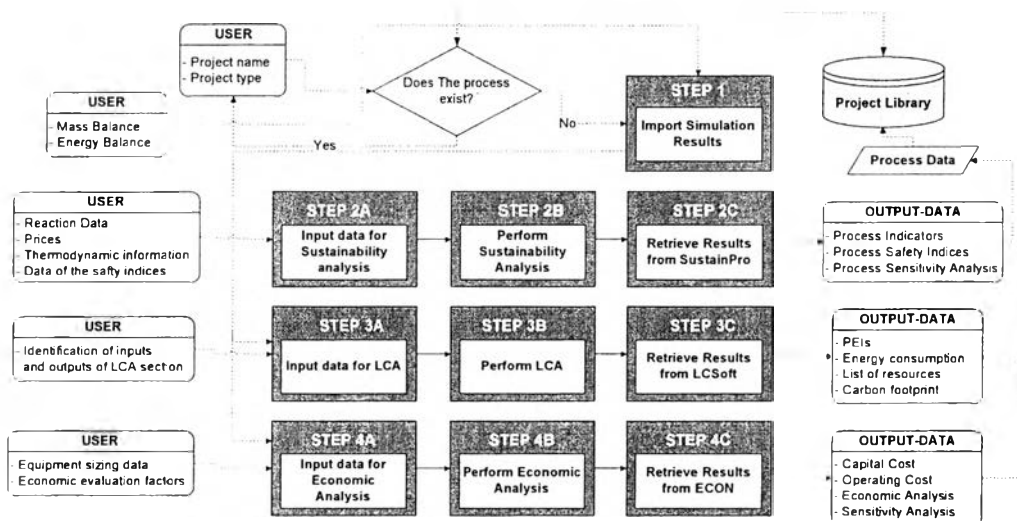
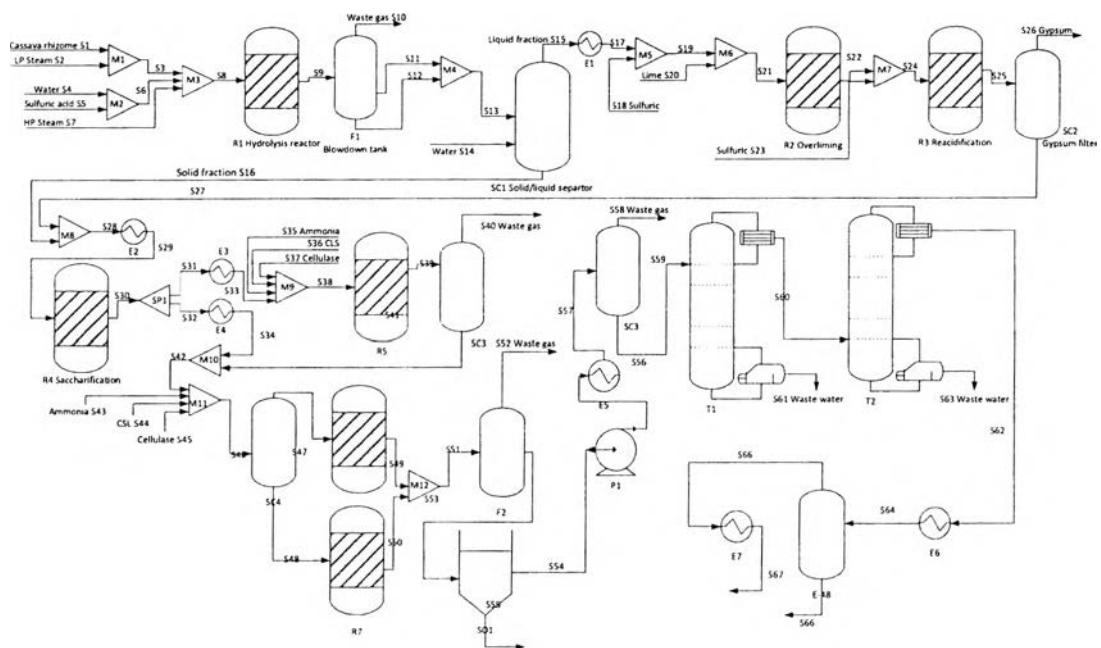


Figure 4.5 The structure of tool integration.

#### 4.4.1 Case study

In order to test this tool, a bioethanol production process using cassava rhizome is used as a case study (Mangnimit, 2013). The mass and energy flows are taken from the simulation results which are developed according to NREL study. Input wet biomass is 377 tons/day and bioethanol product is 119 tons/day to with addition of cellulose enzyme. The flowsheet is illustrated in Figure 4.6. Process data for sustainability analysis, LCA, and economic evaluation are illustrated in Appendix C. Simulation results are directly imported into the interface, steps to enter sustainability analysis data, LCA data, and economic data are reduced, and results from each software are imported to the interface and clearly presented enabling proficient evaluation of improvement strategies.



**Figure 4.6** Flowsheet of the case study.

#### 4.4.2 SustainPro results

This sustainability analysis tool provides targets from improvement in order to make the process more profitable, safer, and more sustainable. SustainPro calculates indicators for each open-part (OP), and close-path (CP) and orders them from higher to lower potential for improvement. The main indicators are; material value added (MVA), the value generated from the feed to the demand of a certain compound in a certain OP and it can be calculated by the difference between sale

price and purchase price depended on the mass of the component; energy and waste cost (EWC), the sum of the energy cost (the duty times mass of utility and the unit price of the utility needed in sub-operation) and waste cost (the mass of waste times the treatment cost); total value added (TVA), the difference of MVA and EWC.

After entering all necessary data into the software throughout the interface, the red color means that path is the highest potential to be improved. The top five targets for improvement for each indicator are shown in Table 4.5. The second line of each path states the component and OP it refers to. In cases where the component enters the process through means of a reaction it is written “P” followed by the name of the unit where the reactions take place. SustainPro did not calculate indicators for CP since there is no recycle path in the case study.

It is necessary to use a good engineering judgment to evaluate which of the targets could actually be improved. From Table 4.2, EWC of OP 67, OP 43, and OP 50 indicate that these paths need to be reduced their duties since EWC depends on mass of utility and utility price. MVA and TVA of OP 322, OP 15, and OP 326 indicate that corn steep liquor (CSL), lignin, and cellulase (enzyme) lose their value they exit the process. Therefore the excess flow of CSL should be reduced and cellulase should be recovered and recycled, if possible. However, cellulase is difficult to be recovered and recycled and therefore, other options, such as, use of the lignin or waste and recycle of water needs to be investigated.

**Table 4.5** Indicator results of the case study after ordering in SustainPro.

Path	MVA	Propability	Path	EWC	Propability	Path	TVA	Propability
OP 322 Corn Steep Liquor-44-61	-553.41	High	OP 67 Ethanol-P R6-67	795.4 9	Medium	OP 322 Corn Steep Liquor-44- 61	- 1348.9	High
OP 206 Water-14-52	-505.97	High	OP 43 Xylose -P R1-61	270.9 5	Low	OP 206 Water-14-52	- 776.92	High
OP 15 Lignin-1-55	-440.5	High	OP 50 Xylose-P R1-61	145.3 5	Low	OP 15 Lignin-1-55	- 585.85	High
OP 318 Corn Steep Liquor-36-61	-376.32	High	OP 35 Glucose-P R4-61	102.8 1	Low	OP 318 Corn Steep Liquor-36- 61	- 479.13	High
OP 326 Cellulase-45- 55	-299.59	High	OP 62 Ethanol-P R5-67	74.92	High	OP 326 Cellulase- 45-55	- 374.51	High

#### 4.4.3 LCSoft results

This study is a cradle-to-gate LCI of bioethanol production from cassava rhizome. Production of cassava phase, transportation and manufacturing are analyzed. In order to calculate the contribution of each section in the process, the case study is divided into 5 sections which are; (1) Pretreatment, to make the lignocellulosic material enable to be hydrolyzed; (2) Detoxification, the compounds that are toxic for the fermentation microorganisms are treated; (3) SSCF, to convert glucose and other sugars to ethanol; (4) Distillation, to distil the process stream from SSCF section until a mixture of nearly azeotropic water and ethanol is obtained; and (5) Dehydration, the ethanol from distillation section is purified using vapor-phase molecular sieves in order to obtain bioethanol within the specifications (see Appendix C). From this information, the emissions and environmental impacts, carbon footprint from the process, and energy consumption of bioethanol production are estimated.



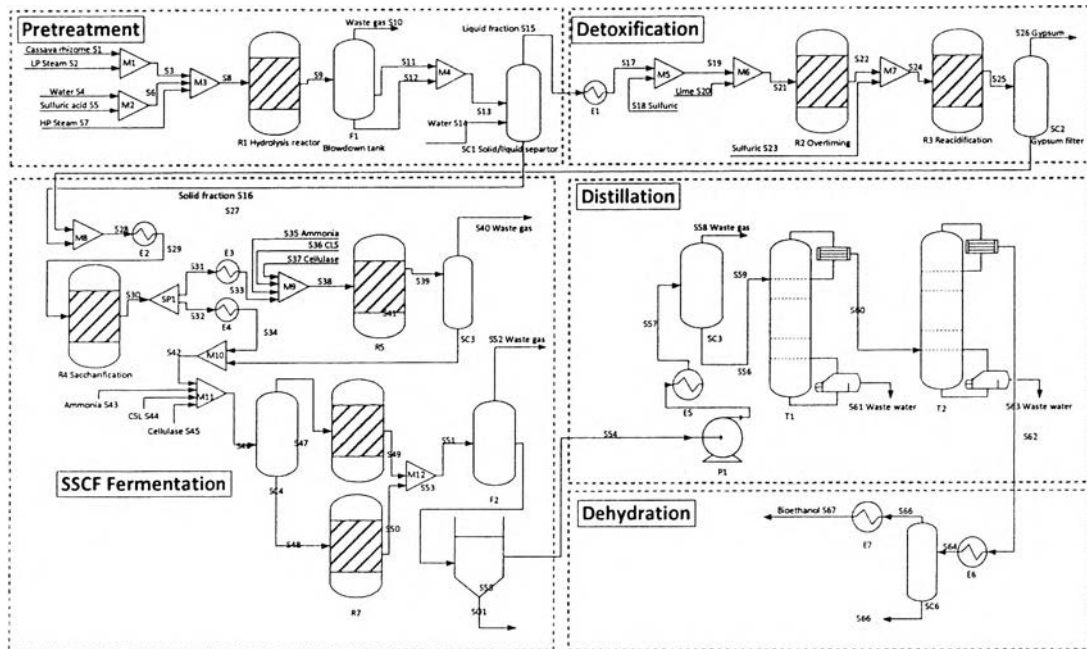


Figure 4.7 LCA boundaries of the case study.

#### 4.4.3.1 Energy consumption

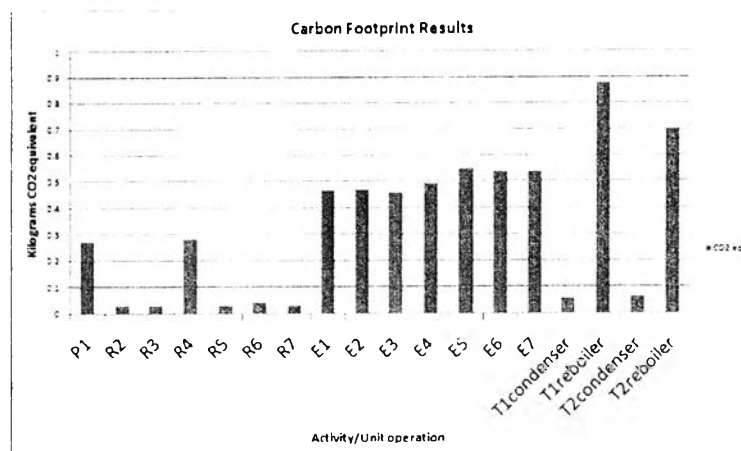
Table 4.6 represents the most energy consumption section which is distillation section which is agreeable with SustainPro results.

Table 4.6 Energy consumption results of the case study in LCSof

Section	Energy consumption (MJ/kg product)	% renewable
(1) Pretreatment	0.24	0.00
(2) Detoxification	0.44	39.20
(3) SSCF	1.22	58.39
(4) Distillation	9.07	99.81
(5) Dehydration	1.94	100.00
Total	12.91	92.03

#### 4.4.3.2 Carbon footprint

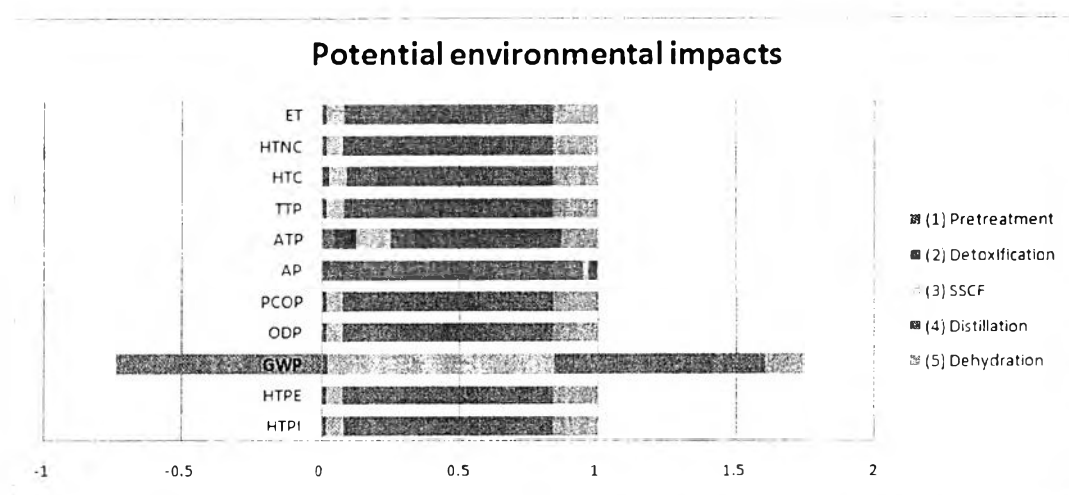
Carbon footprint results are calculated from the emissions of green house gas from utility consumption in the process are shown in Figure 4.8. The emissions from utility consumption mainly come from reboiler steam of distillation column T1 and T2. Therefore, this section should be improved.



**Figure 4.8** Carbon footprint results.

#### 4.4.3.3 Impact assessment results

Environmental impacts contributed from each section are calculated and represented each impact in the bar chart in LCSofT as shown in Figure 4.9. Distillation section has high contribution in every impact categories. Therefore, from LCSofT results, this section should be improved.



**Figure 4.9** Impact assessment results.

#### 4.4.4 ECON results

Economic feasibility is necessary for process design to ensure the economical sustainability of the process before searching for the improvement strategies in order to find the optimal design. After entering dimensioning of equipments, the prices of product and raw materials, and economic related data into ECON throughout the interface, total capital investment cost, operating cost, and other economic evaluation parameters will be calculated and imported from ECON to the interface.

After application of ECON, total capital investment is \$53,692,808, the details are shown in Figure 4.10; and total operating cost is \$20,792,726, the details are shown in Figure 4.11. From these result, the largest fractions of the operating costs are found to involve the raw materials and utilities. 70 % of the utility cost are reboiler steam from the distillation column T1(44 %) and T2 (26 %) as shown in Figure 4.12, and therefore, distillation units need to be improved. However, net present value (NPV) of this process is \$ 95,125,049.00 with 15% expected internal rate of return (IRR). Therefore, this process has high potential for economic feasibility.

Manufacturing Fixed-capital Investment (Direct Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result
Purchased Equipment Delivered	11 %	\$ 10,611,227.00
Purchased Equipment Installation	0.47 %	\$ 4,987,276.69
Instrumentation and Controls (installed)	0.36 %	\$ 3,820,041.72
Piping (Installed)	0.68 %	\$ 7,215,634.36
Electrical Systems (Installed)	0.11 %	\$ 1,167,234.97
Buildings (Including Services)	0.18 %	\$ 1,910,020.86
Yard Improvement	0.1 %	\$ 1,061,122.70
Service Factors (Installed)	0.7 %	\$ 7,427,658.90
	2.8 %	
<b>Total Direct Cost</b>		<b>\$ 38,200,417.20</b>
Nonmanufacturing Fixed-capital Investment (Indirect Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result
Engineering and Supervision	0.33 %	\$ 3,501,704.91
Construction Expenses	0.41 %	\$ 4,350,603.07
Legal Expenses	0.04 %	\$ 424,449.08
Contractor's Fees	0.22 %	\$ 2,334,463.94
Contingency	0.44 %	\$ 4,668,939.88
	1.44 %	
<b>Total indirect cost</b>		<b>\$ 15,280,166.88</b>
Fixed-capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result
Fixed-capital Investment (FCI)		\$ 53,480,584.08
Working Capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result
Working Capital Investment (WCI)	0.69 %	\$ 2,222,454.54
<b>Total Capital Investment (TCI)</b>		<b>\$ 55,703,038.62</b>

Figure 4.10 Total capital investment calculation details.

Fixed Capital Investment	\$ 53,480,584.08		
Plant Capacity	33320220 kg/day	Use Default Factor	
Processing Step	0	Recalculate	

Items of Operating Cost	tor ( can change by u	Basis	Cost, \$/year
Raw Material	0		\$ 7,800,517.00
Operating Labor	0	Fixed Capital Investment	\$ -
Operating Supervision	0.15	Operating Labor	\$ -
Utilities	0		\$ 3,459,217.00
Maintenance and Repairs	0.06	Fixed Capital Investment	\$ 3,208,835.04
Operating Supplies	0.15	Maintenance and Supplies	\$ 481,325.25
Laboratory Charges	0.15	Operating Labor	\$ -
Royalties	0.01	Total Product Cost	\$ 207,927.26
	0		
<b>Variable Cost</b>			<b>\$ 14,957,821.55</b>
Property Taxes	0.02	Fixed Capital Investment	\$ 1,069,611.68
Financing (interest)	0	Fixed Capital Investment	\$ -
Insurance	0.01	Fixed Capital Investment	\$ 534,805.84
Rent	0	Fixed Capital Investment	\$ -
<b>Fixed Charges</b>			<b>\$ 1,604,417.52</b>
Plant Overhead	0.6	abor • Supervision • Maintenac	\$ 1,925,301.00
<b>Manufacturing Cost</b>			<b>\$ 16,562,239.07</b>
Administration	0.2	abor • Supervision • Maintenac	\$ 641,767.00
Distribution & selling	0.04	Total Product Cost	\$ 831,709.04
Research & Development	0.04	Total Product Cost	\$ 831,709.04
<b>General Expense</b>			<b>\$ 2,305,185.08</b>
<b>Total Product Cost with Out Depreciation</b>			<b>\$ 20,792,728.00</b>

Figure 4.11 Operating cost calculation details.

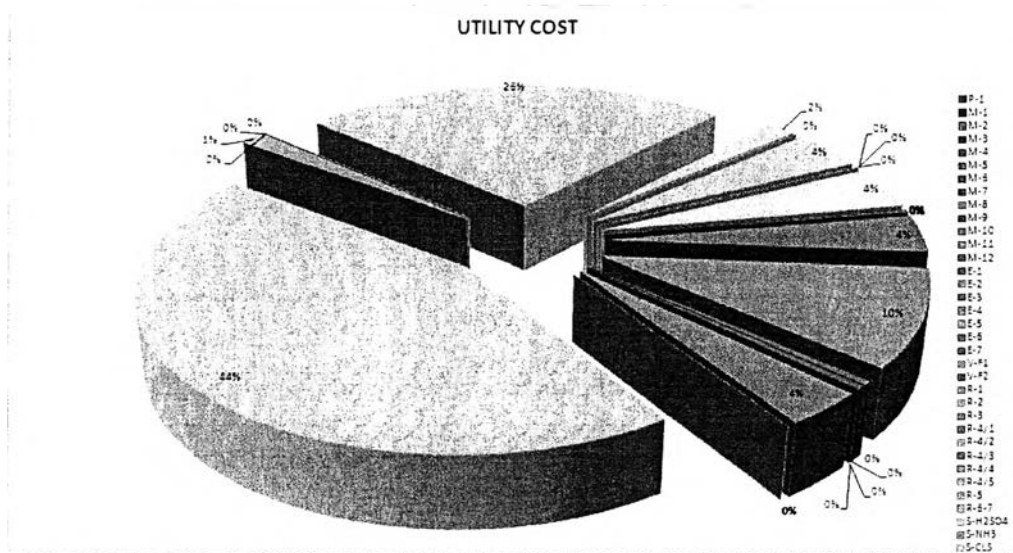


Figure 4.12 Pie chart of utility cost.

## 4.5 Validation of LCSoft version 2.0

This study is a cradle-to-gate LCI of bioethanol production from cassava rhizome. Production of cassava phase, transportation and manufacturing are analyzed. In the manufacturing, the mass and energy flows are taken from the simulation results which are developed according to NREL study (Mangnimit, 2013). Input wet biomass is 377 tons/day and ethanol product is 119 tons/day. From this information, energy consumption, carbon footprint, and environmental impacts of bioethanol production are estimated. The energy consumption and environmental impact calculated from LCSoft will be compared with SimaPro.

### 4.5.1 Modeling consideration in LCSoft

The scope of the case study includes manufacturing phase of raw material which are the cassava cultivation and production of sulfuric acid, ammonia, corn steep liquor (CSL), and cellulase enzyme. In what regards to the components presented in the simulation results, the following ones exist in the LCSoft LCI database: sulfuric acid, ammonia, corn steep liquor (CSL), and cellulase enzyme. Therefore the impacts associated with them are included in the environmental impact assessment. As the cassava cultivation is included, cellulose, hemicelluloses, and lignin presented in the input streams of the process simulation results are modeled as the sum of the mass of cassava rhizome (lignocellulosic matter). The following components do not exist in the LCSoft LCI database: glucose, xylose, cellobiose, furfural, hydroxymethyl furfural (HMF), lactic acid, succinic acid, and glycerol. However these compounds have no influence on the environmental impacts calculated in LCSoft. In order to analyze the environmental impacts from using utilities in the bioethanol production process, the processes are: electricity using natural gas, Natural gas, combusted in industrial boiler and Chilled water, and engine-driven chiller using natural gas.

#### 4.5.2 Modeling consideration in SimaPro

Raw materials such as sulfuric acid and ammonia exist in both LCSoft and SimaPro LCI database. On the other hand, CSL and cellulase enzyme do not exist in SimaPro. The cassava cultivation is modeled by the sum of cellulose, hemicelluloses, and lignin and using LCI data from the literature since LCI data for cassava cultivation does not exist in SimaPro LCI database. The production of energy which are the electricity from natural gas, natural gas, combusted in industrial boiler, and cooling water are considered (SimaPro user manual, 2006).

#### 4.5.3 TRACI method

Tool for the Reduction and Assessment of Chemical and other environmental Impacts (TRACI) is midpoint oriented LCIA methodology of US Environmental Protection Agency (EPA) that supports consistency in environmental decision making. TRACI allows the examination of the potential for impacts associated with the raw material consumption and chemical releases resulting from the processes involved in producing a product. It allows the user to examine the potential for impacts for a single life cycle stage, or the whole life cycle, and to compare the results between products or processes. The purpose of TRACI is to allow a determination or a preliminary comparison of two or more options on the basis of the following environmental impact categories: ozone depletion (ODP), global warming (GWP), acidification (AP), eutrophication (EP), respiratory effects (RE), photochemical oxidation (PCOP), carcinogenics (HTC), non carcinogenics (HTNC), and ecotoxicity (ET).

#### 4.5.4 Cumulative Energy Demand (CED) method

This method is based on the method published byecoinvent version 1.01 and expanded by PRé Consultants for raw materials available in the SimaPro 6 database used to calculate energy consumption calculated from resources used in the system boundaries.

#### 4.5.5 Comparison with commercial software (SimaPro)

The energy consumption from SimaPro using CED method is 14.04 MJ/1 kg of ethanol which is slightly greater than 12.91 MJ/1 kg of ethanol from LCSOFT because heating value of natural gas in LCSOFT is 49.8 MJ/kg which is greater than 46.8 MJ/kg from SimaPro.

Life cycle assessment of bioethanol process using cassava rhizome is conducted using TRACI method. The comparison of environmental impacts is shown in Table 4.6. The insignificant difference SSE and percent differences of GWP and PCOP values from both software indicate that the boundary definitions, assumptions in inventories, material flows, and energy flows are the same. The major differences are AP and HTNC. AP values from SimaPro is greater than those from LCSOFT because Franklin database in SimaPro model yields larger sets of emission factors associated with the combustion fuels compared with those in LCSOFT model. HTNC and ET values from LCSOFT is greater than the one from SimaPro because LCSOFT has HTNC characterization factor of isoprene (estimated from Tool 2) which does not exist in SimaPro. The differences of HTC, ODP, and ET values from both software are considered to be insignificant since these values in the acceptable ranges.

**Table 4.7** Comparative results of bioethanol process between SimaPro and LCSOFT

Environmental impacts	Unit	SimaPro	LCSOFT	Sum squares error (SSE)	Percent difference (%)
Global Warming (GWP)	kg CO <sub>2</sub> eq.	7.29E-01	7.30E-01	2.0427E-06	-0.19
Acidification (AP)	H <sup>+</sup> moles eq.	6.46E-01	1.07E-01	0.29070047	83.50
Carcinogenics (HTC)	kg benzene eq.	8.65E-06	2.89E-07	6.9873E-11	96.65
Non carcinogenics (HTNC)	kg toluene eq.	1.44E+00	2.83E+00	1.90745627	-95.63
Ozone depletion (ODP)	kg CFC-11 eq.	4.09E-10	1.14E-10	8.6918E-20	72.06
Ecotoxicity (ET)	kg 2,4-D eq.	1.24E-03	6.20E-03	2.4535E-05	-397.99
photochemical oxidation (PCOP)	kg NO <sub>x</sub> eq.	2.40E-02	2.61E-02	4.4188E-06	-8.75