CHAPTER IV

RESULTS AND DISCUSSION

4.1 Calculation Model

There were 34 equations used to develop this LCA software (LCSoft). These equations could be divided into three main groups as follow: emission calculation model, energy and resource consumption model and environmental impact model. All equations are shown in Table 4.1. Detail for each equation is discussed further in the next section.

Table 4.1 Equations used to develop LCSoft

Emission calculation models	
Categories	Equation
Emission from raw material	CO_2 Emission = $\sum m_i \times EF_{CO2}$
	CO Emission = $\sum m_i \times EF_{CO}$
	SO_x Emission = $\sum m_i \times EF_{SOx}$
	NO_x Emission = $\sum m_i \times EF_{NOx}$
	N_2O Emission = $\sum m_i \times EF_{N2O}$
	CFC-11 Emission = $\sum m_i \times EF_{CFC-11}$
	HFC-134a Emission = $\sum m_i \times EF_{HFC-134a}$
	CH_4 Emission = $\sum m_i \times EF_{CH4}$
	NH_3 Emission = $\sum m_i \times EF_{NH3}$
	HCl Emission = $\sum m_i \times EF_{HCl}$
	HF Emission = $\sum m_i \times EF_{HF}$
	NMVOC Emission = $\sum m_i \times EF_{NMVOC}$
	PM_{10} Emission = $\sum m_i \times EF_{PM10}$
Emission from energy usage	Emission from coal base fuel = energy from coal × EF_x
	Emission from natural gas base fuel = energy from natural gas × EF_x
	Emission from petroleum base fuel = energy from petroleum fuel × EF_x
	Emission from other fuel = energy from fuel × EF_x
Emission from utility usage	Emission from hot utility = energy from hot utility × EF_x
	Emission from cold utility = quantity of cold utility × EFx
	Emission from electricity = energy from electricity × EFx

Table 4.1 Equations use to develop LCSoft (Cont'd)

Energy and fuel consumption models	
Categories	Equation
Energy and fuel consumption	$E_{total} = \sum$energy use in process
	Energy use per kg of product = $E_{total}/m_{Product}$
	Percent energy from renewable = $(E_{renew} \times 100)/E_{total}$
	Fuel use = energy use/Heating value
Environmental impact calculation models	
Categories	Equation
Carbon footprint	CO_2 equivalent = $m_{GHG} \times GWP$
	Carbon footprint = $\sum CO_2e$ in each activity
Impact assessment	Global warming = $\sum m_i \times GWP_i$
	Ozone depletion = $\sum m_i \times ODP_i$
	Acidification = $\sum m_i \times AP_i$
	Eutrophication = $\sum m_i \times EP_i$
	Photochemical smog = $\sum m_i \times POCP_i$
	Human toxicity = $\sum m_i \times HTP_i$
	Aquatic toxicity = $\sum m_i \times ATP_i$
	Terrestrial toxicity = $\sum m_i \times TTP_i$

4.1.1 Emission Calculation Model

4.1.1.1 Emission from Raw Material

This type of equation is used to calculate amount of pollutant that emitted from use of raw material in a chemical process. There are thirteen equations which are selected for each substance in this study.

Carbon dioxide emission

$$CO_2 \text{ emission from raw materials} = \sum_{i=1}^{n} m_i \times EF_{CO2,i} \quad (4.1)$$

Where

m_i = mass of material i input

$EF_{CO2,i}$ = CO_2 emission factor of material i

Carbon monoxide emission equation

Carbon monoxide emission equation

$$\text{CO emission from raw materials} = \sum_{i=1}^{n} m_i \times EF_{CO,i} \quad (4.2)$$

where

m_i = mass of material i input

$EF_{CO,i}$ = CO emission factor of material i

Sulfur oxide emission equation

$$SO_x \text{ emission from raw materials} = \sum_{i=1}^{n} m_i \times EF_{SOx,i} \quad (4.3)$$

where

m_i = mass of material i input

$EF_{Sox,i}$ = SO_x emission factor of material i

Nitrogen oxide emission equation

$$NO_x \text{ emission from raw materials} = \sum_{i=1}^{n} m_i \times EF_{NOx,i} \quad (4.4)$$

where

m_i = mass of material i input

$EF_{NOx,i}$ = NO_x emission factor of material i

Nitrous oxide emission equation

$$N_2O \text{ emission from raw materials} = \sum_{i=1}^{n} m_i \times EF_{N2O,i} \quad (4.5)$$

where

m_i = mass of material i input

$EF_{N2O,i}$ = N_2O emission factor of material i

CFC-11 emission equation

$$\text{CFC-11 emission from raw materials} = \sum_{i=1}^{n} m_i \times EF_{CFC-11,i} \quad (4.6)$$

where

m_i = mass of material i input

$EF_{CFC-11,i}$ = CFC-11 emission factor of material i

HFC-134a emission equation

$$\text{HFC-134a emission from raw materials} = \sum_{i=1}^{n} m_i \times EF_{HFC-134a,i} \quad (4.7)$$

where

m_i = mass of material i input

$EF_{HFC-134a,i}$ = HFC-134a emission factor of material i

Methane emission equation

$$CH_4 \text{ emission from raw materials} = \sum_{i=1}^{n} m_i \times EF_{CH4,i} \quad (4.8)$$

where

m_i = mass of material i input

$EF_{CH4,i}$ = CH_4 emission factor of material i

Ammonia emission equation

$$NH_3 \text{ emission from raw materials} = \sum_{i=1}^{n} m_i \times EF_{NH3,i} \quad (4.9)$$

where

m_i = mass of material i input

$EF_{NH3,i}$ = NH_3 emission factor of material i

Hydrochloric acid emission equation

$$\text{HCl emission from raw materials} = \sum_{i=1}^{n} m_i \times EF_{HCl,i} \qquad (4.10)$$

where

m_i = mass of material i input

$EF_{HCl,i}$ = HCl emission factor of material i

Hydrofluoric acid emission equation

$$\text{HF emission from raw materials} = \sum_{i=1}^{n} m_i \times EF_{HF,i} \qquad (4.11)$$

where

m_i = mass of material i input

$EF_{HF,i}$ = HF emission factor of material i

Non-methane volatile organic compound emission equation

$$\text{NMVOC emission from raw materials} = \sum_{i=1}^{n} m_i \times EF_{NMVOC,i} \qquad (4.12)$$

where

m_i = mass of material i input

$EF_{NMVOC,i}$ = NMVOC emission factor of material i

Particulate matter emission equation

$$PM_{10}\text{ emission from raw materials} = \sum_{i=1}^{n} m_i \times EF_{PM10,i} \qquad (4.13)$$

where

m_i = mass of material i input

$EF_{PM10,i}$ = PM_{10} emission factor of material i

4.1.1.2 Emission from Utility

These equations used to calculate emission of pollutant from use of utility in this case is steam, cooling water and electricity. Steam and electricity which are generated from co-generation process are not included in the first version of LCSoft because there is no database for co-generation process in the first version.

Emission from electricity equation

$$\text{Emission of substance x from electricity} = \text{kWh} \times EF_x \quad (4.14)$$

where

kWh = unit of electricity use

EF_x = emission factor of substance x per unit electricity generated

Note: x is cover three substances which are CO_2, CH_4 and N_2O

Emission from steam equation

$$\text{Emission of substance x from steam} = E_{steam} \times EF_x \quad (4.15)$$

where

E_{steam} = energy from steam

EF_x = emission factor of substance x per unit energy

Note: x is cover three substances which are CO_2, CH_4 and N_2O

Emission from cooling water equation

$$\text{Emission of substance x from cooling water} = m_{cooling\ water} \times EF_x \quad (4.16)$$

where

$m_{cooling\ water}$ = mass of cooling water

EF_x = emission factor of substance x per unit mass of cooling water

Note: x is cover three substances which are CO_2, CH_4 and N_2O

4.1.1.3 Emission from Energy

LCSoft contain equation to calculate emission substance from energy for three main type of fuel including

- Petroleum base fuel such as diesel, LPG, fuel oil, etc.
- Coal base fuel such as lignite, anthracite, bituminous coal, etc.
- Natural gas base fuel

Equation to calculate emission from energy are shown in equation 4.17 - 4.19

Emission of energy from petroleum base fuel

$$\text{Emission of substance x from petroleum base fuel} = E_{petroleum} \times EF_x \quad (4.17)$$

where

$E_{petroluem}$ = energy from petroleum base fuel (GJ)

EF_x = emission factor of substance x per unit energy of petroleum fuel

Note: x is cover three substances which are CO_2, CH_4 and N_2O

Emission of energy from coal base fuel

$$\text{Emission of substance x from coal base fuel} = E_{coal} \times EF_x \quad (4.18)$$

where

E_{coal} = energy from coal base fuel (GJ)

EF_x = emission factor of substance x per unit energy of coal

Note: x is cover three substances which are CO_2, CH_4 and N_2O

Emission of energy from coal base fuel

$$\text{Emission of substance x from natural gas base fuel} = E_{nat.gas} \times EF_x \qquad (4.19)$$

where

$E_{nat.gas}$ = energy from natural gas base fuel (GJ)

EF_x = emission factor of substance x per unit energy of natural gas

Note: x is cover three substances which are CO_2, CH_4 and N_2O

Emission of energy from other fuel

$$\text{Emission of substance x from other fuel} = E_{fi} \times EF_x \qquad (4.20)$$

where

E_{fi} = energy from fuel i (GJ)

EF_x = emission factor of substance x per unit energy of fuel i

Note: x is cover three substances which are CO_2, CH_4 and N_2O, other fuels in LCSoft are tire derived fuel, waste oil blended with residual fuel oil, waste oil blended with distillate fuel oil and municipal solid waste.

4.1.2 Energy and Fuel Consumption Model

Energy and fuel consumption model is requiring to estimate quantity of energy and fuel use in the process. This model including four equations as follow.

Fuel use estimation equation

$$\text{Quantity of fuel use} = \frac{\text{Energy use}_i}{\text{Heating value of fuel i}} \qquad (4.21)$$

Total energy consumption model

$$E_{process} = \sum \text{energy use in process} \quad (4.22)$$

where

$E_{process}$ = Total energy consumption of the process

Energy consumption for product

$$E_{product,i} = E_{process}/m_{product,i} \quad (4.23)$$

where

$E_{product,i}$ = Energy consumption per unit mass of product i

$m_{product,i}$ = Total mass of product i

Percentage energy from renewable

$$\text{Percentage energy from renewable } (\%E_{renew}) = (E_{renew}/E_{process}) \times 100 \quad (4.24)$$

where

E_{renew} = Total energy from renewable source use in process

4.1.3 Environmental Impact Model

4.1.3.1 Carbon Footprint Estimation

In order to estimate carbon footprint of the entire process, all of greenhouse gas emitted from each step in the chemical process must be converted to carbon dioxide equivalent (CO_2 eq.) by using global warming potential factor. After greenhouse gas conversion, summation of CO_2 eq. in each step must be done to complete carbon footprint estimation of the process. Equation 4.24 and 4.25 were used in this calculation.

Greenhouse gas conversion

$$CO_2\ eq. = m_{GHG} \times GWP_i \qquad (4.25)$$

where

CO_2 eq.= carbon dioxide equivalent

m_{GHG} = mass of greenhouse gas

GWP_i = characterization factor for global warming of greenhouse gas

Carbon dioxide emitted from each step

$$\text{Carbon footprint of each step} = \sum CO_2e \text{ from each equipment/activity} \qquad (4.26)$$

4.1.3.2 Environmental Impact Assessment

Eight categories of environmental impact were selected to implement software in this study. This model will give the final results which are impact indicators of eight impact categories including global warming, ozone depletion, photochemical formation, acidification, eutrophication, human toxicity, aquatic toxicity and terrestrial toxicity. Equations 4.27 - 4.34 represent impact assessment calculation for each impact categories

Global warming

$$\text{Global warming} = \sum m_i \times GWP_i \qquad (4.27)$$

where

m_i = mass of greenhouse gas i (kg)

GWP_i = Characterization factor for global warming of greenhouse gas (kg CO_2 eq./kg i)

Ozone depletion

$$\text{Ozone depletion} = \sum m_i \times ODP_i \quad (4.28)$$

where

m_i = mass of ozone depletion substance i (kg)

ODP_i = Characterization factor for ozone depletion substance i (kg CFC-11 eq./kg i)

Acidification

$$\text{Acidification} = \sum m_i \times AP_i \quad (4.29)$$

where

m_i = mass of acidify substance i (kg)

AP_i = Characterization factor for acidify substance i (kg SO_2 eq./kg i)

Eutrophication

$$\text{Eutrophication} = \sum m_i \times EP_i \quad (4.30)$$

where

m_i = mass of nutrient enrichment substance i (kg)

EP_i = Characterization factor for nutrient substance i (kg PO_4 eq./kg i)

Photochemical formation

$$\text{Photochemical ozone formation} = \sum m_i \times POCP_i \qquad (4.31)$$

where

m_i = mass of photochemical oxidant substance i (kg)

$POCP_i$ = Characterization factor for photochemical oxidant substance i (kg C_2H_4 eq./kg i)

Human toxicity

$$\text{Human toxicity} = \sum m_i \times HTP_i \qquad (4.32)$$

where

m_i = mass of toxic substance i (kg)

HTP_i = Characterization factor for toxic substance i (kg 1,4-dichlorobenzene eq./kg i)

Fresh water aquatic toxicity

$$\text{Fresh water aquatic toxicity} = \sum m_i \times ATP_i \qquad (4.33)$$

where

m_i = mass of toxic substance i (kg)

ATP_i = Characterization factor for toxic substance i (kg 1,4-dichlorobenzene eq./kg i)

Terrestrial toxicity

$$\text{Terrestrial toxicity} = \sum m_i \times TTP_i \qquad (4.34)$$

where

m_i = mass of toxic substance (kg)

TTP_i = Characterization factor for toxic substance i

(kg 1,4-dichlorobenzene eq./kg i)

4.2 Software Design

4.2.1 Software Architecture

Software architecture is the first task for software design and development. This architecture is used as a base structure of LCSoft. In addition, an overview of LCSoft software architecture is presented in Figure 4.1.

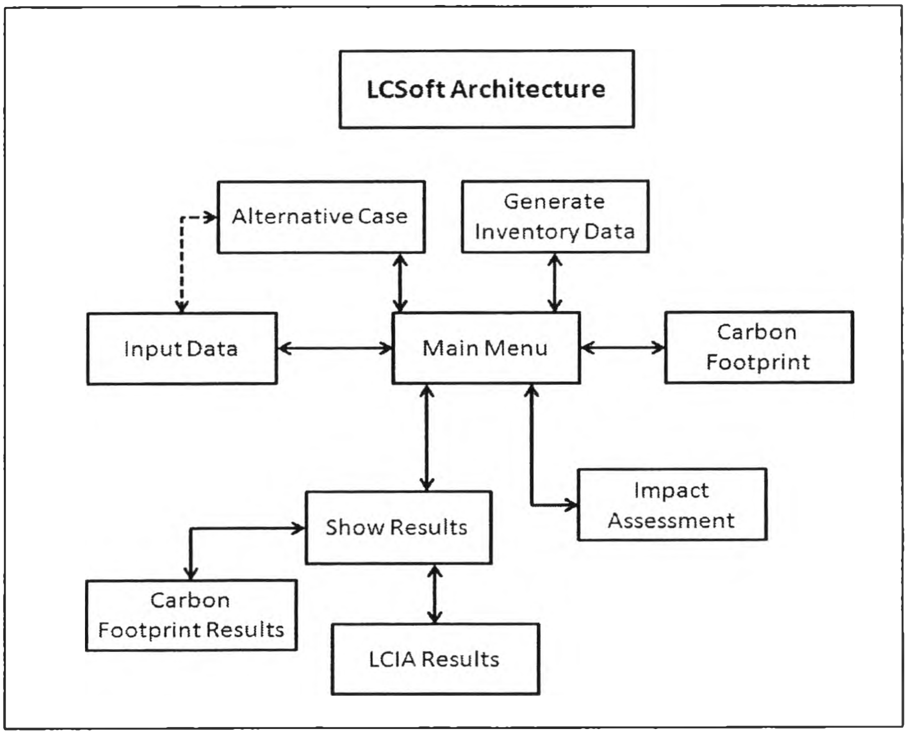


Figure 4.1 LCSoft architecture.

Software architecture is like a map of the software that show how each feature in the software link to another. The software architecture of LCSoft has 6 main sections excluding main menu as described below.

4.2.1.1 Input Data

This section will contain user interface for input all necessary data such as stream table, equipment table, fuel type, etc. to the software. After input all required data user can go back to main menu section to move further in other section

4.2.1.2 Generate Inventory Data

The third section is "generate inventory data". In this section LCSoft will show inventory data of the designed process by calculate inventory data using data from "input data" section and data base of this software. Data tabulate in this section are quantity of chemical in input/output streams, quantity of emitted substance, fuel consumption, total energy consumption and energy consumption for product.

4.2.1.3 Carbon Footprint

Before perform carbon footprint estimation of the process, user must come to this section to define the type of equipment and utility used in each equipment and then LCSoft can perform carbon footprint estimation.

4.2.1.4 Impact Assessment

This section serves the same purpose as carbon footprint section but impact assessment will give results of impact indicator of the process instead of carbon footprint.

4.2.1.5 Carbon Footprint Results

From main menu user can view the carbon footprint of the entire process by access to this section

4.2.1.6 LCIA Results

User can view environmental impact of the process by access to this section

4.2.2 Activity Diagram

The activity diagram that highlights the work flow and data flow is presented in Figure 4.2. As shown in this figure, the calculation procedure consists of six main steps, including: input data step, emission calculation step, energy consumption step, resource consumption step, carbon footprint step and lastly impact assessment step. Description of each step in calculation procedure is on page 35. The calculation procedure has been validated by hand calculation (see the calculation in Appendix C) using acetaldehyde production process as a case study (see detail in Appendix B). The results from hand calculation were further used in the software validation step to compare with the results obtained from LCSoft (Section 4.4).

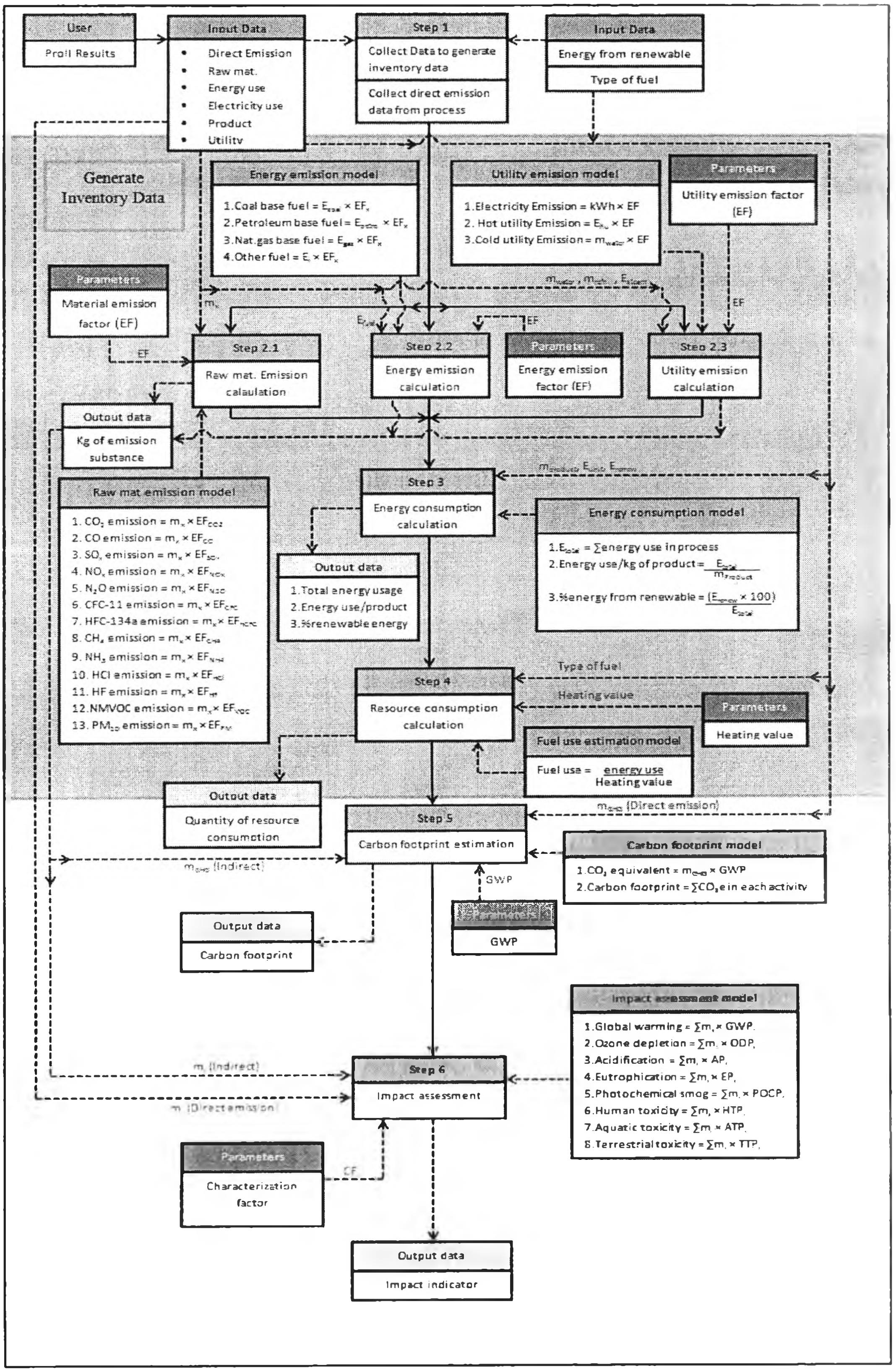


Figure 4.2 Activity diagram of LCSoft.

Step 1 Collect data

In this step all necessary data that require for calculation process will be input by user. This data including direct pollutant emission from the process to use it directly for LCIA

Step 2.1 Emission from raw material calculations

This step will calculate pollutant emission from input chemicals by using emission factor from database and mass balance from ProII result.

Step 2.2 Emission from energy calculations

This step will calculate pollutant emission from the use (combustion) of fuel in the process by using energy consumption results from ProII than multiply by its emission factor to obtain the quantity of pollutant.

Step 2.3 Emission from utility calculations

This step will calculate pollutant emission from utility usage by using emission factor from database and utility usage data from ProII result.

Step 3 Energy consumption calculations

This step will calculate total energy consumption of the entire process by summation of energy use in each unit (boiler, flash drum, reactor etc.). This step also calculates energy use per kg of product and percentage energy from renewable.

Step 4 Resource consumption calculations

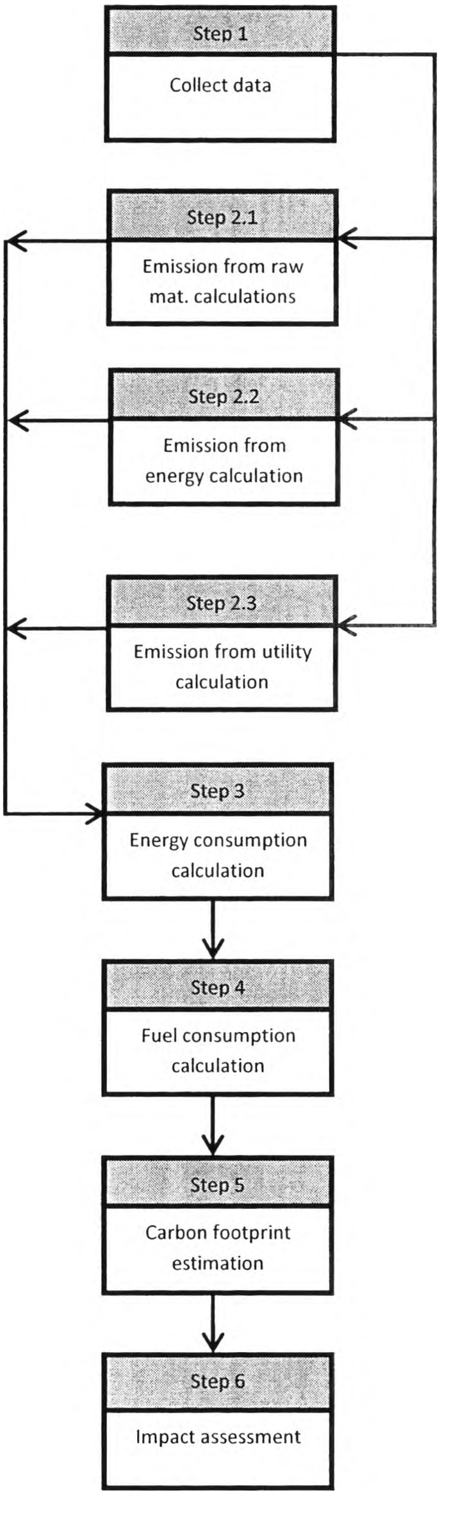
The results from step 3 will be one of data input to this step to calculate quantity of resource use to generate energy for the process.

Step 5 Carbon footprint estimation

Greenhouse gas emit from each unit operation (both direct and indirect) in the process will be convert into CO_2 equivalent in this step to show which step of the process that can generate CO_2.

Step 6 Impact assessment

Use the results from step 2.1, 2.2 and 2.3 and direct emission data to calculate environmental impact of the process the final results will be the impact indicator for each impact category.



4.3 LCSoft Development

LCSoft was developed by VBA which consisted of 20 EXCEL worksheets, the main menu and input data interface were presented in sheets 1-2, while sheets 3-5 were used to define product, hot/cold utility and stream name. Inventory data were shown in sheet 6, while sheets 7 and 8 showed the results of carbon footprint and impact assessment, respectively. The remaining twelve sheets represented the database contained in the software. Figure 3 illustrated the input data interface of LCSoft. This section contains screenshots of LCSoft, showing the way to insert the required data, the different calculation steps and the result section. Full manual for LCSoft is in Appendix A.

4.3.1 Main Menu

The main menu page is presented in one Excel sheet (see Figure 4.3). In this page, there are 5 buttons:

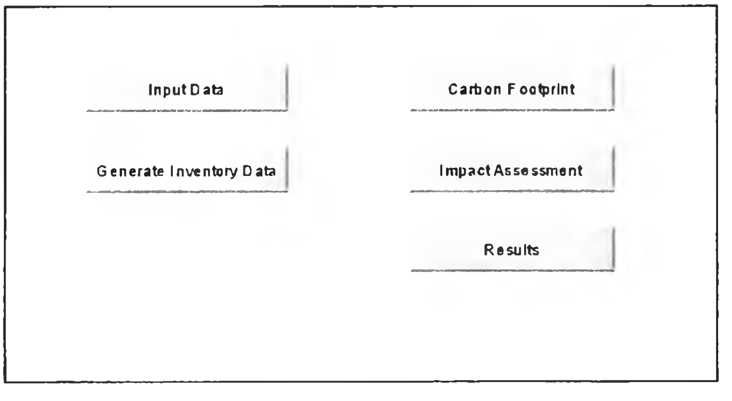


Figure 4.3 Main menu interface.

4.3.1.1 Input Data Button

To force user to input all required data first, this button will be the only button that enable when start up LCSoft. By clicking this button, user will access to input data page to input required data to the software

4.3.1.2 Generate Inventory Data Button

This button will enable after all required data has been input to the program. When click, LCSoft will read information of the process from imported stream table and equipment table and access to "Generate inventory data" page.

4.3.1.3 Carbon Footprint Button

User can start carbon footprint estimation by clicking this button. This button will enable after generate inventory data has been done.

4.3.1.4 Carbon Footprint Button

To calculate environmental impact user must click this button. This button will enable after generate inventory data has been done.

4.3.1.5 Results Button

User can view the results of both carbon footprint and impact assessment by access to "view result" form via this button.

4.3.2 Input Data

Input data page is shown in Figure 4.4. The following data are required to input into the software: stream table of designed process from PROII, equipment table of designed process from PROII, input-output stream name, quantity and type of hot/cold utility, product and/or by product's name, fuel type, location and quantity of renewable energy.

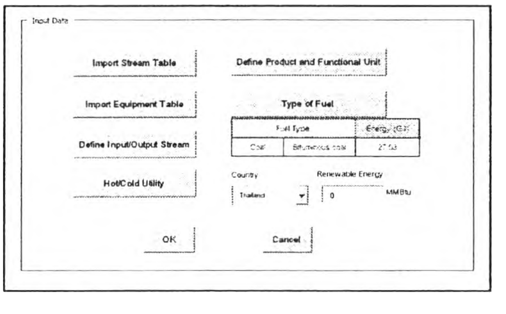


Figure 4.4 Input data interface.

4.3.2.1 Import Stream Table Button

Import stream table by call "import" form with this button

4.3.2.2 Import Equipment Table Button

Import equipment table by call "import" form with this button

4.3.2.3 Define Input/Output Stream Button

By clicking this button, LCSoft will bring user to define stream page (see Figure 4.5) in this page user must define stream name for input stream, output stream to soil, output stream to air, output stream to air and product stream manually.

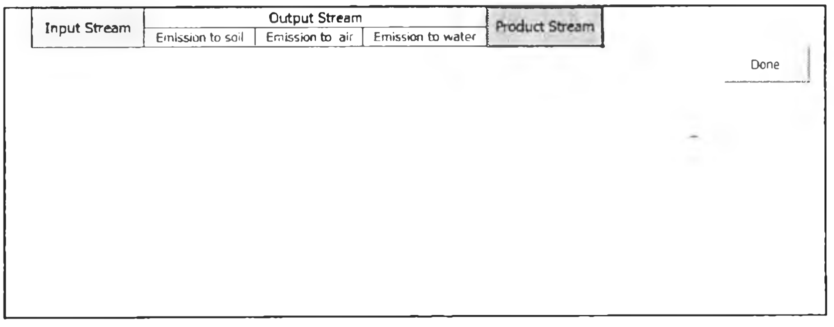


Figure 4.5 Define input/output stream page.

4.3.2.4 Hot/Cold Utility Button

This button use for define type and quantity of hot and cold utility by access to utility entry page. Utility entry page is shown in Figure 4.6.

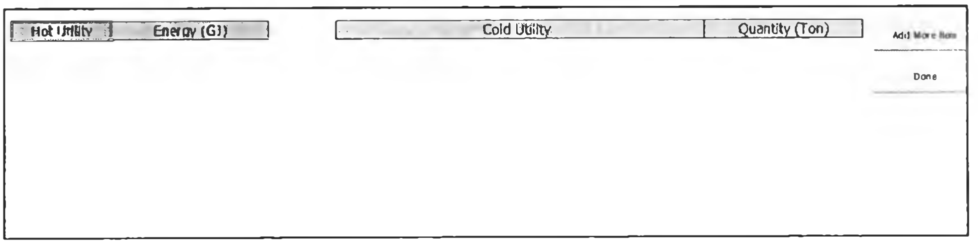


Figure 4.6 Utility entry page.

When access to utility entry page, “Utility entry” form will populate to help user to define hot and cold utility. Type of hot and cold utility available in LCSoft are steam and cooling water but user can flexibly add more database later. Utility entry form is shown in Figure 4.7.

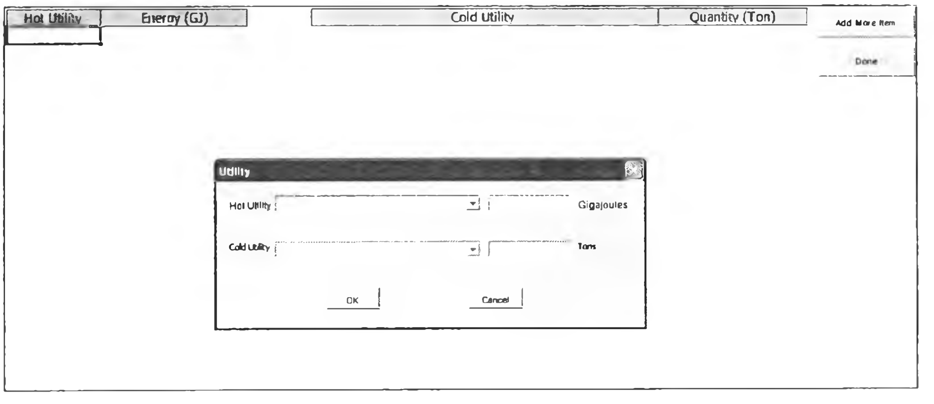


Figure 4.7 Utility entry form.

4.3.2.5 Define Product and Functional Unit Button

After import stream table and define stream LCSoft will read all chemical name from stream table and automatically put it into combo box in “Define product and functional unit” page (see Figure 4.8) so user can choose product name from the combo box. For by product, user can define it by clicking “Add by product” button to call “Add by product” form as shown in Figure 4.9.

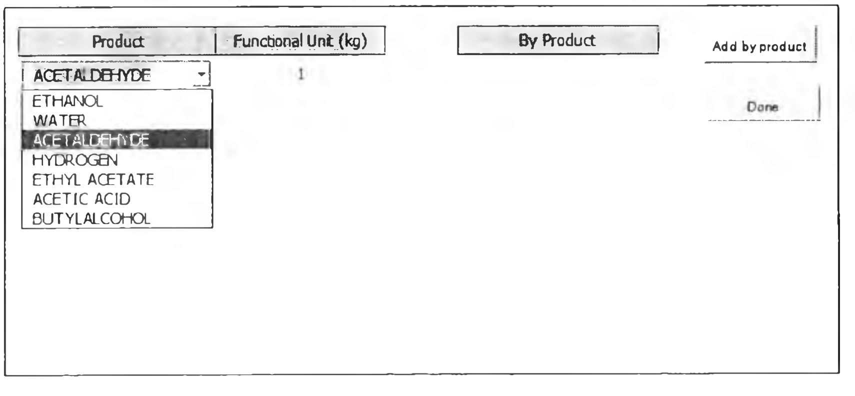


Figure 4.8 Define product and functional unit page.

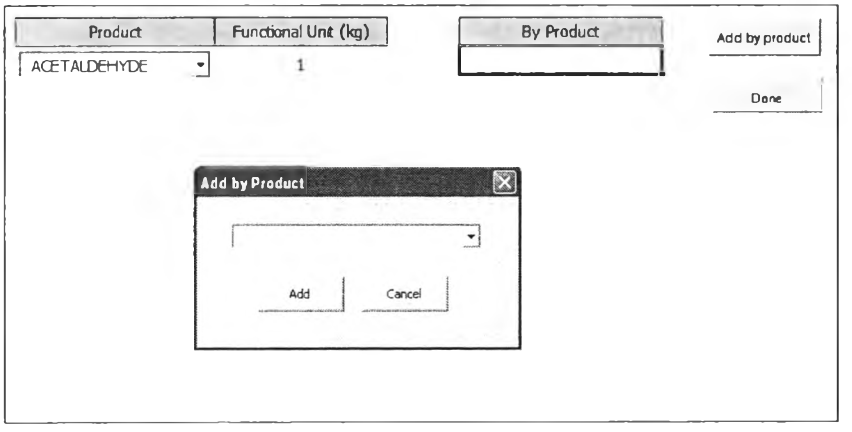


Figure 4.9 Add by product form.

4.3.2.6 Type of Fuel Button

By clicking this button LCSoft will call "Fuel use" form as shown in Figure 4.10 to help user define type and energy of fuel used in the process.

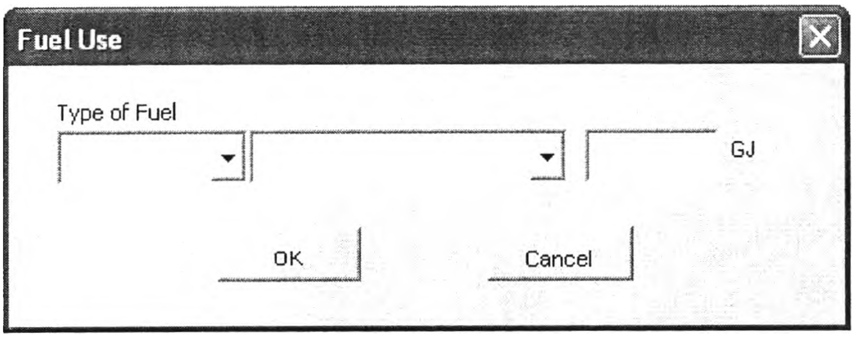


Figure 4.10 Fuel use form.

4.3.2.7 Combo Box Country

This combo box contain list of country for user to choose. This data is required for calculate emission from electricity.

4.3.2.8 Renewable Energy Text Box

This area is available for user to specify energy from renewable used in the process.

4.3.3 Generate Inventory Data

From main menu interface user can access to generate inventory data page after input all required data in input data section. By clicking "Generate inventory data" button on main menu interface, LCSoft will read data from stream table and show it in inventory data page as shown in Figure 4.11.

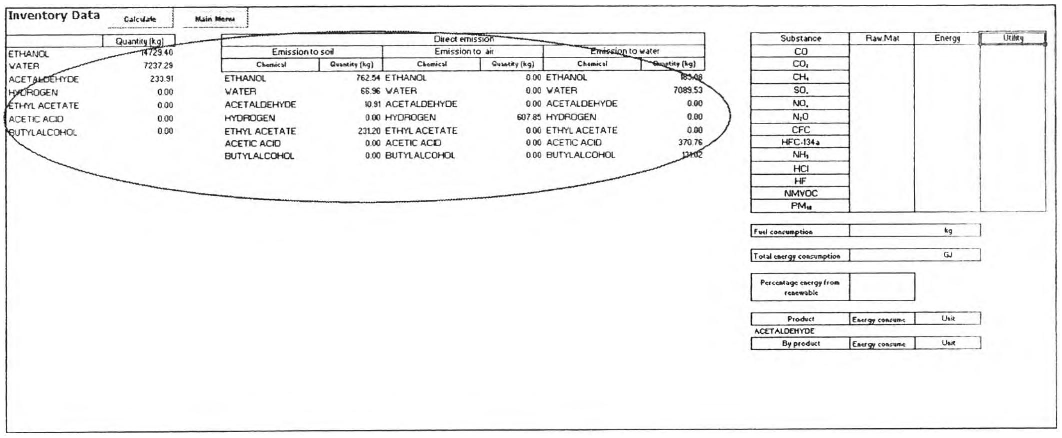


Figure 4.11 Input/Output data show in inventory data page.

To calculate inventory data, click the "Calculate" button on the top left of the page. After clicking, the calculated inventory data will show on the right (see Figure 4.12).

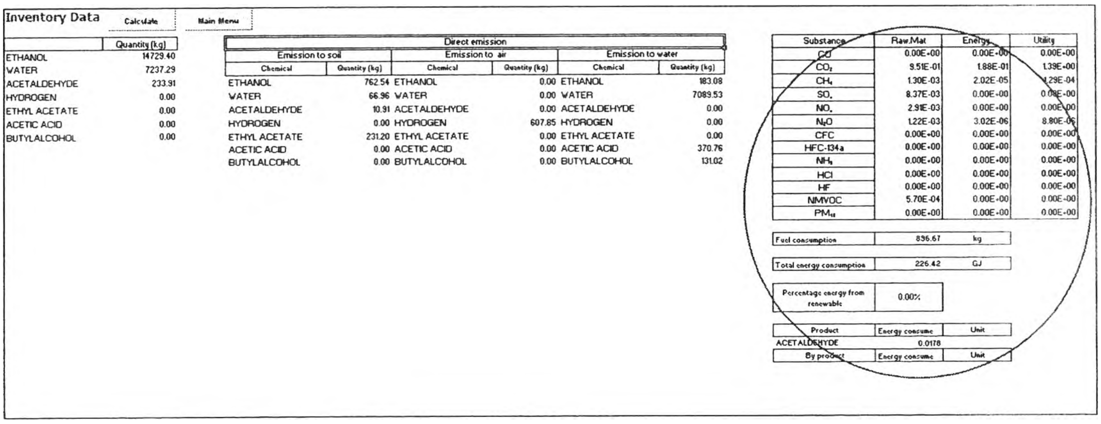


Figure 4.12 Inventory data.

4.3.4 Carbon Footprint

In order to do carbon footprint estimation user must define activity and energy source in each equipment in the process. As shown in Figure 4.13 three main buttons in this page use for carbon footprint estimation are:

4.3.4.1 Import Equipment Name Button

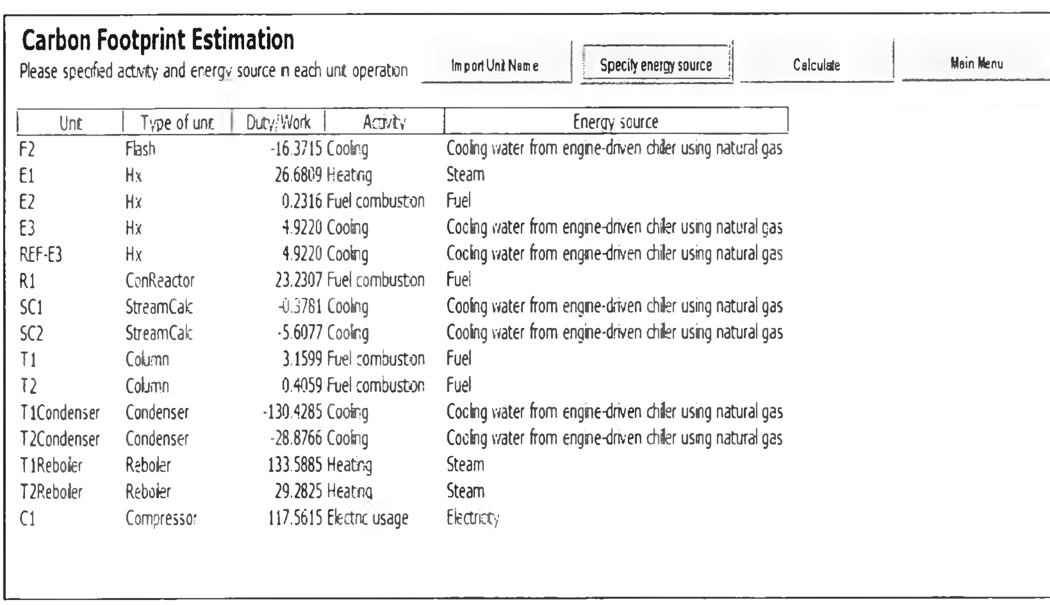
This button use for read type and name of equipment from equipment table.

4.3.4.2 Specify Energy Source Button

This button use for specify activity and energy source in each equipment.

4.3.4.3 Calculate Button

Start calculation for carbon footprint via this button. Results from this calculation will show in result section.


Carbon Footprint Estimation

Please specified activity and energy source in each unit operation

Import Unit Name | Specify energy source | Calculate | Main Menu

Unit	Type of unit	Duty/Work	Activity	Energy source
F2	Flash	-16.3715	Cooling	Cooling water from engine-driven chiller using natural gas
E1	Hx	26.6809	Heating	Steam
E2	Hx	0.2316	Fuel combustion	Fuel
E3	Hx	-4.9220	Cooling	Cooling water from engine-driven chiller using natural gas
REF-E3	Hx	4.9220	Cooling	Cooling water from engine-driven chiller using natural gas
R1	ConReactor	23.2307	Fuel combustion	Fuel
SC1	StreamCalc	-0.3781	Cooling	Cooling water from engine-driven chiller using natural gas
SC2	StreamCalc	-5.6077	Cooling	Cooling water from engine-driven chiller using natural gas
T1	Column	3.1599	Fuel combustion	Fuel
T2	Column	0.4059	Fuel combustion	Fuel
T1Condenser	Condenser	-130.4285	Cooling	Cooling water from engine-driven chiller using natural gas
T2Condenser	Condenser	-28.8766	Cooling	Cooling water from engine-driven chiller using natural gas
T1Reboiler	Reboiler	133.5885	Heating	Steam
T2Reboiler	Reboiler	29.2825	Heating	Steam
C1	Compressor	117.5615	Electric usage	Electricity

Figure 4.13 Carbon footprint estimation page.

4.3.5 Impact Assessment

By clicking "Impact Assessment" on main menu page, LCSoft will start to calculate environmental impact and move to "LCIA Results" section automatically.

4.3.6 Results

On the main menu page user can go to result page by clicking "Results" button. After click, LCSoft will call "Results" form for user to choose which result the user wants to see. "Results" form is shown in Figure 4.14.

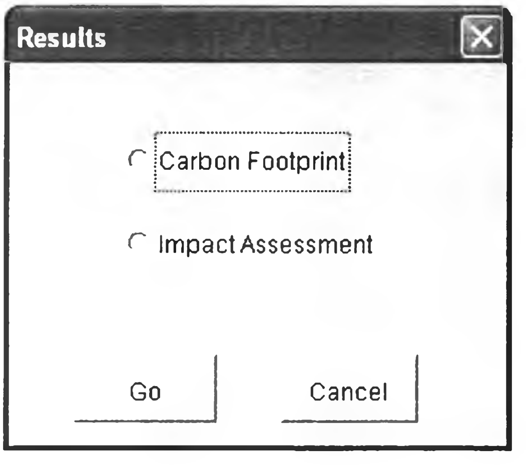


Figure 4.14 Results form.

4.3.6.1 Carbon Footprint Result

This page can access from "Results" form to see carbon footprint result (see Figure 4.15).

4.3.6.2 Environmental Impact Result

This page can access from "Results" form to see impact assessment result (see Figure 4.16).

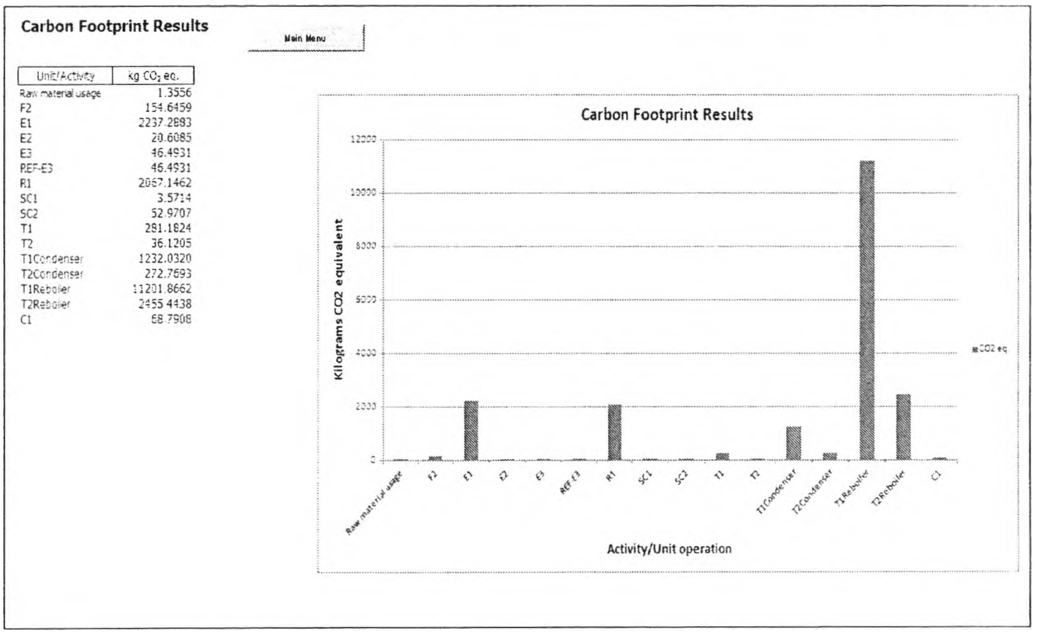


Figure 4.15 Carbon footprint result.

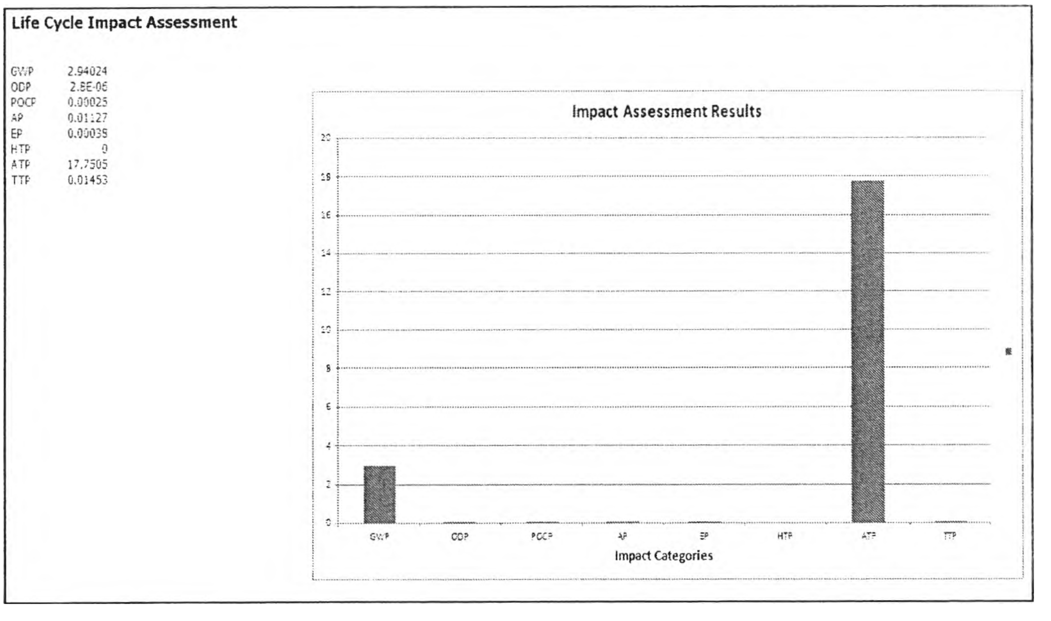


Figure 4.16 Impact assessment results.

4.4 Validation

The software was validated by using acetaldehyde production process. This process was originally created in simulation course year 2010 of the Petroleum and Petrochemical College (PPC) by using PROII simulation program. The process flowsheet is shown in Figure 4.17. By applying LCSoft to perform LCA on this case study, the results obtained from LCSoft were compared with the results from hand-calculation which used the same calculation procedure developed in previous part as shown in activity diagram. The comparison was done for inventory data, carbon footprint result and life cycle impact assessment result, in addition, the result of LCSoft was also compared with the result run by commercial LCA software SimaPro as shown in section 4.4.4.

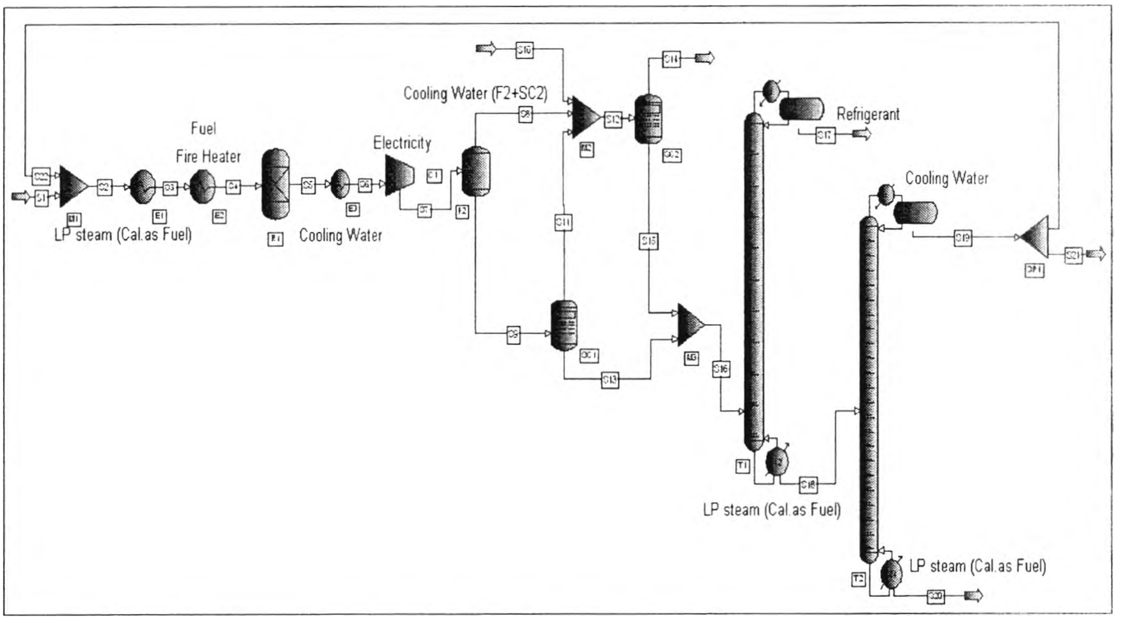


Figure 4.17 Acetaldehyde production process flowsheet.

4.4.1 Comparative Inventory Data

Table 4.2 Comparative emission from raw material of acetaldehyde process between hand calculation and LCSoft

Substance	LCSoft (kg/kg product)	Hand calculation* (kg/kg product)
CO	0	0
CO_2	0.951	0.951
CH_4	1.30E-03	1.30E-03
SO_x	8.37E-03	7.24E-03
NO_x	2.91E-03	2.51E-03
N_2O	1.22E-03	1.22E-03
CFC	0	0
HFC-134a	0	0
NH_3	0	0
HCl	0	0
HF	0	0
NMVOC	5.70E-04	4.93E-04
PM_{10}	0	0

From Table 4.2, it can be noted that LCSoft gives similar values to those obtained by hand calculations except value of sulfur oxide, nitrogen oxide and non-methane volatile organic compound. This is due to LCSoft calculation has included both water input (stream S10) and contaminating water in ethanol (Stream S1). On the other hand, hand calculation concerns only water input stream (S10).

Tables 4.3 - 4.7 represent comparison of emission from energy, emission from utility, total energy consumption, energy consumption for product and fuel consumption respectively. As shown in these tables there are insignificantly different between results from LCSoft and hand-calculation. These results show that LCSoft can give the correct results of emissions from energy and utility, total energy consumption, energy consumption for product and fuel consumption.

Table 4.3 Comparative emission from energy of acetaldehyde process between hand calculation and LCSoft

Substance	LCSoft (kg/kg product)	Hand calculation* (kg/kg product)
CO	0	0
CO_2	0.188	0.188
CH_4	2.02E-05	2.02E-05
SO_x	0	0
NO_x	0	0
N_2O	3.02E-06	3.02E-06
CFC	0	0
HFC-134a	0	0
NH_3	0	0
HCl	0	0
HF	0	0
NMVOC	0	0
PM_{10}	0	0

Table 4.4 Comparative emission from utility of acetaldehyde process between hand calculation and LCSoft

Substance	LCSoft (kg/kg product)	Hand calculation* (kg/kg product)
CO	0	0
CO_2	1.390	1.390
CH_4	1.29E-04	1.29E-04
SO_x	0	0
NO_x	0	0
N_2O	8.80E-06	8.78E-06
CFC	0	0
HFC-134a	0	0
NH_3	0	0
HCl	0	0
HF	0	0
NMVOC	0	0
PM_{10}	0	0

Table 4.5 Comparative total energy consumption of acetaldehyde process between hand calculation and LCSoft

LCSoft (GJ)	Hand calculation* (GJ)
226.42	226.43

Table 4.6 Comparative energy consumption for product of acetaldehyde process between hand calculation and LCSoft

LCSoft (GJ/kg)	Hand calculation* (GJ/kg)
0.0178	0.0178

Table 4.7 Comparative fuel consumption of acetaldehyde process between hand calculation and LCSoft

LCSoft (kg)	Hand calculation* (kg)
896.67	896.67

4.4.2 Comparative Carbon Footprint Results

This validation was also extended to the carbon footprint calculations for the acetaldehyde production process. The result is shown in Table 4.8. From this table, LCSoft gives a close approximate carbon footprint value with hand calculation so it is shown that LCSoft has worked properly to give correct calculations for carbon footprint.

Table 4.8 Comparative carbon footprint of acetaldehyde process between hand calculation and LCSoft

Unit/Activity	kg CO2 eq.	
	LCSoft	Hand calculation*
Raw material usage	1.3556	1.3557
F2	0.0122	0.0122
E1	0.1761	0.1757
E2	0.0016	0.0016
E3	0.0037	0.0037
REF-E3	0.0037	0.0037
R1	0.1627	0.163
SC1	0.0003	2.81E-04
SC2	0.0042	4.17E-03
T1	0.0221	0.0221
T2	0.0028	2.84E-03
T1Condenser	0.0970	0.097
T2Condenser	0.0215	0.0215
T1Reboiler	0.8818	0.8816
T2Reboiler	0.1933	0.1933
C1	0.0054	0.0054

4.4.3 Comparative Impact Assessment Results

Comparison of environmental assessment results between LCSoft and hand-calculation is shown in Table 4.9 below.

Table 4.9 Comparative impact assessment of acetaldehyde process between hand calculation and LCSoft

Impact categories	LCSoft	Hand calculation*
GWP	2.94	2.94
ODP	0.00000285	0.00000285
POCP	0.000246	0.000247
AP	0.011269	0.011269
EP	0.000378	0.000378
HTP	0	0.00
ATP	17.75	17.74
TTP	0.0145	0.0145

The comparison shows that the results from both methods are identical. That means LCSoft can work properly and give the final results of carbon footprint and impact indicator for each impact category.
*Calculation data is shown in appendix C.

4.4.4 SimaPro Comparison

This comparison was done by using bio-ethanol process which far more complicated than acetaldehyde process as a case study. This process was originally created by Mr. Patharutama Nidhinandana in 2012 as a part of his thesis work at PPC. The comparison results are shown in Table 4.10.

Table 4.10 Comparative results of bioethanol process between SimaPro and LCSoft

Impact categories	SimaPro	LCSoft	Percent Difference
Global warming (GWP100)	3.69E+00	3.51E+00	4.79%
Ozone layer depletion	1.17E-08	1.09E-08	6.51%
Human toxicity	1.96E-02	9.25E-03	52.68%
Fresh water aquatic toxicity	1.08E-03	1.31E-03	-21.09%
Terrestrial toxicity	5.27E-05	6.88E-05	-30.56%
Photochemical oxidation	7.26E-03	8.32E-03	-14.61%
Acidification	2.80E-03	1.33E-03	52.51%
Eutrophication	3.59E-03	1.89E-03	47.37%

As we can see from the table, there are some differences between the results from SimaPro and LCSoft. These differences occur because both programs use difference databases. SimaPro has a large database that can generate an inventory data of many substances because database of SimaPro contain a lot of emission factors while LCSoft has a database covering just thirteen substances. Therefore, inventory data generated from SimaPro contain a lot more chemical emissions than inventory data generated from LCSoft. Consequently, this effect results in the difference between impact indicator values of SimaPro and those of LCSoft, even both softwares use the same database of characterization factors.

Moreover, for human toxicity, SimaPro has a database covering toxic emitted from all three sources which are air, soil and water, whereas LCSoft is limitted only toxic substance emitted to air. As a result, human toxicity value from SimaPro is much higher than the value obtained from LCSoft. For freshwater aquatic toxicity and terrestrial toxicity, LCSoft has a database that contains characterization factor of more than 3500 toxic substances obtained from Simplebox 3.0 (Den Hollander et al., (2003), EUSES (1996), USES-LCA (Huijbregts et al., 2000)) and these parameters are still different from the parameters in SimaPro. Since this bio-ethanol process is the fermentation process, the main waste released from this process is wastewater. For SimaPro, the water that is released to environmental has affect both acidification and eutrophication. This means that SimaPro has a characterization factor of water for these two impact categories. However, due to the current limitation of the first version of our nearly developed software, there is no characterization factor of water for acidification and eutrophication in case of LCSoft. That is why both acidification potential and eutrophication potential from these two software are different.