CHAPTER IV
RESULTS AND DISSCUSSION

4.1 Development of Life Cycle Inventory Calculation Function

Life Cycle Inventory calculation was developed for compiling and quantifying input and output (e.g. natural resources, raw materials, emissions, and wastes) of given product corresponding to all relevant processes within the system boundary based on model given in Table 4.14. In Table 4.14, "A" represents the technology matrix that contains commodity flow of all processes. Inflow and outflow are noted by positive and negative values, respectively. "B" represents the intervention matrix that contains chemical substances, natural resources, or energy emitted or consumed by processes, while, "s" is a scaling factor that is used to scale up the unit processes in the technology matrix to the achieve target value defined by a functional unit. In order to validate LCI calculation function, case study of acetic acid, 98 % in H_2O production at plant - RER (Althaus *et al.*, 2007) was used to calculate LCI from cradle-to-gate by using LCSoft and commercial LCA software, SimaPro7.1. Comparison of LCI results was done by using ratio analysis as shown in Figure 4.1. The horizontal axis indicates the elementary flow considered and the vertical axis represents the ratio of LCI results of LCSoft to SimaPro7.1. Figure 4.1 shows the ratio of LCI results, of LCSoft to SimaPro7.1, that distribute around 1. The results indicate the very good match of LCI results from both LCSoft and SimaPro7.1. Table A1 shows LCI calculated from 2 software including elementary names and their values. Therefore, accurate LCI results could be achieved by using LCSoft compared to commercial LCA software, SimaPro7.1.

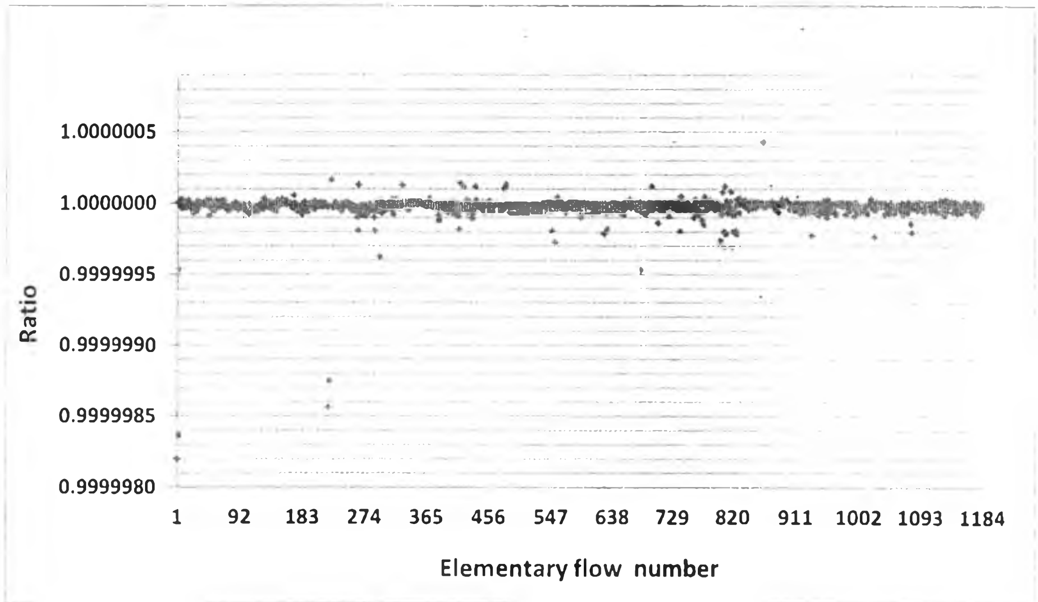

Figure 4.1 Ratio of LCI results of LCSoft to SimaPro7.1 (based on Acetic acid, 98 % in H_2O, at plant – RER, ecoinvent data v2.0).

4.2 Extension of Inventory Database

The application range of LCA calculation in LCSoft was increased widely by enlargement of inventory data in LCSoft database. LCI data from available sources were processed throughout the LCI knowledge base management tool contained in LCSoft. Inventory data in LCSoft database were clearly addressed related details, i.e., input and output information, dataset information, reference function, time period, geography, technology, representative, data generator and publication, sources, and persons, in order to increase the transparency of data. LCSoft database structure was divided into two levels; LCI KB's first level and second level as shown in Figures 4.2-4.3.

4.2.1 LCSoft Database Structure: LCI KB's First Level

LCSoft database was organized to 3 main categories: (1) Material, (2) Utility, and (3) Transportation. Material category was divided into 5 sub-categories that are biomass, chemical manufacturing, crop production, fuel production, and others product manufacturing. Utility was be divided into 5 sub-categories that are heating utility, cooling utility, electricity by fuel, electricity by region, and others utility. Transportation was classified into 5 mode of transportation, e.g., air, pipeline, rail, road, and water. Figure 4.2 shows structure of LCSoft database and all mentioned categories and sub-categories.

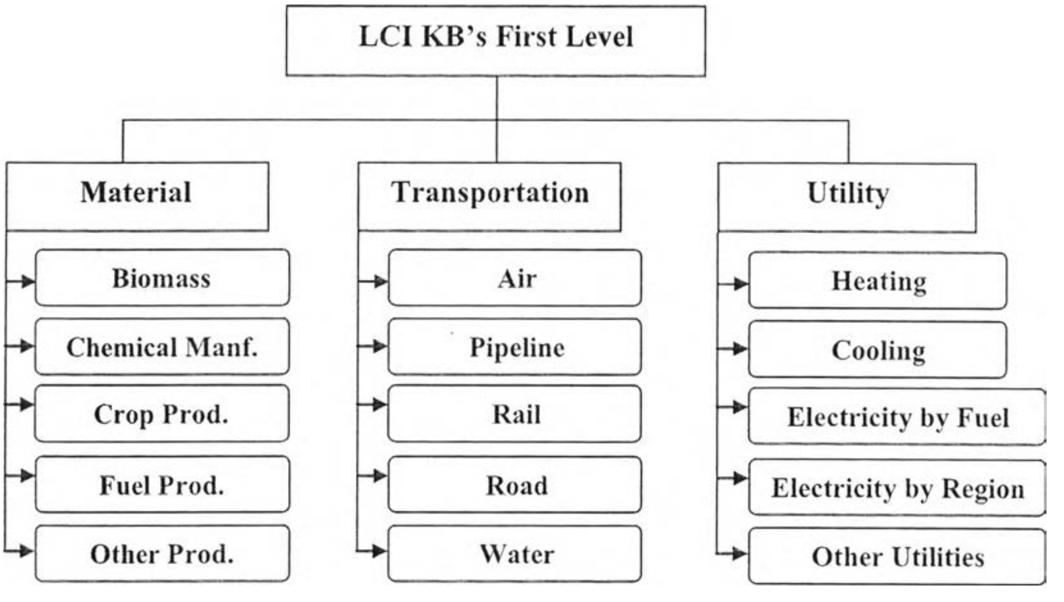

Figure 4.2 LCI KB's first level structure.

4.2.2 <u>LCSoft Database Structure: LCI KB's Second Level</u>

LCI KB's second level consist of: (1) input type, i.e., input processes from technosphere (activities and/or material required from other unit processes) and resources (energy, mineral, water, and other natural resources), (2) output type, i.e., energy, emission (air, soil, and water), waste, and by-product as shown in Figure 4.3.

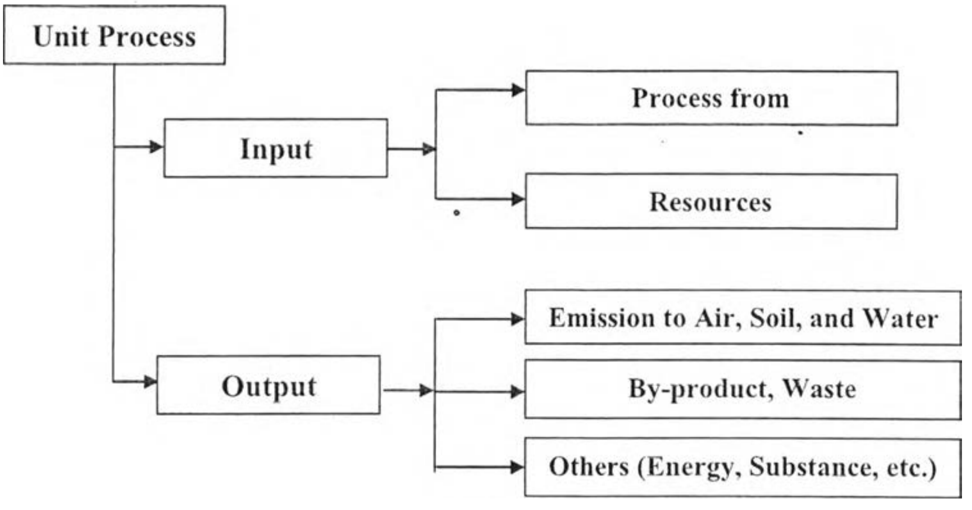

Figure 4.3 LCI KB's second level structure.

Table 4.1 shows the list of input LCI of Corn steep liquor production that consists of energy resources, minerals, and water. Output LCI, such as emission to air and water of Corn steep liquor, are shown in Table 4.2.

Table 4.1 Input LCI of Corn steep liquor production unit process

Name	Compartment	Sub-compartment	Unit	Amount
Coal, hard, unspecified, in ground	Resource	In ground	kg	0.00037736
Gas, natural, in ground	Resource	In ground	m3	0.00148
Limestone, in ground	Resource	In ground	kg	0.0027155
Oil, crude, in ground	Resource	In ground	kg	0.00057581
Phosphate ore, in ground	Resource	In ground	kg	0.0013295
Potassium oxide	Resource	In ground	kg	0.0003308
Uranium, in ground	Resource	In ground	kg	1.0488E-08
Water, process, unspecified natural origin/kg	Resource	In ground	kg	1.15

Table 4.2 Output LCI of Corn steep liquor production unit process

Name	Compartment	Sub-compartment	Unit	Amount
Acids, unspecified	Water	Unspecified	kg	6.0202E-08
Aldehydes, unspecified	Air	Unspecified	kg	6.1085E-09
Ammonia	Air	Unspecified	kg	0.00012017
Ammonia	Water	Unspecified	kg	8.3327E-08
Antimony	Air	Unspecified	kg	5.6285E-12
Arsenic	Air	Unspecified	kg	1.2898E-10
Barium	Air	Unspecified	kg	4.3915E-12
Benzene	Air	Unspecified	kg	2.9121E-08
BOD5, Biological Oxygen Demand	Water	Unspecified	kg	1.5419E-06
Cadmium	Air	Unspecified	kg	1.0494E-11
Carbon dioxide, fossil	Air	Unspecified	kg	0.006861
Carbon monoxide, fossil	Water	Unspecified	kg	0.000020511
Chloride	Water	Unspecified	kg	0.00000722
Chromium	Air	Unspecified	kg	5.216E-10
Cobalt	Air	Unspecified	kg	1.2849E-11
COD, Chemical Oxygen Demand	Water	Unspecified	kg	6.2012E-06
Copper	Air	Unspecified	kg	1.7306E-12
Dinitrogen monoxide	Air	Unspecified	kg	6.2058E-06
Fluoride	Air	Unspecified	kg	1.1181E-07
Fluoride	Water	Unspecified	kg	1.5817E-09
Formaldehyde	Air	Unspecified	kg	1.7323E-09
Hydrocarbons, unspecified	Air	Unspecified	kg	0.00000764
Hydrocarbons, unspecified	Water	Unspecified	kg	1.6507E-09
Hydrogen chloride	Air	Unspecified	kg	1.2101E-07
Hydrogen fluoride	Air	Unspecified	kg	1.8732E-08
Hydrogen sulfide	Air	Unspecified	kg	3.5735E-09
Iron	Water	Unspecified	kg	3.1525E-12
Lead	Air	Unspecified	kg	2.6013E-10
Magnesium	Air	Unspecified	kg	8.6981E-10
Manganese	Air	Unspecified	kg	3.2155E-10
Mercury	Air	Unspecified	kg	9.6382E-12
Metallic ions, unspecified	Water	Unspecified	kg	1.2958E-08
Methane, fossil	Air	Unspecified	kg	0.000010554
Molybdenum	Air	Unspecified	kg	7.2755E-13
Nickel	Air	Unspecified	kg	5.3312E-10
Nitrate	Water	Unspecified	kg	0.00053401
Nitrogen oxides	Air	Unspecified	kg	0.00002991
Oils, unspecified	Water	Unspecified	kg	1.6358E-07

Table 4.2 Output LCI of Corn steep liquor production unit process (cont'd)

Name	Compartment	Sub-compartment	Unit	Amount
Organic substances, unspecified	Air	Unspecified	kg	4.98E-06
Particulates	Air	Unspecified	kg	0.0002029
Phenol	Water	Unspecified	kg	5.35E-09
Salts, unspecified	Water	Unspecified	kg	1.41E-06
Sodium, ion	Water	Unspecified	kg	9.30E-06
Sulfate	Water	Unspecified	kg	3.45E-10
Sulfur dioxide	Air	Unspecified	kg	0.0082154
Suspended substances, unspecified	Water	Unspecified	kg	1.32E-06
Toluene	Air	Unspecified	kg	2.75E-11
Vanadium	Air	Unspecified	kg	1.30E-11
Waste water/m3	Water	Unspecified	m3	8.25E-09
Waste, industrial	Waste	Unspecified	kg	5.80E-07
Waste, unspecified	Waste	Unspecified	kg	0.0004204
Xylene	Air	Unspecified	kg	1.10E-12
Zinc	Air	Unspecified	kg	2.33E-11

LCSoft originally contains 239 unit processes. In order to extend LCSoft database, LCI data from U.S. LCI database powered by National Renewable Energy Laboratory (NREL, 2015) and other literatures were collected and processed through the new LCI calculation function in order to get the input and output information for each unit process. LCI database was extended to 703 unit processes cover 965 products include 3 biomass products, 133 chemical products, 62 crop products, 23 fuel products, 129 utilities, 110 transportation, and 505 other product manufacturing.

4.3 Improvement of Impact Categories in LCIA Calculation

4.3.1 Impact Category in LCSoft

LCSoft originally contains 11 impact categories consist of 8 impact categories from U.S. Environmental Protection Agency (EPA); and 3 impact categories from USEtox as shown in Table 4.3. The predictive model in the study of "Estimation of Environment-Related Properties of Chemicals for Design of Sustainable Processes: Development of Group-Contribution$^+$ (GC^+)" Property Models and Uncertainty Analysis" (Hukkerikar *et al.*, 2012) have been used to extend characterization factors data of chemical substances contained in 11 impact categories. In order to enlarge the assessment of environmental impacts, 3 new impacts categories, water resource consumption, mineral extraction, deposited wastes, and one renovate impact categories, energy consumption, as shown in Table 4.3 were necessary to be added to LCSoft.

Table 4.3 Detail of impact categories contained in LCSoft

Impact Category	Characterization Factor	Unit	CF Source
Acidification	$CF^{AP}_{t,c}$	kg H+ eq	USEPA
Aquatic toxicity	$CF^{ATP}_{t,c}$	$1/LC_{50}$	
Global warming potential	$CF^{GWP}_{t,c}$	kg CO_2 eq	
Human toxicity by exposure	$CF^{HTPE}_{t,c}$	1/TWA	
Human toxicity by ingestion	$CF^{HTPI}_{t,c}$	$1/LD_{50}$	
Ozone depletion	$CF^{ODP}_{t,c}$	kg CFC-11 eq	
Photochemical oxidation	$CF^{POCP}_{t,c}$	kg C_2H_2 eq	
Terrestrial toxicity	$CF^{TTP}_{t,c}$	$1/LD_{50}$	
Fresh water ecotoxicity	$CF^{ET}_{t,c}$	kg 2,4-D eq	USEtox
Human toxicity-carcinogenics	$CF^{HTC}_{t,c}$	kg benzene eq	
Human toxicity-noncarcinogenics	$CF^{HTNC}_{t,c}$	kg toluene eq	
Energy consumption	$CF^{Energy}_{t,c}$	MJ eq	Cumulative Energy Demand
Mineral extraction	$CF^{Mineral}_{t,c}$	kg Sb eq	CML-IA
Deposited wastes	$CF^{Waste}_{t,c}$	UBP	Ecological scarcity
Water resource consumption	$CF^{Water}_{t,c}$	UBP	

4.3.2 Source for New Impact Categories

In order to add new impact categories to LCSoft, characterization factors from "Swiss Eco-Factors 2013 according to the Ecological Scarcity Method" (Frischknecht and Büsser-Knöpfel, 2013) was used for assessment of deposited wastes and water resource consumption. The key metrics of this method are eco-factors that evaluate the environmental impacts of pollutant emissions or resource consumption in eco-point (UBP) per unit of quantity. Cumulative Energy demand was use for assessment of energy resource depletion.

4.3.2.1 Deposited Wastes

Deposited wastes consists of 3 major types of waste, i.e., wastes in above-ground landfills, hazardous wastes, and radioactive wastes.

(A) Above-ground Landfill Wastes

The key indicator of wastes stored in landfill with regard to ecological scarcity method (eco-factor) is carbon content of material. However. LCSoft cannot use this eco-factor (5.5 UBP/g C) directly because LCSoft database does not state carbon content of wastes, so Long-term TOC emissions are used as proxy instead. In LCSoft database, sanitary landfill is the only source of long-term TOC emissions. The transfer coefficient of sanitary landfills for carbon in waste to carbon as long-term TOC is 0.25 (Doka, 2009). Hence, the eco-factor of long-term TOC emissions is 8.4 UBP/g of long-term TOC as shown in Table B3.

(B) Hazardous Wastes in Underground Disposal Sites

Around one-third of hazardous wastes can be incinerated, recycled, consigned to physical-chemical treatment or stored in landfill for stabilized residues, while the rest is. Removal of soil for cleaning up contaminated sites is the source of hazardous wastes (FOEN, 2011). The characterization factors of hazardous wastes are shown in Table B3.

(C) Radioactive Wastes

Eco-factors for radioactive wastes are evaluated on the basis of legal provisions and scientific calculations by using the radiotoxicity index (NAGRA, 2008). According to the Swiss strategy for a final repository, radioactive wastes were classified to two categories that are; (1) short-lived low-level and medium-level wastes (LMLW) and (2) alpha-toxic wastes (ATW), high-level wastes

(HLW) and spent fuel elements (SF). The characterization factors of radioactive waste are shown in Table B3.

4.3.2.2 Water Resource Consumption

Ecological scarcity (water) is recommended method for assessment of water resource use and consumption (EC-JRC, 2011). This method is based on the availability and the scarcity of water resource. Eco-factors are based on national or watershed based levels of water consumption and the acceptable water stress index suggested by the OECD (2004) (Flury *et al.*, 2012). The characterization factors of water resource consumption are shown in Table B4. Calculation of water resource consumption uses characterization factors, expressed by specific country, proportion of consumptive water use, and amount of water consumption, expressed in volume.

4.3.2.3 Mineral Extraction

The CML method, representing the current recommendation in the ILCD framework (EC-JRC, 2011), uses the Abiotic Depletion Potential (ADP), to be multiplied with amount of resource extracted. CML method is based on scarcity, by including extraction and reserves of resource (ultimate reserve, reserve base, and economic reserve). Characterization factors of element extraction, as a part in ADP, were used to assess the impact of mineral extraction based on ultimate reserve, which is directly related to environmental problem of resource depletion (Van Oers, 2002). The characterization factors of mineral extraction, expressed in unit of kg antimony equivalent, are shown in Table B2.

4.3.2.4 Cumulative Energy Demand

LCSoft originally calculate energy resource consumption by conversion of mass of utilized resource to consumed energy using its heating value defined in LCI database. The energy consumption was divided into renewable and non-renewable resource. In order to investigate the energy consumption in specific category and simplify the energy consumption calculation (saving time of defining heating values in LCI database), energy consumption calculation in LCSoft was restructured by using Cumulative Energy Demand method.

Cumulative Energy Demand (CED) is widely used as a primary screening indicator for the assessment of environmental impact in terms of energy performance including direct and indirect consumption of energy (Frischknecht *et al.*, 2007). The characterization factors in CED method are determined from the amount of energy withdraw from the nature and expressed in MJ equivalent. .In LCSoft, CED is divided into 5 categories as shown in Table 2.3.

4.3.3 Validation of New Impact Categories

Production of 1kg acetic acid (98 %), at plant – RER from ecoinvent data v2.0 (Althaus *et al.*, 2007) was used to calculate environmental impacts, including deposited wastes, energy resource consumption, and mineral extraction. The validation of new impact categories was done by comparing the assessment results with SimaPro7.1.

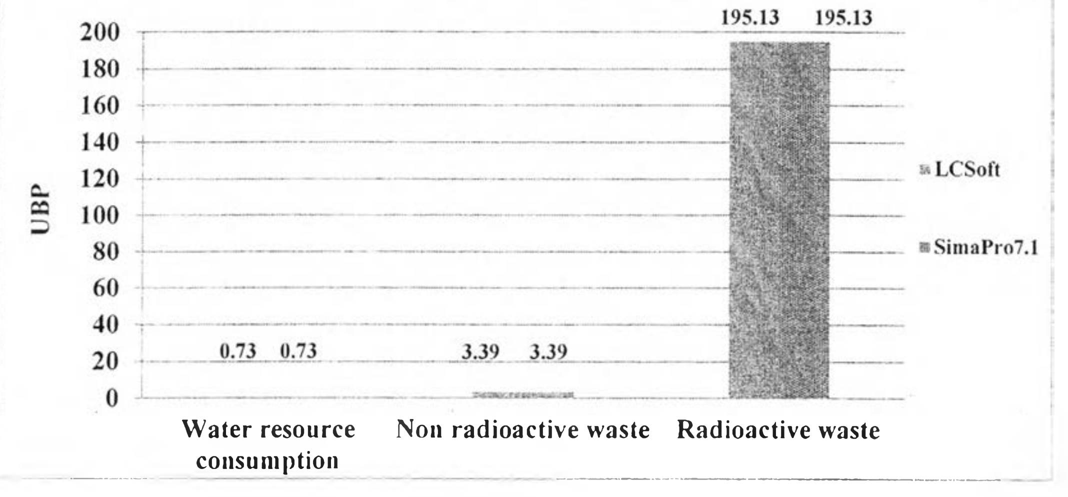

Figure 4.4 Water resource consumption and deposited wastes results of 1 kg Acetic acid, 98 % in H_2O, at plant – RER production.

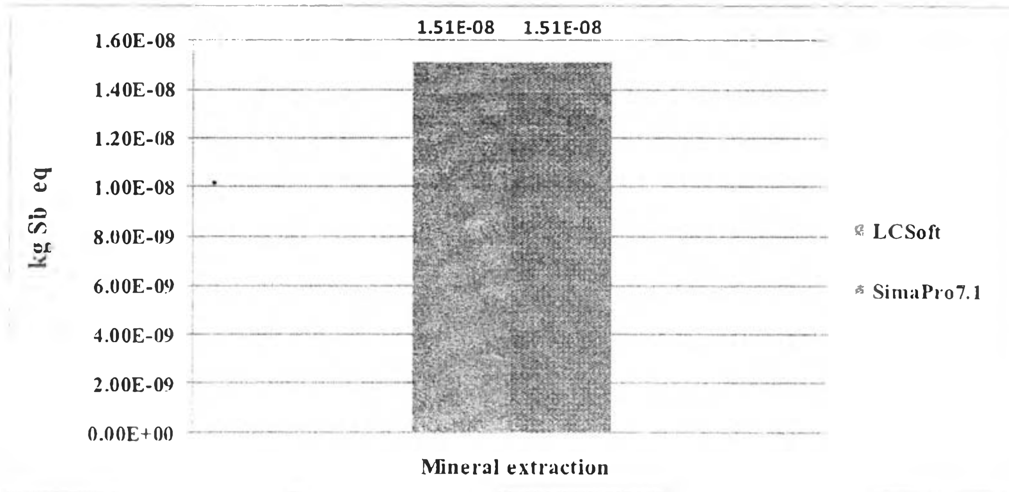

Figure 4.5 Mineral extraction result of 1 kg Acetic acid, 98 % in H_2O, at plant – RER production.

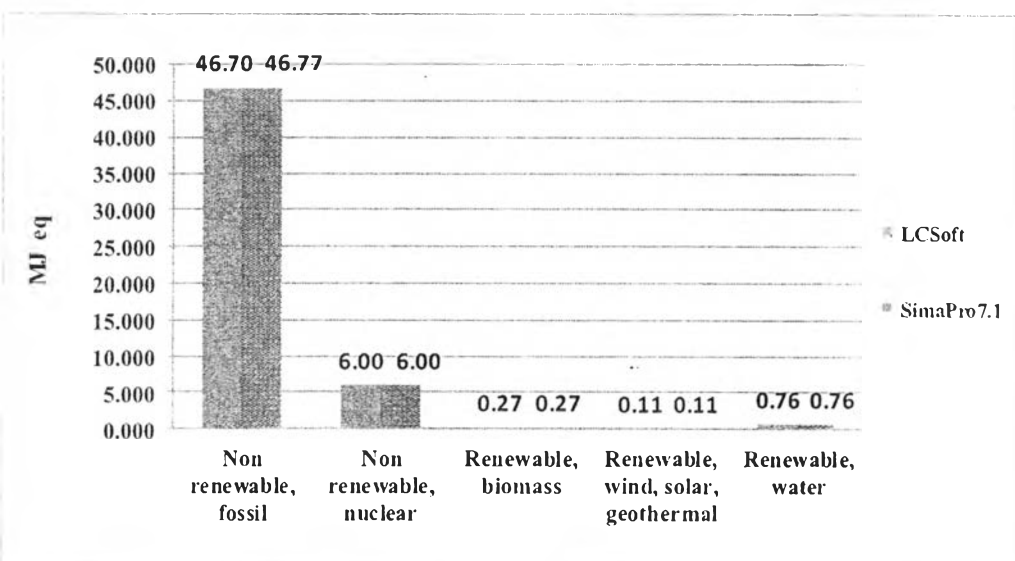

Figure 4.6 Energy resource consumption of 1 kg Acetic acid, 98 % in H_2O, at plant – RER production.

Figure 4.4 shows good match of water resource consumption result (based on regions of Denmark) and deposited wastes result, that is divided into two groups, which are non-radioactive wastes (landfill and hazardous wastes) and radioactive wastes. Figures 4.5-4.6 show good match of mineral extraction result and energy resource consumption result as well.

4.4 Development of Contribution Analysis

According to ISO 14040 (ISO, 2006a) contribution analysis is in the interpretation phase and gives useful information for analysis of assessment results. We can investigate how the assessment results contribute in studied system and find which processes are playing important role in term of environmental performance point of view.

4.4.1 Contribution Analysis Function in LCSoft

In LCSoft, development of contribution analysis was distinguished into 3 parts that are process contribution, LCI contribution, and LCIA contribution.

4.4.1.1 Process Contribution

The quantity of unit processes used to produce designed products or materials was recorded and shown in both graphic and table results in order to investigate how unit processes contribute in each production stage of studied system.

4.4.1.2 LCI Contribution

The contribution of LCI result provides useful information for realizing on how elementary contribute in each production stage. Hence, undersigned elementary or targeted elementary can be decreased or increased by improvement of process and/or product design.

4.4.1.3 LCIA Contribution

Contribution of environmental impact result from LCIA can be analyzed by LCIA contribution. With this function, processes and/or production stages that have significant contributed environmental impact ("Hot spot") can be determined for further product and/or process development. For instance, alternative materials, processes, or products, which have low environmental impacts, can be considered to replace the existing one that may be a danger substance.

4.4.2 Validation of Contribution Analysis Function

Validation of new contribution analysis was done by performing LCA using LCSoft and SimaPro7.1 through the case study. The results from comparison were investigated to identify the deficiencies in function for further improvement. Bioethanol process using cassava rhizome as a feed stock was used as a case study. The mass and energy flows were taken from simulation results developed by Mangnimit (2013). Input biomass was 377 tons per day and the target amount of ethanol production was 199 tons per day. Amount of related input and output streams are given in Table C1. Detail of used equipment and necessary equipment information are given in Table C2.

The process was divided into 5 production stages that are; (1) Pretreatment, (2) Detoxification; (3) SSCF fermentation; (4) Distillation; and (5) Dehydration as shown in Figure 3.2. The boundary system of LCA study focused on cradle-to-gate of bioethanol production covering cassava cultivation, chemicals manufacturing, and utilities production. Name of all related unit processes and sources of data were listed in Table 3.1. In SimaPro7.1 database, LCI of cassava root, corn steep liquor, and Enzyme, cellulose do not exist, therefore, LCI data from the other sources were added to SimaPro7.1 in order to decrease data gap.

4.2.1.1 Process Contribution Results

Tables 4.4-4.5 and Figure 4.7 show process contribution results in exact value, percentage, and graphical format respectively. The results indicate the amount of processes contribute to each production stage. Table 4.6 shows validation result using ratio analysis with very good match results.

Table 4.4 Process contribution result performed by using LCSoft

No	Process	Unit	Total	Production Stage				
				Pretreatment	Detoxification	SSCF	Distillation	Dehydration
1	Ammonia, steam reforming, liquid, at plant	kg	3.31	-	-	3.31	-	-
2	Cassava root	kg	15008.13	15008.1	-	-	-	-
3	Cooling energy, natural gas, at cogen unit with absorption chiller 100 kW	MJ	47938.30	-	497.3	9380.6	38060.4	-
4	Corn steep liquor	kg	147.47	-	-	147.47	-	-
5	Electricity, natural gas, at power plant, US	MJ	20.52	-	-	-	20.5	-
6	Enzyme, cellulase	kg	8.32	-	-	8.32	-	-
7	Natural gas, burned in industrial furnace 100kW	MJ	60584.60	-	859.3	5141.4	44939.5	9644.4
8	Sulphuric acid, at plant	kg	258.34	99.4	158.9	-	-	-

Table 4.5 Process contribution result performed by using LCSoft (Percentage)

No	Process	Unit	Total	Production Stage				
				Pretreatment	Detoxification	SSCF	Distillation	Dehydration
1	Ammonia, steam reforming, liquid, at plant	%				100.00		
2	Cassava root	%		100.00				
3	Cooling energy, natural gas, at cogen unit with absorption chiller 100 kW	%			1.04	19.57	79.39	
4	Corn steep liquor	%				100.00		
5	Electricity, natural gas, at power plant, US	%					100.00	
6	Enzyme, cellulase	%				100.00		
7	Natural gas, burned in industrial furnace 100kW	%			1.42	8.49	74.18	15.92
8	Sulphuric acid, at plant	%		38.49	61.51			

Table 4.6 Ratio of process contribution result of LCSoft to SimaPro7.1

No	Process	Production Stage				
		Pretreatment	Detoxification	SSCF	Distillation	Dehydration
1	Ammonia, steam reforming, liquid, at plant	-	-	1.00	-	-
2	Cassava root	1.00	-		-	-
3	Cooling energy, natural gas, at cogen unit with absorption chiller 100 kW	-	1.00	1.00	1.00	-
4	Corn steep liquor	-	-	1.00	-	-
5	Electricity, natural gas, at power plant, US	-	-		1.00	-
6	Enzyme, cellulase	-	-	1.00	-	-
7	Natural gas, burned in industrial furnace 100kW	-	1.00	1.00	1.00	1.00
8	Sulphuric acid, at plant	1.00	1.00		-	-

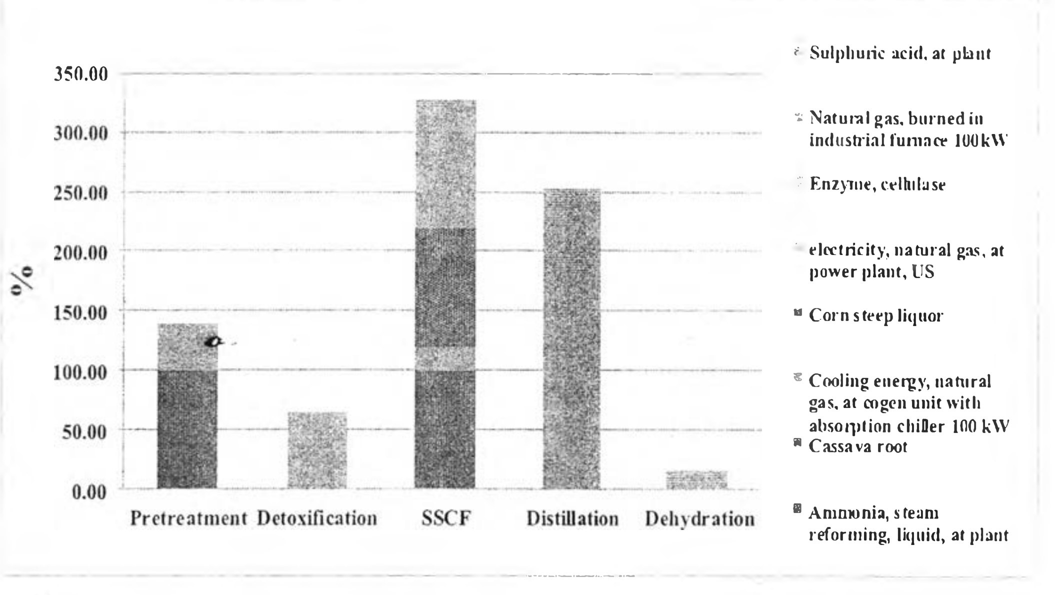

Figure 4.7 Process contribution result performed by using LCSoft.

4.2.1.2 LCI Contribution Result

Table 4.7 shows part of LCI contribution result performed by LCSoft and Table D1 shows full result of LCI contribution. Figure 4.8 shows the validation results of LCI contribution by comparing the results from LCSoft with SimaPro7.1. The results indicate the good match of LCI contribution result between LCSoft and SimaPro7.1.

Table 4.7 Part of LCI contribution result performed by LCSoft

No	Substance	Compartment	Subcompartment	Unit	Total	Pretreatment	Detoxification	SSCF	Distillation	Dehydration
1	1,4-Butanediol	air	high population density	kg	2.49E-08	7.98E-10	1.51E-09	4.50E-09	1.81E-08	5.10E-12
2	1,4-Butanediol	water	river	kg	9.97E-09	3.19E-10	6.04E-10	1.80E-09	7.24E-09	2.04E-12
3	2,4-D	soil	agricultural	kg	3.88E-07	1.68E-09	7.39E-09	5.41E-08	2.94E-07	3.05E-08
4	2-Propanol	air	high population density	kg	4.66E-04	1.49E-05	2.83E-05	8.42E-05	3.39E-04	8.47E-08
5	4-Methyl-2-pentanone	water	unspecified	kg	2.35E-08	1.23E-11	2.47E-11	9.45E-11	2.34E-08	7.35E-13
6	Acenaphthene	air	high population density	kg	5.68E-10	9.69E-12	2.17E-11	9.00E-11	4.23E-10	2.43E-11
7	Acenaphthene	air	low population density	kg	8.33E-11	4.92E-13	1.60E-12	1.48E-11	6.58E-11	5.47E-13
8	Acenaphthene	air	unspecified	kg	5.40E-11	2.83E-14	5.67E-14	2.17E-13	5.37E-11	1.69E-15
9	Acenaphthene	water	ocean	kg	4.64E-09	3.23E-10	5.59E-10	7.08E-10	2.89E-09	1.64E-10
10	Acenaphthene	water	river	kg	1.10E-08	6.67E-10	1.17E-09	1.65E-09	7.05E-09	4.52E-10
11	Acenaphthylene	water	ocean	kg	2.90E-10	2.02E-11	3.50E-11	4.43E-11	1.81E-10	1.02E-11
12	Acenaphthylene	water	river	kg	6.88E-10	4.17E-11	7.33E-11	1.03E-10	4.41E-10	2.82E-11

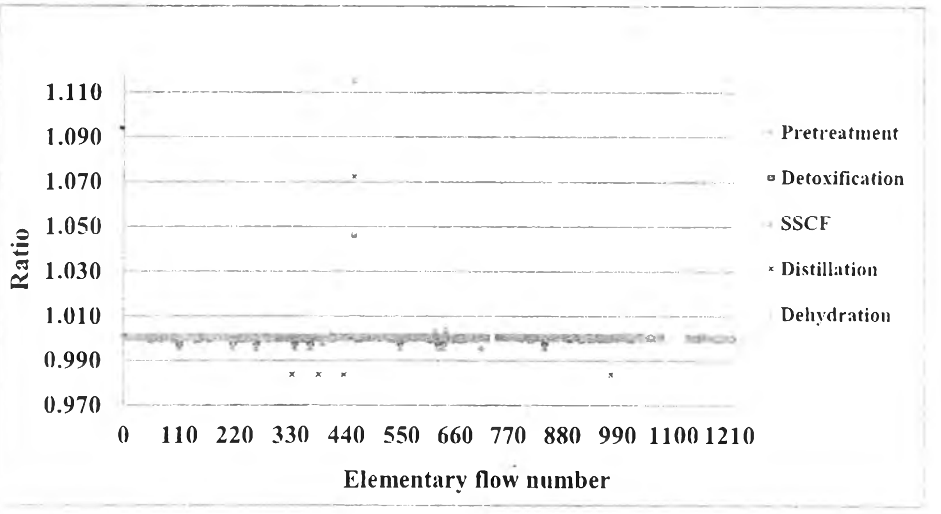

Figure 4.8 Ratio of LCI contribution result of LCSoft to SimaPro7.1.

4.2.1.3 LCIA Contribution Result

Table 4.8 shows LCIA contribution results performed by LCSoft and validation results is shown in Table 4.9. From Table 4.9, the ratio of LCSoft to SimaPro7.1 results show the good match with energy resource consumption, deposited wastes, mineral extraction, water resource consumption and some impact in WAR algorithm such as acidification (AP), global warming potential (GWP), and photochemical oxidation (POCP). Some impact shows different value between LCSoft and SimaPro7.1 because characterization factors that were used to calculate environmental impact came from different models and different sources. Characterization factors of AP, ATP, GWP, HTPE, HTPI, HTNC, ODP, POCP, and TTP contained in LCSoft were collected from WAR algorithm similar to HTC, HTNC, and ET that were collected from USEtox and were extended by Group Contrition method (Hukkerikar *et al.*, 2012), which does not exist in SimaPro7.1. Thus, the characterization factors in LCSoft cover more related chemical substances than characterization factors that were used to calculate AP, HTC, HTNC, ET, GWP, ODP, POCP in SimaPro7.1 which is TRACI2 in this case study. LCIA contribution can also be displayed in graphical results as shown in Figures 4.9.

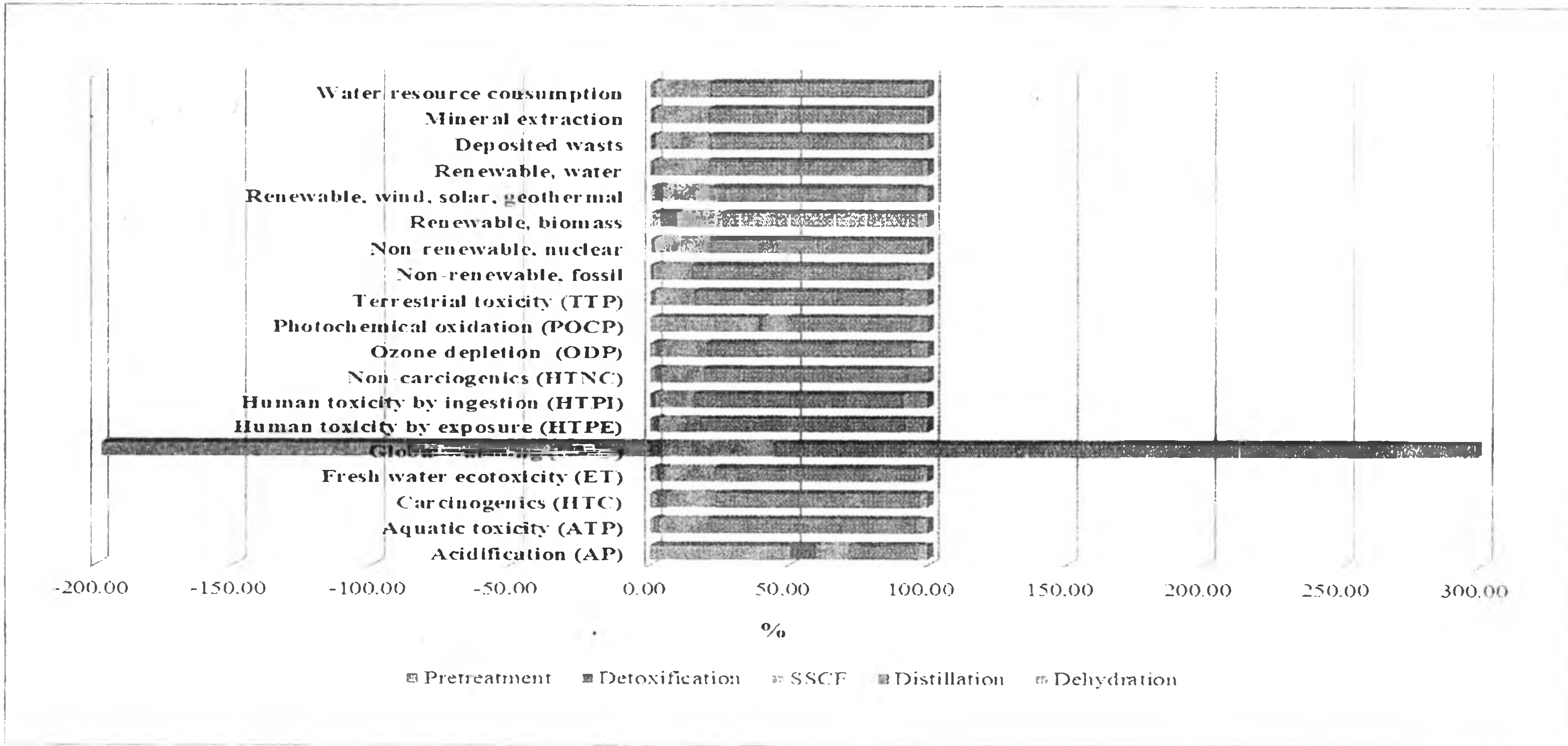

Figure 4.9 LCIA contribution result performed by LCSoft.

Table 4.8 LCIA contribution results performed by LCSoft

No	Impact Category	Unit	Total	Production Stage				
				Pretreat-ment	Detoxifi-cation	SSCF	Distilla-tion	Dehydra-tion
1	Non-renewable, fossil	MJ eq	1.17E+05	190.76	1780.71	15283.87	88310.39	11444.15
2	Non-renewable, nuclear	MJ eq	8.22E+03	33.04	138.88	1544.92	6434.00	71.66
3	Renewable, biomass	MJ eq	1.21E+02	4.20	7.93	19.43	86.32	3.40
4	Renewable, wind, solar, geothe	MJ eq	4.22E+01	0.58	1.39	6.98	31.76	1.45
5	Renewable, water	MJ eq	1.85E+03	5.36	28.13	345.24	1451.83	21.26
6	Acidification (AP)	kg H+ eq	1.14E+03	575.00	114.26	125.27	295.8145	28.87254
7	Aquatic toxicity (ATP)	1/LC_{50}	2.74E+00	0.02743	0.073823	0.455274	2.085993	0.098984
8	Carcinogenics (HTC)	kg C_6H_6 eq	2.76E+01	0.56121	1.176609	4.68677	20.58413	0.559335
9	Fresh water ecotoxicity (ET)	kg 2,4-D eq	1.28E+03	22.707	49.27104	219.4649	962.131	31.18588
10	Global warming (GWP)	kg CO_2 eq	2.29E+03	-4536.22	108.4729	910.2314	5155.799	651.6773
11	Human toxicity by exposure (HTPE)	1/TWA	2.53E-02	0.000238	0.000684	0.003467	0.018966	0.001993
12	Human toxicity by ingestion (HTPI)	1/LD_{50}	4.37E+00	0.016768	0.080327	0.57861	3.312941	0.381202
13	Non-carciogenics (HTNC)	kg C_6H_6 eq	3.33E+04	428.1362	1067.804	4801.734	24799.29	2161.331
14	Ozone depletion (ODP)	kg CFC-11 eq	5.77E-03	7.73E-05	0.000189	0.000876	0.00431	0.000315
15	Photochemical oxidation (POCP)	kg C_2H_2 eq	8.61E+00	3.335767	0.194496	0.692282	3.92514	0.465772
16	Terrestrial toxicity (TTP)	1/LD_{50}	4.37E+00	0.016768	0.080327	0.57861	3.312941	0.381202
17	Deposited wastes	UBP	2.49E+05	1209.372	4546.974	46295.50164	194250.5	2709.95
18	Mineral extraction	kg Sb eq	2.08E-05	8.81E-08	3.58E-07	3.90E-06	1.63E-05	1.81E-07
19	Water resource consumption	UBP	1.16E+03	58.8	105	196	794	3.67

Table 4.9 Ratio of LCIA contribution results of LCSoft to SimaPro7.1

No	Impact Category	Total	Production Stage				
			Pretreatment	Detoxification	SSCF	Distillation	Dehydration
1	Non-renewable, fossil	1.00	1.00	1.00	1.00	1.00	1.00
2	Non-renewable, nuclear	1.00	1.00	1.00	1.00	1.00	1.00
3	Renewable, biomass	1.00	1.00	1.00	1.00	1.00	1.00
4	Renewable, wind, solar, geothe	1.00	1.00	1.00	1.00	1.00	1.00
5	Renewable, water	1.00	1.00	1.00	1.00	1.00	1.00
6	Acidification (AP)	1.03	1.04	1.00	1.01	1.01	1.00
7	Aquatic toxicity (ATP)						
8	Carcinogenics (HTC)	3.46	4.64	4.30	3.18	3.39	11.63
9	Fresh water ecotoxicity (ET)	0.81	0.81	0.81	0.81	0.81	0.82
10	Global warming (GWP)	0.97	1.00	1.00	0.99	0.99	0.99
11	Human toxicity by exposure (HTPE)	-	-	-	-	-	-
12	Human toxicity by ingestion (HTPI)	-	-	-	-	-	-
13	Non-carciogenics (HTNC)	1.73	0.49	0.68	1.55	1.86	6.21
14	Ozone depletion (ODP)	5.76	58.56	12.86	6.74	5.67	3.33
15	Photochemical oxidation (POCP)	1.04	1.00	1.03	1.02	1.08	1.08
16	Terrestrial toxicity (TTP)						
17	Deposited wastes	1.00	1.00	1.00	1.00	1.00	1.00
18	Mineral extraction	1.00	1.00	1.00	1.00	1.00	1.00
19	Water resource consumption	1.00	1.00	1.00	1.00	1.00	1.00

LCSoft also provides LCIA contribution results in specific impact category. For instance, Tables 4.10-4.11 show LCIA contribution results of non-renewable, fossil in exact value and percentage respectively. Figures 4.10-4.11 shows LCIA contribution of non-renewable fossil in graphical result. Furthermore, LCSoft can display the LCIA contribution results in specific category and specific production stage as shown in Figures 4.12-4.13.

Table 4.10 LCIA contribution results of non-renewable, fossil

No	Process	Unit	Total	Production stage				
				Pretreat-ment	Detoxifi-cation	SSCF	Distillati-on	Dehydration
1	Ammonia, steam reforming, liquid, at plant	MJ eq	130.29			130.29		
2	Cassava root	MJ eq	0.00					
3	Cooling energy, natural gas, at cogen unit with absorption chiller 100 kW	MJ eq	43980.06		456.24	8606.05	34917.77	
4	Corn steep liquor	MJ eq	13.31			13.31		
5	electricity, natural gas, at power plant, US	MJ eq	66.94				66.94	
6	Enzyme, cellulase	MJ eq	433.38			433.38		
7	Natural gas, burned in industrial furnace 100kW	MJ eq	71890.32		1019.65	6100.84	53325.68	11444.15
8	Sulphuric acid, at plant	MJ eq	495.57	190.76	304.82			
Total			117009.88	190.76	1780.71	15283.87	88310.39	11444.15

Table 4.11 LCIA contribution results of non-renewable, fossil (Percentage)

No	Process	Unit	Total	Production stage				
				Pretreat-ment	Detoxifi-cation	SSCF	Distillation	Dehydration
1	Ammonia, steam reforming, liquid, at plant	%	0.11			0.85		
2	Cassava root		0.00					
3	Cooling energy, natural gas, at cogen unit with absorption chiller 100 kW		37.59		25.62	56.31	39.54	
4	Corn steep liquor		0.01			0.090		
5	electricity, natural gas, at power plant, US		0.06				0.08	
6	Enzyme, cellulase		0.37			2.84		
7	Natural gas, burned in industrial furnace 100kW		61.44		57.26	39.92	60.38	100.00
8	Sulphuric acid, at plant		0.42	100.00	17.12			
Total			100.00	100.00	100.00	100.00	100.00	100.00

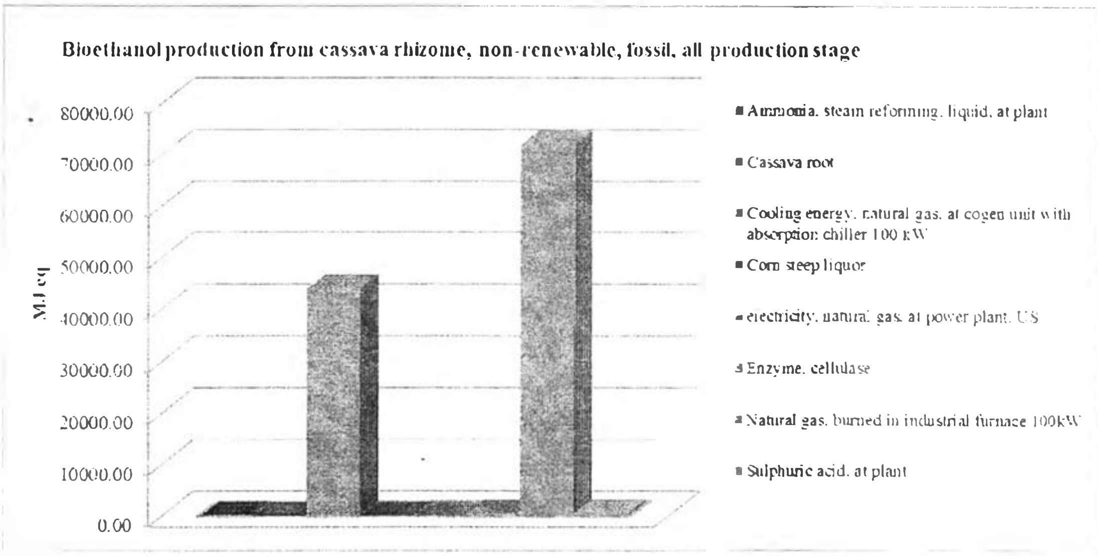

Figure 4.10 LCIA contribution results in bar chart (non-renewable, fossil, all production stage).

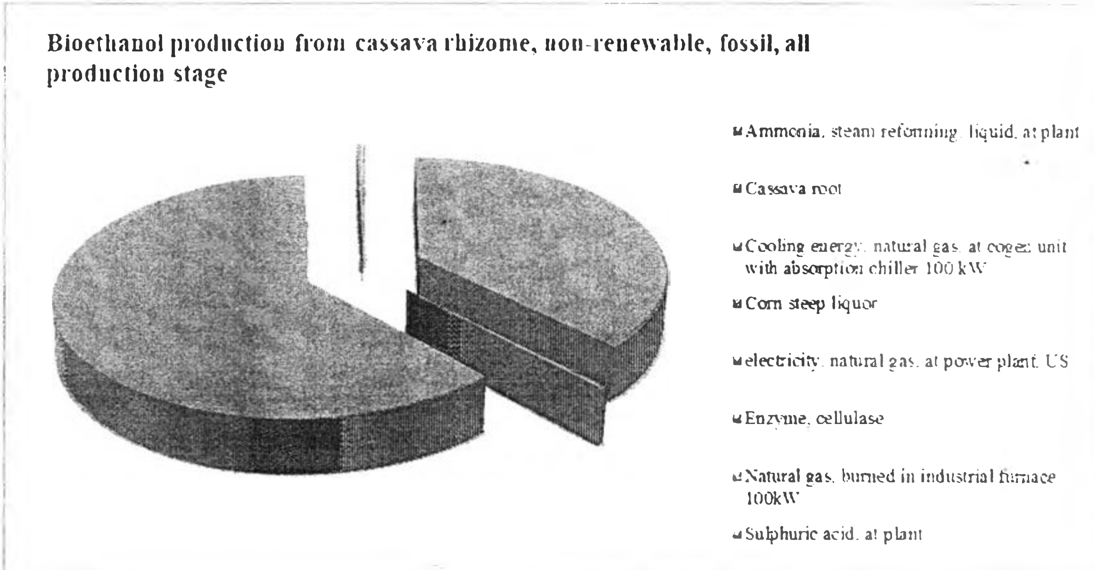

Figure 4.11 LCIA contribution results in pie chart (non-renewable, fossil, all production stage).

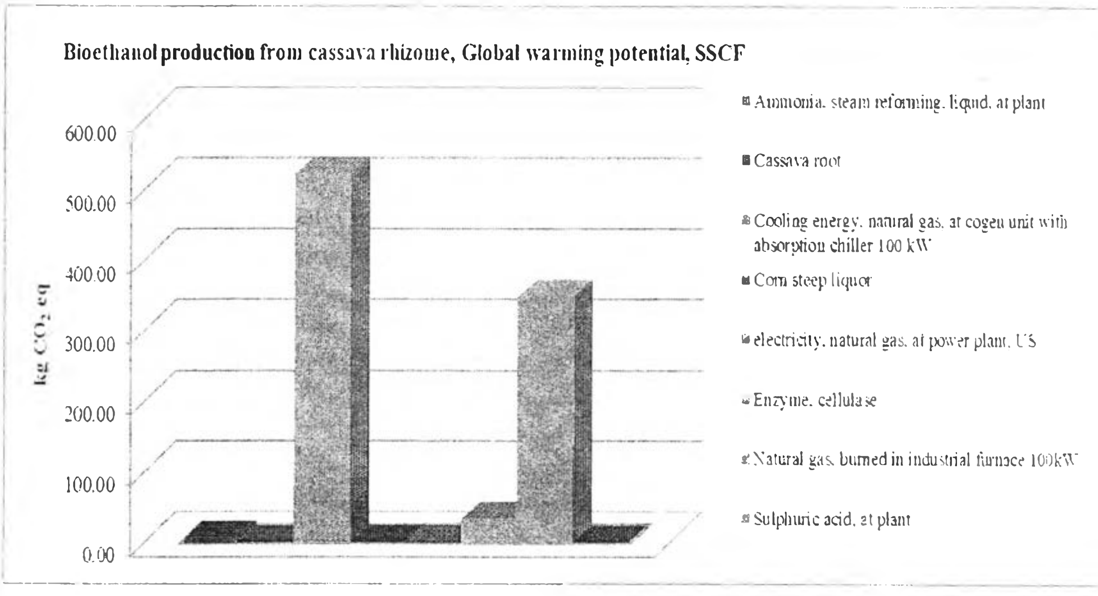

Figure 4.12 LCIA contribution results in bar chart (non-renewable, fossil, SSCF production stage).

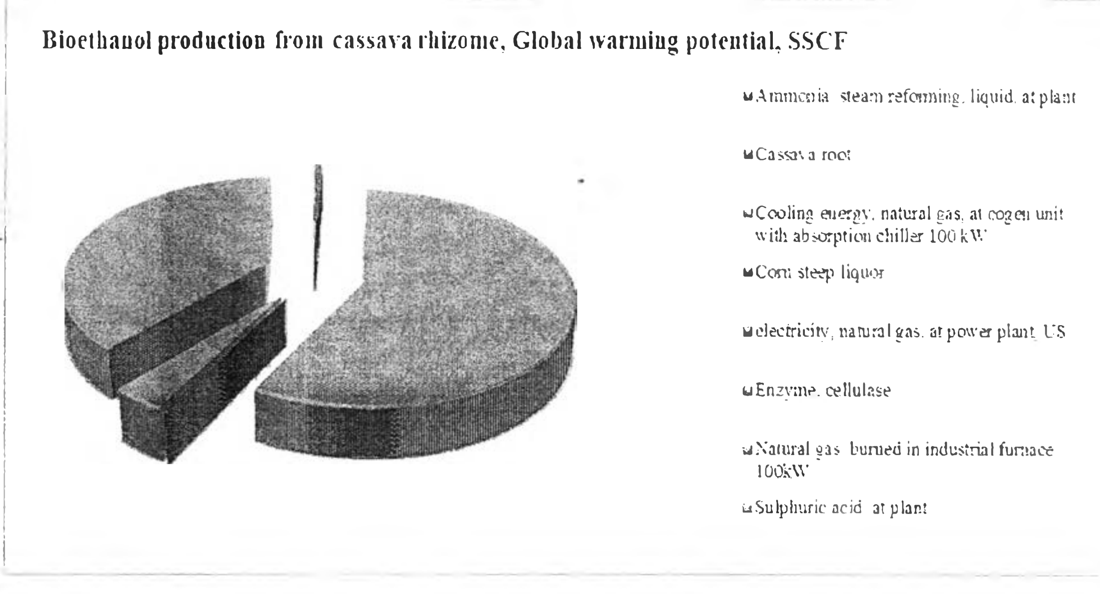

Figure 4.13 LCIA contribution results in pie chart (non-renewable, fossil, SSCF production stage).

4.5 LCSoft-new Version System Structure

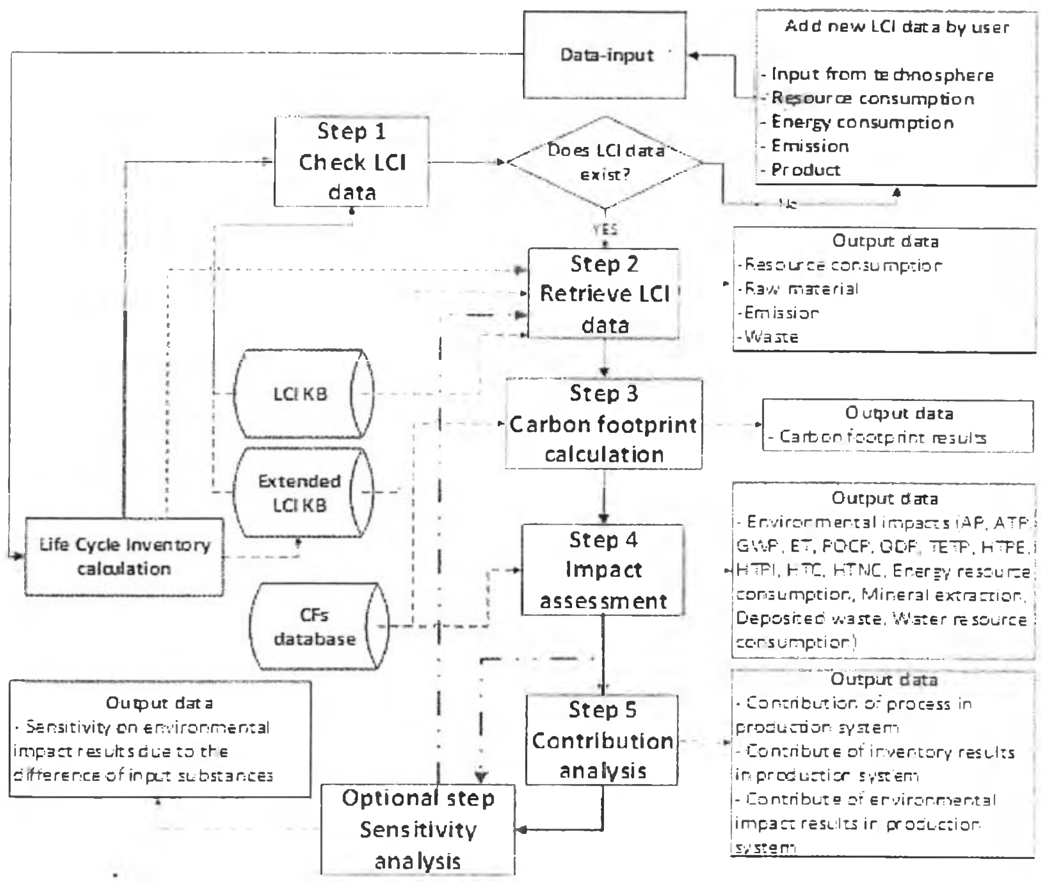

Figure 4.14 LCSoft system structure.

Figure 4.15 shows the new LCSoft version system structure. Calculation model and data in LCSoft2.0 were improved and expanded. Grey colour represents the improved area. LCA calculation in LCSoft new version consists of 5 main steps and optional steps which are described below.

4.5.1 Step1: Check LCI Data

LCI data of products or processes contained in database will be checked and displayed to software interface in order to notice user which data are existing. Adding or modification of LCI data are available, then added or modified data will recalculate the LCI results by LCI calculation function contained in software.

4.5.2 Step2: Retrieve LCI Data

LCI data are retrieved from LCI KB and Extended LCI KB. Retrieved LCI data such as input processes, raw materials, natural resources, energy, and emissions are promptly to be used in LCIA calculation next step.

4.5.3 Step3: Carbon Footprint Calculation

Carbon footprint is described as amount of carbon dioxide and greenhouse gas associated with functional unit. Carbon footprint is estimated using global warming potential (GWP) as an impact indicator. GWP is used to convert the greenhouse gas emitted from utility consumption in production system to be unit of carbon dioxide (CO_2 equivalent) per functional unit. Equations 4.1-4.2 used to estimate carbon footprint. Characterization factors used to estimate GWP are taken from Characterization factor database contained in software.

$$CO2_{eq} = (m^{PRO}_{GHC,air} \times CF^{GWP}_{GHC,air})/m_{product} \quad (4.1)$$

$$Carbon\ footprint = \sum CO2_{eq} \quad (4.2)$$

Where GHG indicates Greenhouse gas, $m^{PRO}{}_{GHG,air}$ is referred to mass flow rate of greenhouse gas (GHG), $CF^{GWP}{}_{GHG,air}$ is global warming characterization factor of emitted greenhouse gas, and CO_{2eq} is carbon dioxide equivalent per 1 kg of product (Kalakul, 2013).

4.5.4 Step4: Impact Assessment

Environmental impact assessment is calculated by using Equation 2.3. 15 impact categories are contained in software as shown in Table 4.3.

4.5.5 Step5: Contribution Analysis

Contribution analysis is divided into three parts which are processes contribution, LCI results contribution, and LCIA calculation. The results are mentioned above. This feature allow user to investigate the contribution of result in production system that can give information for further development.

4.5.6 Optional Step: Sensitivity Analysis

For investigating the influence of different assumption on impact assessment results, LCSoft allow user to perform sensitivity analysis which user can change assumption, such as type of utility, type of raw material, amount of input process, and see the variation of impact assessment results with ability to compare results with other assumption.

Table 4.12 LCSoft calculation step

Calculation Step	Description	Input Data/ Output Data/ Calculation Model
Step1: Check LCI Data	The LCI data of related products or processes are checked in this step with permission to add or modify LCI data. If input from technosphere is existing in added data or modified data, the LCI results can be achieve by LCI calculation function contained in software.	Input Data: - Mass balance (stream table) - Energy balance and duty of equipment (equipment table) Calculation model: (Heijung and Suh, 2002). $A*s = f$ (2.1) $g = B*s$ (2.2)
Step2: Retrieve LCI Data	Resource consumption, raw material consumption, and emission of related products or processes are received from LCI KB for next step calculation and displaying of LCI results	Output data: - Emission - Waste - Resource - Energy
Step3: Carbon Footprint Calculation	All amount of CO2 and greenhouse gas in production process are quantified and characterized by using Global warming potential (GWP) as an indicator.	Calculation Model: (Guinee *et al.*, 2002). $CO2_{eq} = (m^{PRO}_{GHG,air} \times CF^{GWP}_{GHG,air})/m_{product}$ (4.1) $\text{Carbon footprint} = \sum CO2_{eq}$ (4.2)
Step4: Impact Assessment	The LCI results are classified and characterized to each impact category based on their effect on environmental	Calculation Model : (Guinee *et al.*, 2002) $I^k = \sum_{i,c} EM_{i,c}\, x\, CF^k_{i,c}$ (2.3)
Step5: Contribution Analysis	The process, LCI results, and impact assessment results are shown obviously in each production system in order to investigate the contribution	Input Data: - Amount of product used in production system - LCI results - LCIA results
Optional Step: Sensitivity Analysis	The influence of different assumption on the assessment results could be observed.	Input Data: Alternative input material