CHAPTER II
BACKGROUND AND LITERATURE REVIEW

Environmental and sustainability awareness, through the increasing of natural resource consumption, process operations, and product manufacturing together with waste disposal, have been concerned significantly in modem society. Life Cycle Assessment (LCA) has been shown to be an effective tool for quantifying environmental impacts of products, processes, services, and activities throughout the entire life cycle. Furthermore, LCA has been extensively used worldwide to support decision making and policy development towards sustainable production and consumption.

2.1 Life Cycle Assessment (LCA)

LCA framework is standardized by the International Organization for Standardization (ISO) including ISO 14040: Principles and Framework and ISO 14044: Requirements and Guidelines. The framework is organized into four main phases including: (1) Goal and scope definition; (2) Life Cycle Inventory analysis; (3) Life Cycle Impact Assessment; and (4) Interpretation as shown in Figure 2.1.

2.1.1 Goal and Scope Definition

The objective of LCA study is defined as clearly as possible in this stage. In the defining of goal, the intended application, significant of the study, the intended audience, and the purpose of results usage should be described clearly and unambiguously. For the scope of study, product system (studied system) and function of system are defined as system boundary and functional unit respectively. System boundary is defined in term of the life cycle stages, geographic and time boundary. Life cycle stage can be divided into four levels.

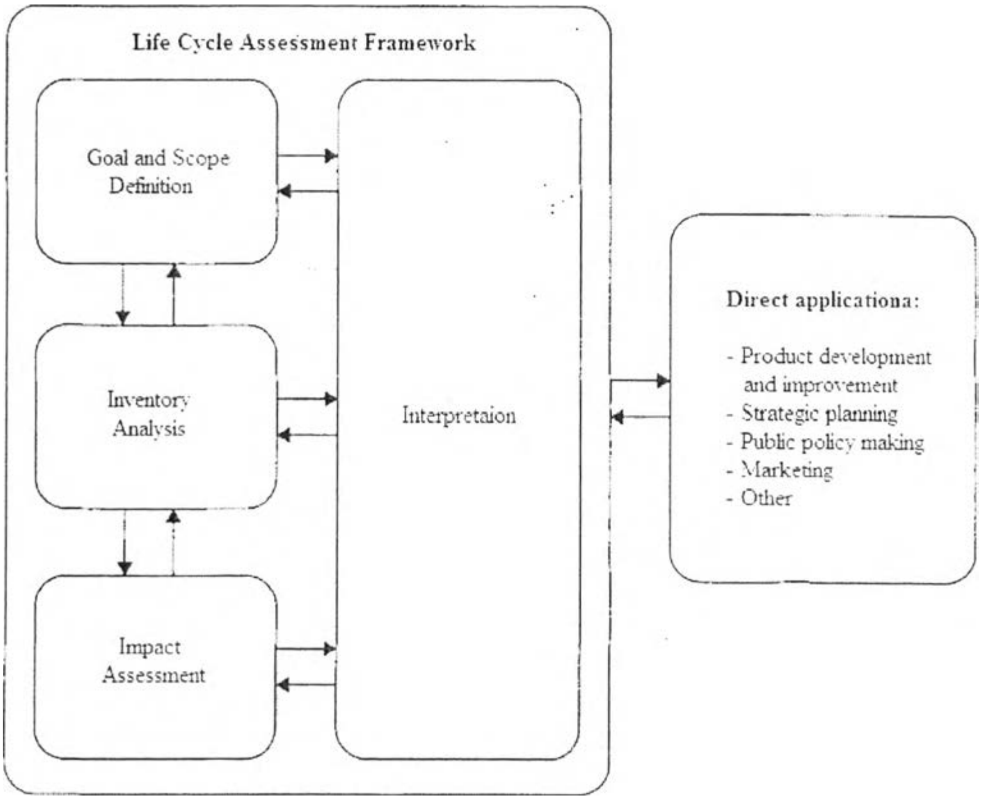


Figure 2.1 The principle framework for LCA (ISO, 2006b).

2.1.1.1 Cradle to Grave

This is a complete LCA starting from raw material extraction (cradle) through the manufacturing, transportation, use, and disposal phase (grave).

2.1.1.2 Cradle to Gate

This is a partial LCA starting from raw material extraction (cradle) to manufacturing phase (gate of factory).

2.1.1.3 Gate to Gate

This is a partial LCA which used to determine environmental impacts at only one value-added process or production stage in the entire production chain.

2.1.1.4 Gate to Grave

This is an assessment of product or process from use to end-of-life phases (behind the manufacturing phase).

Functional unit (comparison basis) is defined in this stage. The purpose is to quantify identified function of product to be the reference for product comparison, such as weight of designed product and energy produced by fuel.

2.1.2 Life Cycle Inventory Analysis

Life Cycle Inventory analysis (LCI) involves the complication and quantification of input (raw material, natural resource, waste for treatment) and output (product, by-product, emissions, waste, energy) of all relevant processes in system boundary. The LCI is built on the basis of the unit process, where the inputs are converted to outputs (Heijungs and Guineév, 2012).

2.1.2.1 Life Cycle Inventory (LCI) Calculation

There are three major methods used in LCI calculation which are: (1) LCI based on process analysis, such as Process flow diagram, Matrix inversion; (2) Input-output based LCI; (3) Hybrid LCI, such as Tiered hybrid analysis, IO-based hybrid analysis, and Integrated hybrid analysis (Suh and Huppes, 2003).

(A) Process Flow Diagram

Process flow diagram represents the connection of processes in product system through the commodity flows. The LCI of product system can be calculated from multiplication of amount of environmental intervention generated to produce a certain amount of commodities, that is fulfilling a functional unit. The solution of this method is more complexity, when the product system contains “loop”. For instance, production of electricity requires steel and production of steel also requires electricity. Consoli *et al.* (1993) suggest using an iterative method to solve this problem which speed of convergence is affected by increasing of iterations. Infinite geometric progression can be used to solve this problem as well (Suh and Huppes, 2003).

(B) Matrix Inversion

Heijungs and Suh (2002) purposed the matrix inversion method for LCI calculation without using iterative or geometric progression method.

$$As = f \tag{2.1}$$

$$g = Bs \tag{2.2}$$

Equations 2.1 and 2.2 are used to calculate LCI where "A" is referred to "Technology Matrix" that contains flows of commodities (economic flows) of processes. "B" is referred to "Intervention Matrix" that contains flows of environmental intervention (i.e. emissions or natural resources consumed or emitted from unit processes). "f" represents "final demand vector", which is the given amount of designed product produced by system. "s" is referred to "scaling factor", that scale up economic flows contained in technology matrix to meet with target amount defined by final demand vector. "g" represents "Total intervention vector" that contains set of all environmental intervention flows given by intervention matrix and scaling factor.

(C) IO-based LCI

Using of LCI based on process analysis cannot gives completely LCI result due to the ability of process-specific data collection for the entire economy system ; however, this problem can be handled by using Input–Output analysis (Suh and Huppes, 2003). Input-Output analysis (IOA) describes the inter-relation of production and consumption of industry outputs, which is represented by monetary transaction flow between industries (Leontief, 1936). There are limitation of using IO based LCI which are: (1) IOA provide LCI only in pre-consumer stage of the product life cycle and leave the rest of product life cycle outside the system boundary; (2) amount of imported commodities should be negligible to prevent the misspecification of imports; (3) IO-based LCI data is normally older than LCI data in process-based due to the time consuming of industry survey and publication; (4) The lack of environmental data in most countries. Although, the IO-based LCI can provide the complete boundary system using less resource and time, the using of IO-based method is rather limited (Suh and Huppes, 2003).

(D) Hybrid Analysis

Hybrid analysis is combination of process-based, which provides more accurate and detailed process information with more recent data, and IO-based, which provide more complete upstream boundary in natural level with less time consuming but there is complexity in order to perform hybrid method. LCI database and the environmental data in IO are still available in few countries and it is needed to be further developed into global level (Suh and Huppes, 2003).

. *2.1.2.2 Life Cycle Inventory (LCI) Data Source*

Inventory data sources can be primary source (interviews, questionnaires or surveys, bookkeeping or enterprise resource planning (ERP) system, data collection tools, and on-site measurements) or secondary source, which are database, statics and open literature (Curran, 2012). There are many data sources provided including open sources and closed sources. These data sources are mostly gathered from Northeast Asia, North America, and Western Europe as shown in Tables 2.1-2.2.

Table 2.1 Available life cycle inventory database (Curran and Notten, 2006)

Name	Website	Availability	Language	Date Focus (if any)	Number of Datasets	Geographic Origin
Australian Life Cycle Inventory Data Project	http://www.auslci.com.au/	Free	English		100	Australia
BUWAL250	http://svi-Verpackung.ch/de/Services/1&Publikationen /	Fee or included with SimaPro	German, French	Packaging materials		Switzerland
Canadian Raw Material Database	http: / /crmd.uwaterloo.ca/	Free with registration	English, French	Aluminum, glass, plastics, steel, and wood	17	Canada
ecoinvent	www.ecoinvent.ch	License fee	English		4000	Global/Europe/Switzerland
EDIP	www.lca-center.dk	License fee	Danish		100	Denmark
German Network on Life Cycle Inventory Data	www.lci-network.de	On-going	German, English			Germany
Japan National LC A Project	http://www.jemai.or.jp/ english/lca/project.cfm	FEE	Japanese		600	Japan
Korean LCI	http://www.kncpc.re.kr	On-going	Korea, English	Energy/ chemicals, metal, paper, rubber, polymers, electronic/ electric, construction, production, process, delivery, disposal, and utility	158	Korea

Table 2.1 Available life cycle inventory database (Curran and Notten, 2006) (cont'd)

Name	**Website**	**Availability**	**Language**	**Date Focus (if any)**	**Number of Datasets**	**Geographic Origin**
LCA Food	www.lcafood.dk	Free	Danish, English	Food products and processes		Denmark
SPINE@CPM	http://cpmdatabase.cpm.chalmers.se/	Free	English		700	Global
Swiss Agricultural Life Cycle Assessment Database (SALCA)	http://www.agroscope.admin.ch/oekobilanzen/	Available through ecoinvent or with project cooperation	German, English, French, Italian	Agriculture	700	Switzerland
Thai National LCI Database	http://www.thailcidatabase.net		Thai, English			Thailand
US LCI Database Project	www.nrel.gov/lci	Free with contact	English		300	USA

Table 2.2 Industry Organization's Database (Curran and Notten, 2006)

Industry Organization	**Website**	**Availability**	**Language**	**Product Group or Sector**	**Geographic Coverage**
American Plastics Council (APC)	Available from US LCI	Free	English	Polymers	America
EPD-Norway	www.epd-norge.no	Free	Norwegian, English	Norwegian business (several sectors)	Norway and Europe
European Aluminium Association (EAA)	www.aluminium.org	Free	English	Aluminium production	Europe
European Copper Institute (ECI)	www.copper-life-cycle.org	Free with contact	English	Copper tubes, sheets and wire	Europe
European Federation of Corrugated Board Manufacturers (FEFCO	www.fefco.org	Free	English	Corrugated Board	Europe
International Iron and Steel Institute (IISI)	www.worldsteel.org	Free with contact	English	Steel	Global
International Zinc Association	info@iza.com	Available to LCA practitioners on request	English	Zinc	Global
ISSF International Stainless steel Forum (ISSF)	www.worldstainless.org/	Free with contact	English, Chinese, Japanese	Stainless steel	Global
KCL(EcoData)	http://www.kcl.fi/	Free	English	Pulp and paper	Finish/ Nordic
Nickel Institute	http://www.nickelinstitute.org	Free with contact	English	Nickel	Global
PlasticsEurope (formerly APME)	www.plasticseurope.org	Free	English	Plastic	Europe

Table 2.2 Industry Organization's Database (Curran and Notten, 2006) (cont'd)

Industry Organization	Website	Availability	Language	Product Group or Sector	Geographic Coverage
Volvo EPDs	http://www.volvotruck.com/dealers-vtc/en-gb/VTBC-EastAnglia/aboutus/environment/environmental_product_declaration	Free	English	Trucks and busses	Europe
World Steel Carbon Footprint	http://www.worldautosteel.org/Environment/Life-Cycle-Assessment/worldsteel-releases-datasets-to-help-lower-carbon-footprint.aspx	Free by request	English	Steep Products	Global

2.1.3 Life Cycle Impact Assessment (LCIA)

Life cycle impact assessment or LCIA is the of potential environmental impacts of product or process throughout its life cycle in order to achieve better understanding of relationship between product or process and its potential environmental impacts such as resource depletion, global warming, acidification, etc. LCIA consist of 3 mandatory elements and 3 optional elements regarding to the ISO 14044 (Margni and Curran, 2012) as shown in Figure 2.2. Mandatory elements consist of: (1) selection of impact categories, category indicators and characterization models; (2) assignment of LCI results (classification); (3) calculation of category indicator results (characterization). Optional elements consist of: (1) normalization; (2) grouping; and (3) weighting.

2.1.3.1 Selection of Impact Categories, Category Indicators and Characterization Models

The selection of impact categories, category indicators and characterization models should be related to goal and scope of performing LCA. The impact categories are referred to the classes that represent environmental issue such as global warming, acidification, natural resource depletion, etc. Category indicator is the result of simplified model of a very complex reality (Margini and Curran, 2012), that is used to represents the potential of environmental impacts. Characterization models derive the characterization factor, which represent the effect of each element in LCI results on related impact category, by indicating the relationship between LCI results and category indicators. Table 2.3 shows the main

LCIA methodology, which is normally used to perform impacts assessment. Each methodology contains impact categories, category indicators, and characterization factors. Numbers in parentheses (n) indicate the number of category indicators contained in methodology.

Table 2.3 Main LCIA methodology (Margini and Curran, 2012)

Distance-to-Target	Midpoint	Endpoint
Critical Volumina	CML (9+)	EPS (5)
Ecological Scarcity	EDIP (9)	Eco-indicator 99 (3)
	TRACI (12)	
	ILCD Handbook (15)	ILCD Handbook (3)
	Midpoint-Endpoint	
	IMPACT 2002+ (14-4)	
	LIME (11-4)	
	ReCiPe (18-3)	
	IMPACT World+ (30-3)	

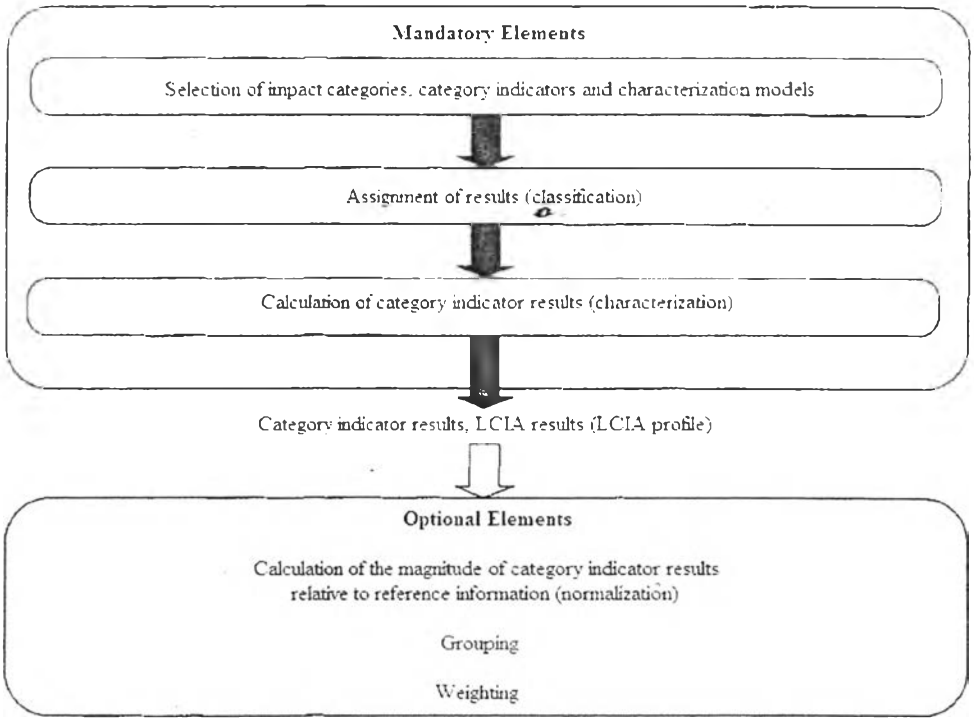


Figure 2.2 Mandatory and optional elements of LCIA (ISO, 2006b).

New implemented environmental impacts in LCSoft new version consists of deposited wastes, energy consumption, mineral extraction, and water consumption. For assessment the impact of deposited waste and water consumption, Ecological Scarcity 2013 was used. Cumulative Energy Demand was used to calculate impact of energy resource consumption. Mineral extraction was assessed by using CML-IA method.

(A) Ecological Scarcity

Ecological scarcity method is based on "distance-to-target" principle defined by SETAC (de Haes, 1996). The ecological scarcity method weights environmental impacts, emissions and resource consumption, by eco-factor. The eco-factor is derived from setting the current level of emissions or consumption of resources (current flow) into relation with the environmental law or corresponding political targets (critical flow).

- Ecological Scarcity – Deposited Wastes

Deposited waste consists of 3 major types of waste, i.e., wastes in above-ground landfills, hazardous wastes, and radioactive wastes. In term of landfill wastes, the key indicator of waste stored in landfill with regard to Ecological Scarcity method is carbon content of material. The current flow consist of the quality of carbon in landfill wastes including inert materials and stabilized residues, bioreactive landfill and slag compartments. Table 2.4 shows eco-factor for carbon in bioreactive landfill wastes in UBP/g C, average slags, and other bioactive land fill wastes. For hazardous wastes, around one-third can be incinerated, while the rest is, wherever possible, recycled, consigned to physical-chemical treatment or stored in landfill for stabilized residues (Frischknecht and Büsser-Knöpfel, 2013). Soil removed when cleaning up contaminated sites is the source of hazardous waste. Table 2.5 shows eco-factors for the consignment of hazardous wastes to disposal sites. In term of radioactive wastes, the hazardousness of radioactive wastes depends on their half-life, type, and intensity of their radiation. Types of radioactive waste are classified to two categories with regard to the Swiss strategy including Short-lived low-level and medium-level wastes (LMLW) and Alpha-toxic wastes (ATW), high-level wastes (HLW) and spent fuel elements (SF). Eco-factors are determined on the basis of legal provisions and scientific calculations by radiotoxicity index (NAGRA 2008). Table 2.6 shows eco-factors for LMLW/SF/ATW/HLW wastes.

Table 2.4 Eco-factors for carbon in wastes consigned to landfills (Frischknecht and Büsser-Knöpfel, 2013)

	Edition 2013	Q	Notes	Edition 2006
Normalization (t C/a)	183,222	B	(TVA, 2011), (VSA, 2012)	97,410
Current flow (t C/a)	183,222	B	(TVA, 2011), (VSA, 2012)	97,410
Critical flow (t C/a)	183,222	b	(TVA, 2011), (VSA, 2012)	79,420
Weighting (-)	1.00			1.50
Eco-factor (UBP/g C)	5.50		C content: 2 %; TVA (2011)	15.00
Eco-factor (UBP/g slags)	0.11			0.61
Eco-factor (UBP/g other bioactive landfill wastes)	0.27			2.30
Q=data quality, for explanation, see Part2, Chapter 6				

Table 2.5 Eco-factors for the consignment of hazardous wastes to disposal sites (Frischknecht and Büsser-Knöpfel, 2013)

	Edition 2013	Q	Notes	Edition 2006
Normalization (t waste/a)	37,223	A		36,900
Current flow (t waste/a)	37,223	A	(BAFU 2011b)	36,900
Critical flow (t waste/a)	37,223	c		36,900
Weighting (-)	1.00			1.00
Eco-factor (UBP/g waste)	27.00			27.00
Eco-factor (UBP/cm^3 waste)	43.00		Density 1600 kg/m3 in accordance with Doka (2003b, Part III, p.41	43.00
Q=data quality, for explanation, see Part2, Chapter 6				

Table 2.6 Eco-factors for LMLW/SF/ATW/HLW wastes (Frischknecht and Büsser-Knöpfel, 2013)

	Edition 2013	Q	Characterization Factor (cm^3 HLW-eq./cm^3)	Edition 2006
Low-level and medium-level wastes (LMLW)	2.1	A	0.000045	3,300
High-level and alpha-toxic wastes (HLW, SF & ATW)	35000	A	0.76	18,000
High-level wastes (HLW & SF)	46000	A	1	
Alpha-toxic wastes (ATW)	69	A	0.0015	
Q=data quality, for explanation, see Part2, Chapter 6; Densities of conditioned and encased wastes: LMLW: 5t/m^3; HLW, SF & ATW: 6.85 t/m^3				

- Ecological Scarcity – 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). In term of application of life cycle inventory data, the life cycle inventory data should include entre water balance. Table 2.7 shows elementary flows for complete inventory of water used in processes. The life cycle inventory in LCSoft database includes only data on water withdrawal and not on consumptive water use. The correction factors are introduced in the assessment of consumptive water use. They quantify the average proportion of consumptive water use in water withdrawal for each individual elementary flow as shown in Table 2.8. Figure 2.3 shows elementary flows for complete inventory of water used in processes.

Table 2.7 Elementary flows for complete inventory of water used in processes (Frischknecht and Büsser-Knöpfel, 2013)

No.	Elementary Flow	Industrial Process	Agricultural Process
Input			
1	Water, unspecified natural origin, country XY	Water for production process (e.g. cleaning devices, containers, etc.)	Water for irrigation
-	Water, rain	Not taken into account	Taken into account for complete inventory
2	Water, embodied, in product, country XY	Water embodied in raw materials	Water embodied in seeds
Output			
3	Water, country XY (emitted in the air)	Emission: water vaporized during the production process	Emission: evaporated water from farmed fields
4	Water, river/lake	Discharged directly from the industry into surface waters	Discharged from fields into surface waters
5	Water, sea	Discharged directly from industry into the sea	Discharged from the fields into the sea
6	Water, soil	Direct infiltration in the soil	Infiltration in the soil from fields
7	Water, embodied, in product, country XY	Water embodied in the product	Water embodied in the product
Total			
Water withdrawal		1	
Consumptive water use		3+7-2	

Table 2.8 Standard values for the proportion of consumptive water use (Frischknecht and Büsser-Knöpfel, 2013)

Elementary Flow in the Ecoinvent v.2.2 Database	Proportion of Consumptive Water Use	Source
Water, cooling, in unspecified natural origin	5 %	(Muñoz *et al.*, 2010; Rosiek *et al.*, 2010; Jefferies *et al.*, 2011; Gleick, 1994; Shaffer, 2008; Stiegel *et al.*, 2008; Scown *et al.*, 2011)
Water, lake	10 %	(Shaffer, 2008; Statistics Canada, 2010)
Water, river	10 %	
Water, well, in ground	10 %	
Water, unspecified natural origin	10 %	
Water, salt, ocean	0	
Water, salt, sole	0	
Water, turbine use, in unspecified natural origin	0	

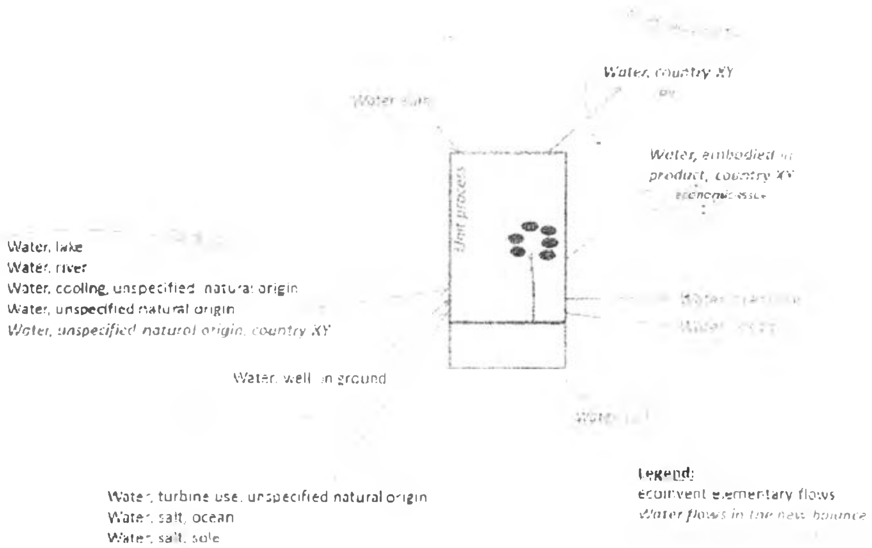


Figure 2.3 Elementary flows for complete inventory of water used in processes (Flury *et al.*, 2012).

(B) Cumulative Energy Demand – Energy Consumption

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 2.9.

Table 2.9 Detail of CED implemented in LCSoft

Category	Subcategory	Resources
Non-renewable Resource	fossil	crude oil, coal mining off-gas, hard coal, lignite, natural gas, peat
	nuclear	uranium
Renewable Resources	biomass	wood, food product, biomass from agriculture
	wind, solar, geothermal	wind energy, solar energy, geothermal energy
	water	hydro power energy

(B) CML-IA – 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).

- Economic Reserve

Measure of the metal content in deposits can be economically extracted at the time of determination including current prices, state of technology, etc. (Schneider *et al.*, 2015).

- Reserve Base

The reserve base is used to estimate of the size of those parts of resources that had reasonable potential for becoming economic within planning horizons. Reserve base is based on expert opinion rather than on actual data (Schneider *et al.*, 2015).

- Ultimate Reserve

The quantity of resource that is ultimately available, estimated by multiplying the average natural concentration of the resource in the primary extracted media (Guinee, 1995).

The reserve base and economic reserve is that the estimate of the size of the reserve involves a variety of respectively technical and economic consideration not directly related to the environmental problem of resource depletion. 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 *et al.*, 2002).

2.1.3.2 Assignment of LCI Results (Classification)

This step is classification of inventory data that are grouped into relevant impact categories based on their effects on environmental damage. For example, CO_2 and CH_4, which are the greenhouse gases, are both classified to the Global warming. Scientific Applications International Corporation (SAIC) (2006) illustrates commonly used life cycle impact categories, scale of effects, related LCI data and characterization factors as shown in Table 2.10. Impact categories can be organized in two levels which are midpoint and endpoint, for instant, ReCiPe shows the relationship between the inventory and the midpoint categories and the endpoint categories as shown in Figure 2.4.

Table 2.10 Example of impact categories (Scientific Applications International Corporation (SAIC), 2006)

Impact Category	Scale	Examples of LCI Data (i.e. classification)	Common Possible Characterization Factor	Description of Characterization Factor
Global Warming	Global	Carbon Dioxide (CO_2) Nitrogen Dioxide (NO_2) Methane (CH_4) Chlorofluorocarbons (CFCs) Hydrochlorofluorocarbons (HCFCs) Methyl Bromide (CH_3Br)	Global Warming Potential	Converts LCI data to carbon dioxide (CO_2) equivalents Note: global warming potentials can be 50, 100 or 500 year potentials.
Stratospheric Ozone Depletion	Global	Chlorofluorocarbons (CFCs) Hydrochlorofluorocarbons (HCFCs) Halons Methyl Bromide (CH_3Br)	Ozone Depleting Potential	Converts LCI data to trichlorofluoromethane (CFC-11) equivalents.
Acidification	Regional Local	Sulfur Oxides (SOx) Nitrogen Oxides (NOx) Hydrochloric Acid (HCL) Hydroflouric Acid (HF) Ammonia (NH_3)	Acidification Potential	Converts LCI data to hydrogen (H^+) ion equivalents.
Eutrophication	Local	Phosphate (PO_4) Nitrogen Oxide (NO) Nitrogen Dioxide (NO_2) Nitrates Ammonia (NH_3)	Eutrophication Potential	Converts LCI data to phosphate (PO_4) equivalents
Photochemical Smog	Local	Non-methane hydrocarbon (NMHC)	Photochemical Oxident Creation Potential	Converts LCI data to ethane (C_2H_6) equivalents.
Terrestrial Toxicity	Local	Toxic chemicals with a reported lethal concentration to rodents	LC_{50}	Converts LC_{50} data to equivalents. uses multi-media modeling, exposure pathways
Aquatic Toxicity	Local	Toxic chemicals with a reported lethal concentration to fish	LC_{50}	Converts LC_{50} data to equivalents: uses multi-media modeling, exposure pathways.
Human Health	Global Regional Local	Total releases to air, water, and soil.	LC_{50}	Converts LC_{50} data to equivalents. uses multi-media modeling, exposure pathways
Resource Depletion	Global Regional Local	Quantity of minerals used Quantity of fossil fuels used	Resource Depletion Potential	Converts LCI data to a ratio of quantity of resource used versus quantity of resource left in reserve.
Land Use	Global Regional Local	Quantity disposed of in a landfill or other land modifications	Land Availability	Converts mass of solid waste into volume using an estimated density.
Water Use	Regional Local	Water used or consumed	Water Shortage Potential	Converts LCI data to a ratio of quantity of water used versus quantity of resource left in reserve.

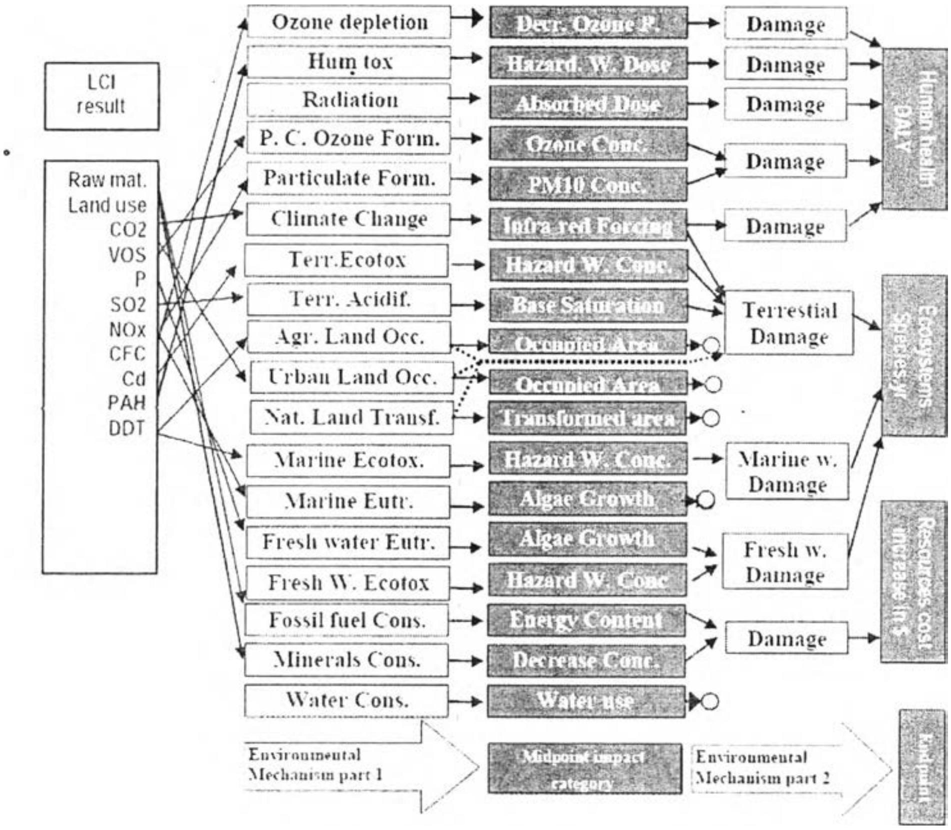


Figure 2.4 Relationship between the inventory and the midpoint categories (environmental mechanisms) and the endpoint categories, ReCiPe 2008 (Eco-efficiency Action Project, 2010).

2.1.3.3 Calculation of Category Indicator Results

The step that every substances in LCI results that are classified into each category of environmental impact is run through a model to calculate its potential impact. For example, Global warming potential is typically based on 1 kg of CO_2 emitted (CO_2-equivalents). The characterization factors (CFs) of each related substance based on impact category are multiplied with amount of each emitted substance and the resulting values are summed for the respective impact category as shown in Equation 2.3.

$$I^{k} = \sum_{t,c} EM_{t,c}\, x\, CF^{k}_{t,c} \tag{2.3}$$

Where "c" indicates impact category, "I" is referred to indicator results for category "*k*", "$CF^{k}_{t,c}$" represents the characterization factor of substance "*t*" emitted to compartment "*c*" of the impact category "*k*", and "$EM_{t,c}$" indicate amount of substance *t* emitted to compartment *c*.

For various substances in LCI database, CFs may not cover for all kind of substances, so the characterization factors estimation can be applied for the case. The study of "Estimation of Environment-Related Properties of Chemicals for Design of Sustainable Process: Development of Group-Contribution^{+} (GC^{+}) Property Models and Uncertainty Analysis" (Hukkerikar *et al.*, 2012) shows the development of systematic model to estimate the pure component properties which are function of structurally dependent parameters representing the molecules and their contributions and the property estimations by (GC^{+}) are included in life cycle impact assessment data of LCSoft2.0 (Kalakul, 2013).

2.1.3.4 Optional Elements

2.1.3.4.1 Normalization

Normalization is the calculation of magnitude of category indicator results compared to reference information to solve the incompatibility of units. For instance, impact category indicator results of climate change and eutrophication are "A" kg CO_2 equivalent and "B" kg P equivalent respectively. After two results were normalized to unit of year (y) for example, the climate change impact can be compared with eutrophication impact to investigate how climate impact are relatively low or high compared to eutrophication impact.

2.1.3.4.2 Grouping

Grouping is "sorting with the purpose of possibly reducing the number of impact categories, as well as possibly ranking them in order of important" (Margni and Curran, 2012).

2.1.3.4.3 Weighting

Weighting is the creation of environmental impact scores by multiplying weighting factor to category indicator results. Weighting can be applied to normalized or non-normalized scores.

2.1.4 Interpretation

The interpretation of LCA is the evaluation of results of inventory analysis and also life cycle impact assessment results associated with goal and scope of the study to help in decision making such as to selecting of products, improvement of processes or services, etc., with clear understanding of the uncertainty and the assumption used (Margni and Curran, 2012).

2.1.4.1 Contribution Analysis

Contribution analysis represents the contribution of the LCA results which are process contribution, LCI results and LCIA results in the production system in order to determine the processes which play a significant role in the production system.

2.1.4.3 Sensitivity Analysis

Sensitivity analysis is used to investigate the influence of different assumption, such as system boundaries, allocation basis, temporal and spatial effect on both LCI and LCIA (Guinée *et al.*, 2002), and characterization method, to the assessment results. The principle is recalculation of LCA with the changed assumption (Goedkoop *et al.*, 2008).

2.2 LCSoft Overview

2.2.1 LCSoft1.0

LCSoft was firstly developed on Microsoft Visual Basic for Application (VBA)-Excel based program (Piyarak, 2012) as shown in Figure 2.5. It was developed to be integrated with process simulation program (ProII) to quantify the environmental impacts of products or processes from cradle to gate especially for chemical and biochemical processes. LCSoft1.0 contains 8 impact categories (global warming, ozone depletion, acidification, eutrophication, photochemical smog, human toxicity, aquatic toxicity, and terrestrial toxicity) for LCIA and carbon footprint estimation, as shown in Figure 2.7 and energy and fuel consumption, as shown in Figure 2.6. Inventory data are gathered from Commission of the European Communities (Commission of the European Communities, 1996), USES-LCA (Huijbregts *et al.*, 2000), and Simplebox 3.0 (den Hollander *et al.*, 2004)

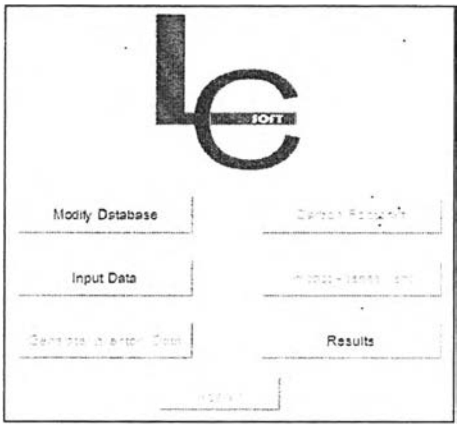
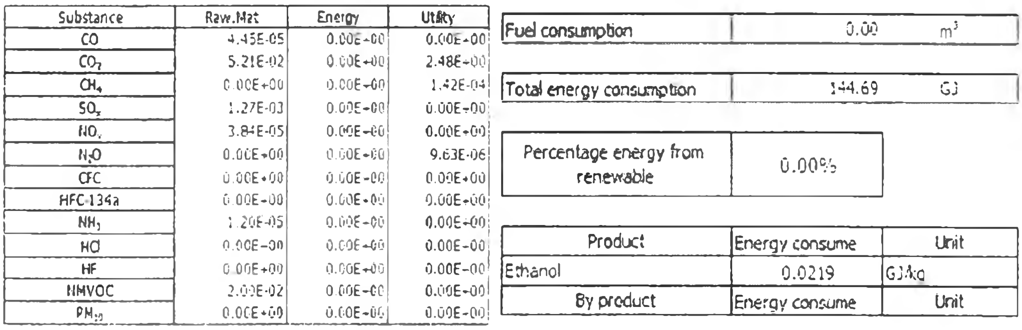


Figure 2.5 LCSoft1.0 interface (Piyarak, 2012).



Substance	Raw.Mat	Energy	Utility
CO	4.45E-05	0.00E+00	0.00E+00
CO_2	5.21E-02	0.00E+00	2.48E+00
CH_4	0.00E+00	0.00E+00	1.42E-04
SO_x	1.27E-03	0.00E+00	0.00E+00
NO_x	3.84E-05	0.00E+00	0.00E+00
N_2O	0.00E+00	0.00E+00	9.63E-06
CFC	0.00E+00	0.00E+00	0.00E+00
HFC-134a	0.00E+00	0.00E+00	0.00E+00
NH_3	1.20E-05	0.00E+00	0.00E+00
HCl	0.00E+00	0.00E+00	0.00E+00
HF	0.00E+00	0.00E+00	0.00E+00
NMVOC	2.00E-02	0.00E+00	0.00E+00
PM_{10}	0.00E+00	0.00E+00	0.00E+00

Fuel consumption	0.00	m^3
Total energy consumption	144.69	GJ

Percentage energy from renewable	0.00%

Product	Energy consume	Unit
Ethanol	0.0219	GJ/kg
By product	Energy consume	Unit

Figure 2.6 Input-output data show in inventory data section in LCSoft 1.0 (Kalakul, 2013).

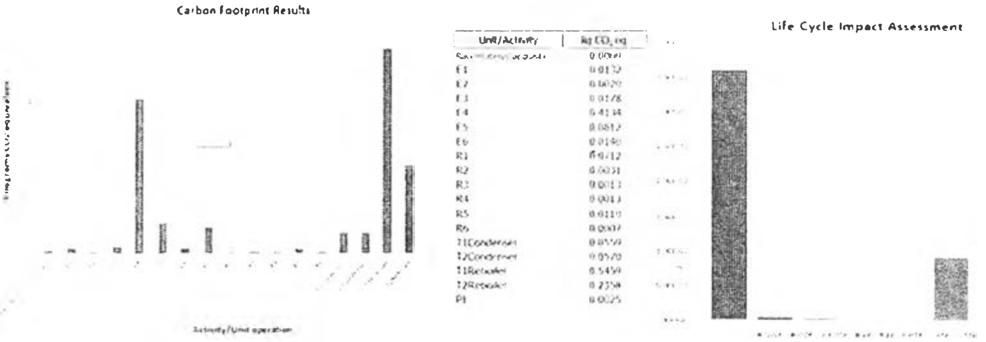


Figure 2.7 Carbon footprint and environmental impacts results in LCSoft1.0 (Kalakul, 2013).

Table 2.11 Environmental impacts comparing between LCSoft1.0 and SimaPro (Piyarak, 2012)

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%

The validation of software was performed by comparing LCIA results which are calculated from hand calculation and LCSoft1.0 by using acetaldehyde production as a case study and comparing assessment results of LCSoft1.0 with SimaPro using bio-ethanol production as a case study as shown in Table 2.11. The results from hand calculation and LCSoft are nearly the same but there are some difference between LCSoft1.0 and SimaPro such as environmental impact of human toxicity, acidification, and eutrophication that has different percentage 52.68, 52.51, and 47.37 respectively. Piyarak (2012) explained that: the variation of result come from amount of emission factors that are contained in database (only 13 emission factors are contained in LCSoft1.0) and environmental impact of human toxicity in LCSoft1.0 cover only emission to air. Piyarak (2012) concluded that: LCSoft1.0 is simple, time saving, easy to handle, cheap suit for personal or academic purpose, and inventory data has flexibility due to user can change or add the value upon the situation. However, inventory data and characterization factor should be extended for supporting various chemical processes and evaluating environmental impact efficiently.

2.2.2 LCSoft2.0

The next version of LCSoft (LCSoft v2.0) was developed to be integrated with process design tools in order to perform multi-objective process evaluation and other tools used in sustainable process design (Kalakul *et al.*, 2014). There are sustainable process design software, SustainPro (Carvalho *et al.*, 2013) and economic analysis software, ECON (Saengwirun, 2011). Software interface is shown in Figure 2.8. LCSoft2.0 framework is divided to four parts which are

2.2.2.1 Tool-1 Knowledge Management

The inventory data was gathered from U.S. LCI (NREL, 2012), other open sources, and option for further data expansion. The structure of LCSoft database is shown in Figure 2.9.

2.2.2.2 Tool-2 Characterization Factor Estimation

LCSoft2.0 contains characterization factor data from U.S. Environmental Protection Agency (USEPA), USEtox^{TM} database (Rosenbaum *et al.*, 2008) and high accuracy developed predictive property model (Hukkerikar *et al.*, 2012), for 11 environmental impacts categories ("human toxicity by ingestion, human toxicity by exposure, aquatic toxicity, terrestrial toxicity, global warming, ozone depletion, photochemical oxidation, acidification, human toxicity-carcinogenic, human toxicity-non carcinogenic, and fresh water eco-toxicity", (Kalakul *et al.*, 2014)

2.2.2.3 Tool-3 Calculation of LCA including Resource and Energy Consumption, Carbon Footprint, and Environmental Impacts

This tool is for calculation of LCA including 5 major steps; that are check existence, retrieve LCI data, calculate resource and energy consumption, calculate carbon footprint, and assess impacts. LCSoft 2.0 has 1 optional step that is additional features including sensitivity analysis and alternative comparison

2.2.2.4 Tool-4 Integration of LCSoft, ECON and SustainPro

The environmental impacts are evaluated by using LCSoft, economical performances are evaluated by using ECON software, and process sustainability is evaluated by using SuntainPro software. Kalakul *et al.* (2014)

explained that "The advantages of this tool are that it makes the data transfer from one software-tool to another very smooth, efficient and consistent, thereby, reducing time spent in performing the calculations. Through Tool-4, the user can easily enter the necessary prerequisites for the integrated software in the main interface in one step as shown in Figure 2.10. The prerequisites for all software components are mass and energy balances from process stream table and the corresponding equipment table. The additional prerequisites for LCSoft are the definitions of the system boundaries. The additional prerequisites for ECON are equipment sizing parameters, and price of materials. The additional prerequisites for SustainPro are component properties and reaction data".

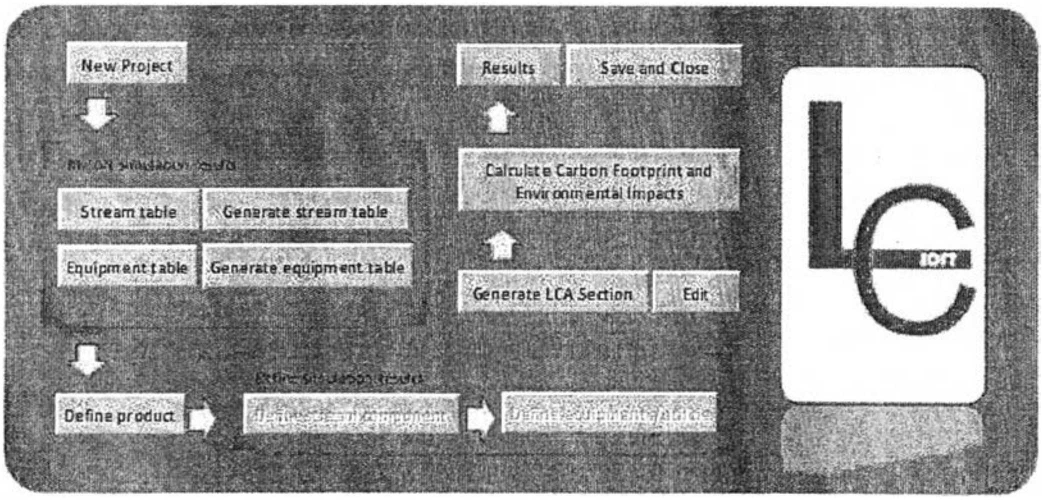


Figure 2.8 LCSoft2.0 interface (Kalakul, 2013).

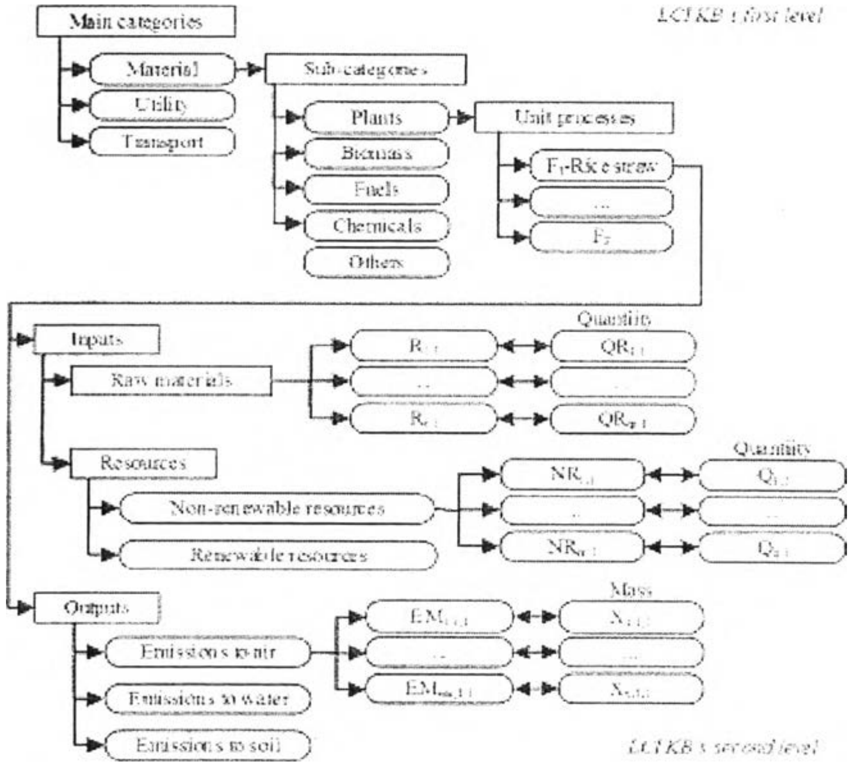


Figure 2.9 Structure of LCI KB (Kalakul *et al.*, 2014).

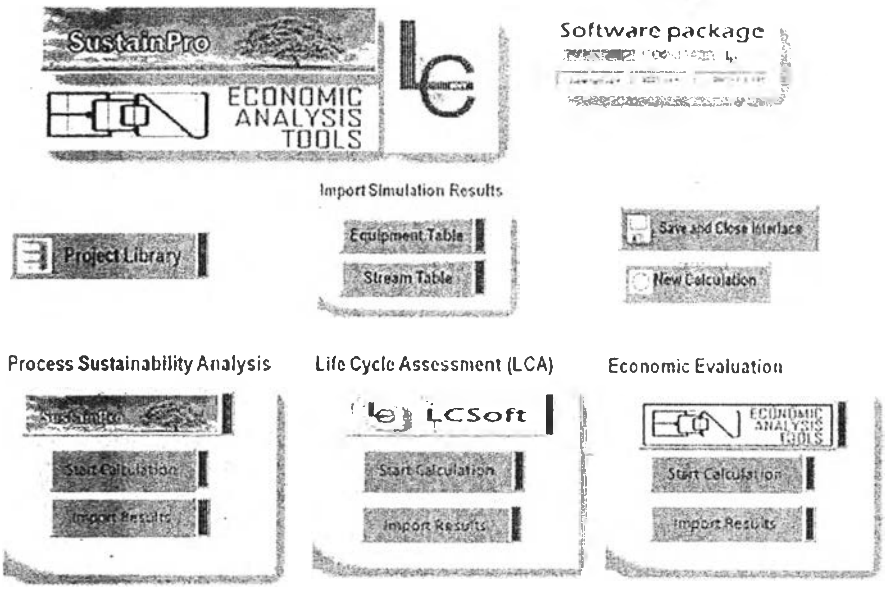


Figure 2.10 Main interface of integrated software (Kalakul *et al.*, 2014).

LCSoft2.0 contains additional tools such as alternative comparison, function which allow user to compare LCA result from different process design, sensitivity analysis, function which allow user to investigate changing of LCA result according to variation of raw materials and energy sources used in the process, and generate LCI data in LCSoft, function which allow user to define new LCI data as shown in Figure 2.11.

The validation of LCSoft2.0 was performed by comparing environmental impact results by using case study of bioethanol production from cassava rhizome in Thailand from cradle-to-gate with SimaPro7.1 as shown in Figures 2.12-2.13. Kalakul *et al.* (2014) mentioned that "The SSE and percent different of GWP (global warming potential) and PCOP (Photochemical oxidation) from LCSoft and SimaPro7.1 is not significant difference, so the boundary definition and assumption in inventories, material flows, and energy flows are the same. The major differences are values of AP (Acidification), HTNC (human toxicity-non-carcinogenics), and ET (eco-toxicity). Difference in AP value due to the larger sets of characterization factors associated with the combustion fuels contained in Franklin database in SimaPro7.1 compared with LCSoft model. HTNC is greater than SimaPro7.1 because LCSoft has isoprene's characterization factor which does not exist in SimaPro7.1. The differences of HTC, ODP, and ET are in the acceptable ranges" (Kalakul *et al.*, 2014).

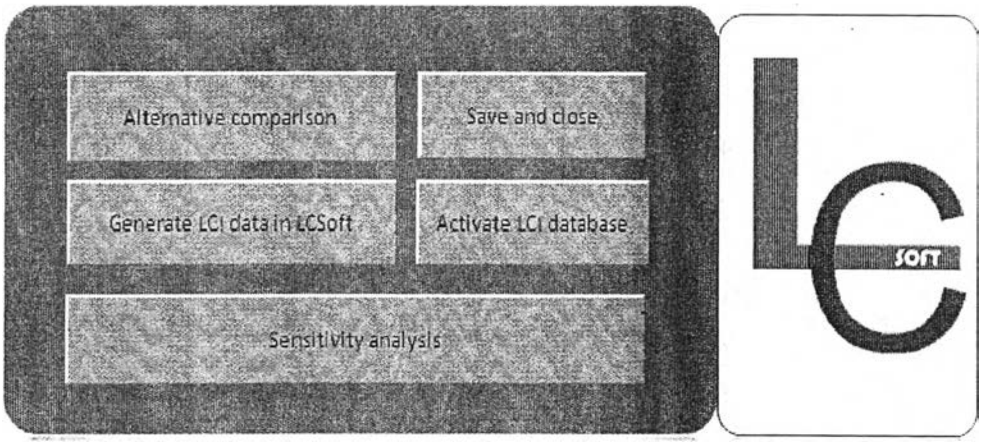


Figure 2.11 Additional tools contained in LCSoft2.0 (Kalakul, 2013).

Environmental impacts	Unit	SimaPro	LCSoft	Sum squares error (SSE)	Percent difference (%)
Global Warming (GWP)	kg CO_2 eq.	7.29E-01	7.30E-01	2.04E-06	0.19
Acidification (AP)	H^+ moles eq.	6.46E-01	1.07E-01	0.29070047	83.5
Carcinogenics (HTC)	kg benzene eq.	8.65E-06	2.89E-07	6.99E-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	8.69E-20	72.06
Ecotoxicity (ET)	kg 2,4-D eq.	1.24E-03	6.20E-03	2.45E-05	397.99
Photochemical oxidation (PCOP)	kg NO_x eq.	2.40E-02	2.61E-02	4.42E-06	8.75

Figure 2.12 Comparative environmental impacts of bioethanol production between LCSoft and SimaPro7.1 (Kalakul *et al.*, 2014).

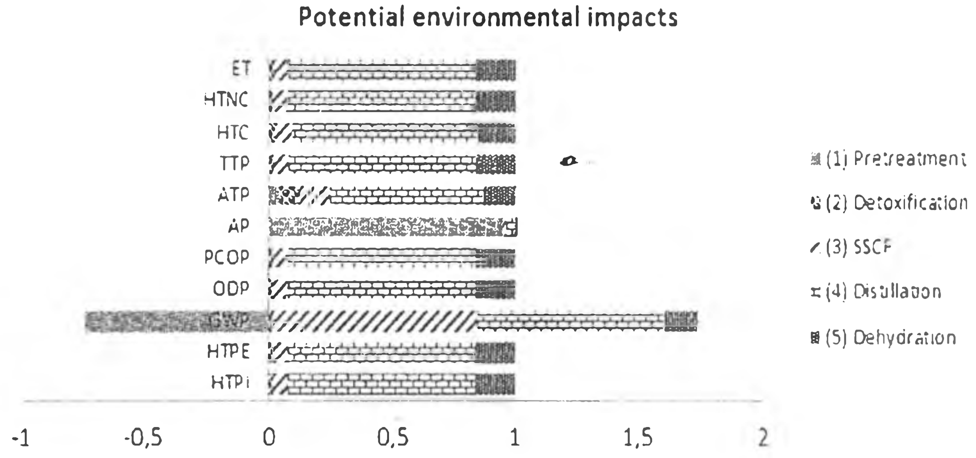


Figure 2.13 Environmental impact results calculated by LCSoft2.0 (Kalakul *et al.*, 2014).

The validation of LCSoft2.0 with commercial LCA program, SimaPro.1, shows the abilities of identifying and quantifying environmental impacts of product or process with complacent results.

2.2.3 Features Comparison of LCSoft2.0 and SimpaPro7.1

Table 2.12 shows the comparison of software features between LCSoft2.0 and SimaPro7.1. LCSoft2.0 has no automatic LCI calculation function so it is really important to add LCI calculation function to LCSoft, in order to perform LCI calculation that is required for LCIA calculation. For expansion of LCI data boundary, inventory data can be added to LCI database especially for chemical and biochemical process. For improving and covering more impact categories, energy consumption is needed to be developed. Water resource consumption, mineral extraction, and deposited waste are needed to be added. Contribution analysis is necessary to be performed in order to investigate the contribution of processes, LCI results, and LCIA results in each stage of production system, and to find the significant contributed impacts or substances for further products or processes development.

Table 2.12 Comparison of features in LCSoft2.0 and SimaPro7.1

Available Features in Software	**LCSoft2.0**	**SimaPro7.1**	**Remarks**
Life cycle inventory			
Life Cycle Inventory Database	Small	Large	Need to be improved
Life Cycle Inventory Calculation	-	/	Need to be improved
Impact Assessment			
Life Cycle Impact Assessment	**WAR algorithm with group contribution** Humantoxicity by ingestion Humantoxicity by exposure Aquatic toxicity Terrestrial toxicity Global warming Ozone depletion Photochemical oxidation Acidification Carciogenics Non carcinogenics Fresh water ecotoxicity	Depend on characterization factor data set	No change
Energy Consumption	/		Need to be improved
Water Consumption	-		Need to be improved
Mineral Extraction	-		Need to be improved
Deposited Wastes	-		Need to be improved
Optional Impact Assessment			
Carbon Footprint	/	-	No change
Interpretation			
Process Contribution	-	/	Need to be improved
LCI results Contribution	-	/	Need to be improved
LCIA results Contribution	/	/	Need to be improved
Sensitivity Analysis	/	/	No changing