IMPROVEMENT OF LIFE CYCLE ASSESSMENT SOFTWARE AND ITS APPLICATIONS

Yodsathorn Chavewanmas

A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Science
The Petroleum and Petrochemical College, Chulalongkorn University
in Academic Partnership with
The University of Michigan, The University of Oklahoma,
Case Western Reserve University, and Institut Français du Pétrole
2017

Thesis Title:	Improvement of Life Cycle Assessment Software and Its Applications
By:	Yodsathorn Chavewanmas
Program:	Petrochemical Technology
Thesis Advisors:	Asst. Prof. Pomthong Malakul Prof. Rafiqul Gani

---

Accepted by The Petroleum and Petrochemical College, Chulalongkorn University, in partial fulfillment of the requirements for the Degree of Master of Science.

.... College Dean

(Prof. Suwabun Chirachanchai)

Thesis Committee:

....

(Asst. Prof. Pomthong Malakul)

....

(Prof. Rafiqul Gani)

....

(Assoc. Prof. Thumrongrut Mungcharoen)

....

(Asst. Prof. Kitipat Siemanond)

ABSTRACT

5871023063: Petrochemical Technology Program

Yodsathorn Chavewanmas: Improvement of Life Cycle Assessment Software and Its Applications.

Thesis Advisors: Asst. Prof. Pomthong Malakul, and Prof. Rafiqul Gani 85 pp.

Keywords: Life cycle assessment/ Life cycle inventory/ Life cycle impact assessment

LCSoft is Life Cycle Assessment (LCA) software which developed for perform LCA together with process design. It is a stand-alone tool with ability to be integrated with other process design tools such as process simulation software (PROII/ASPEN), economic analysis tool (ECON), and sustainable process design tool (SustainPro). In addition, several optional interpretation features are available such as, sensitivity analysis, alternative comparison, and eco-efficiency evaluation. In this research, LCSoft had been improved in performance and application range. The development framework consisted of four tasks. The first task deals with improvement of LCI and LCIA calculation which new pathway for calculation and allocation had been added. The second task deals with new features development which including normalization, parameter sensitivity analysis, data quality indicator, and endpoint impact categories. The third task deals with extension of LCI data in order to cover all of impact categories calculation. The fourth task deals with validation of LCSoft software. The integrated software was validated and verified by comparing assessment results for bioethanol production from cassava rhizome process and for Para-xylene production by Toluene Methylation as case studies and compared with other commercial LCA software. The results indicated that the new feature of LCSoft provided reliable calculations very efficiently, and were especially useful for chemical and biochemical sustainable process design studies.

บทคัดย่อ

ยศธร ฉวีวรรณมาศ : การพัฒนาโปรแกรมประเมินวัฏจักรชีวิตและการนำไปประยุกต์ใช้งาน (Improvement of Life Cycle Assessment Software and Its Applications) อ. ที่ปรึกษา : ผศ. ดร. ปมทอง มาลากุล และ ศ. ดร. ราฟิก กานี 85 หน้า

ซอฟต์แวร์แอลซีซอฟต์คือซอฟต์แวร์ที่ใช้ประเมินวัฏจักรชีวิต ซึ่งถูกพัฒนาเพื่อเป็นเครื่องมือในการคำนวณและประเมินวัฏจักรชีวิตควบคู่ไปกับการออกแบบกระบวนการต่างๆ แอลซีซอฟต์เป็นเครื่องมือที่สามารถใช้งานร่วมกับซอฟต์แวร์อื่นได้ เช่น ซอฟต์แวร์จำลองกระบวนการ ซอฟต์แวร์วิเคราะห์ความคุ้มค่าทางเศรษฐกิจ และซอฟต์แวร์การประเมินความยั่งยืนของกระบวนการ นอกจากนี้แอลซีซอฟต์ยังมีฟังก์ชันในการนำเสนอผลการวิเคราะห์ในรูปแบบต่างๆให้เลือกใช้ เช่น การวิเคราะห์ความอ่อนไหวของข้อมูล การเปรียบเทียบกระบวนการทางเลือก และการประเมินประสิทธิภาพเชิงนิเวศเศรษฐกิจ ในงานวิจัยนี้ซอฟต์แวร์แอลซีซอฟต์ได้ถูกพัฒนาประสิทธิภาพและขยายขอบเขตการประยุกต์ใช้งานให้กว้างขึ้น โดยแบ่งกรอบการวิจัยออกเป็นสี่ส่วน ได้แก่ ส่วนที่หนึ่ง การพัฒนาฟังก์ชันการคำนวณผลกระทบทางสิ่งแวดล้อม โดยสร้างทางเลือกในการคำนวณให้แก่ผู้ใช้ และเพิ่มการคำนวณด้วยวิธีการปันส่วนผลกระทบทางสิ่งแวดล้อม ส่วนที่สอง การพัฒนาฟังก์ชั่นใหม่ๆ เช่น ฟังก์ชันการลดความซับซ้อนของข้อมูล ฟังก์ชันการวิเคราะห์ความอ่อนไหวในแต่ละปัจจัยที่เกี่ยวข้อง ฟังก์ชันประเมินคุณภาพของการเก็บข้อมูล และการประเมินผลกระทบขั้นปลาย ส่วนที่สาม การขยายฐานข้อมูลและการจัดการข้อมูลให้ครอบคลุมผลกระทบต่อสิ่งแวดล้อมทุกชนิด ส่วนที่สี่ การตรวจสอบความถูกต้องและความน่าเชื่อถือของซอฟต์แวร์แอลซีซอฟต์ โดยจะทำการตรวจสอบผ่านการเปรียบเทียบผลการประเมินจากกรณีศึกษา กระบวนการผลิตเอทานอลจากเหง้ามันสำปะหลัง และกระบวนการผลิตพาราไซลีนด้วยวิธีโทลูอีนเมทิลเลชัน เปรียบเทียบผลกับซอฟต์แวร์อื่นที่ใช้ในเชิงพาณิชย์ ซึ่งผลลัพธ์แสดงให้เห็นว่าฟังก์ชันใหม่ของแอลซีซอฟต์ มีการคำนวณที่น่าเชื่อถือและมีประสิทธิภาพ โดยเฉพาะในการออกแบบกระบวนการเคมี และการออกแบบกระบวนการเคมีทางชีวภาพ

ACKNOWLEDGEMENTS

This work would not have been possible without the assistance of the following individuals:

First and foremost, I would like to express my sincere gratitude to my advisor, Asst. Prof. Pomthong Malakul, for his beneficial suggestion, providing valuable knowledge, and supervision from the very early stage of this research. He also provided me unflinching encouragement, patience, and all helpful supports throughout my research.

I would also like to appreciate Prof. Rafiqul Gani for funding and offering me the best opportunity of visiting Department of Chemical and Biochemical Engineering at Technical University of Denmark (DTU) and his invaluable knowledge, and guidance, which very helpful for shaping up my ideas and kind support throughout my research.

I would like to thank Asst. Prof. Kitipat Siemanond and Assoc. Prof. Thumrongrut Mungcharoen for being my thesis committee. Their suggestions and comments are certainly important and helpful for me and this work.

I am grateful for the partial scholarship and partial funding of the thesis work provided by the Petroleum and Petrochemical College.

I greatly appreciate all PPC staffs and my friends who gave me support and encouragement.

I would like to thank Ms. Chanakran Homla-or and Ms. Sawitree Kalakul for her suggestion and help.

Finally, I would like to express my sincere gratitude to thank my whole family for their love, their encouragement, and for understanding every single part of my mind.

TABLE OF CONTENTS

CHAPTER **PAGE**

LIST OF TABLES

TABLE **PAGE**

TABLE **PAGE**

LIST OF FIGURES

CHAPTER I
INTRODUCTION

Nowadays, environmental awareness has become the global issue due to the growth of population, incresing in demand of people, and depletion of natural resources. Industries and businesses organization must be awared and developed the efficient and sustainable process. Thus, the environmental impact assessment is introduced as the key factor for developing or retrofiting the process to be more economical and environmental friendly. One of effective tool that widely used for environmental impact assessment is Life Cycle Assessment or LCA.

Life cycle assessment is an application that provides analysis function of environmental impacts through entire life cycle of the products (starting from production of raw materials to product disposal). LCA is used to identify and improvement the whole process or part of the process in order to minimize the environmental problems and decision making. In particular, LCA are needed to deal with the complicate and numerous data which are required the software for calculation. At present, several commercial software are available such as SimaPro (developed by Pre Consultants, Netherland), and Gabi (developed by PE International, Deutschland). However, in the view of process design, there still need the software which has cooperation function with other process design tools.

Accordingly, our research group has developed LCSoft as the software with an applicable life cycle assessment and integrated to other process design tools such as process simulation, economic analysis tool, and sustainable process design (Piyarak, 2012; Kalakul, 2013; and Supawanich, 2014; Kaesinee, 2015). LCSoft could provide systematically calculation of both Life Cycle Inventory (LCI) and Life Cycle Impact Assessment (LCIA), and evaluated environmental impact result in 21 midpoint impact categories and also carbon footprint results with respect to the production stage. The software could also show the contribution of processes, LCI, and LCIA. In addition, several optional interpretation features were available, such as, sensitivity analysis, alternative comparison, and eco-efficiency evaluation. However, in this research, LCSoft was developed in order to improve the performance and wider range of application.

In this research, LCSoft software was further developed in various aspects by improving LCIA calculations, developing new features, extending and managing the database, and also developing the interface of software to be more user-friendly. In addition, the improved software was validated and verified by comparing assessment results for bioethanol production from cassava rhizome and for para-xylene production by toluene methylation with commercial LCA software, SimaPro.

CHAPTER II
BACKGROUND AND LITERATURE REVIEW

LCSoft is simple LCA software that has user-friendly features to perform LCA study with reliability and effectiveness. Nevertheless, user needs to review LCA principle in order to understand concepts and results from the software. Therefore, this chapter describes two main topics which are principle of LCA, and previous development of LCSoft software.

2.1 Life Cycle Assessment (LCA)

Life Cycle Assessment is specific process for evaluating the environmental impacts of product along the product's life time by identifying and quantifying energy consumption, material used, and also emission that released to the environment. The entire product's life that starting from raw materials acquisition through manufacturing process, transportation, used, disposal and also material recycle is shown by life cycle stages in Figure 2.1. LCA result is used in various objectives such as planning the environmental management strategies, decision making on sustainable process design, pollution prevention for government policy and being important indicator in order to get "Ecolabelling" or environmental friendly certification for products and/or services.

The methodology of LCA study consists of four phases. According to the worldwide standard, International Organization for Standardization (ISO), describes the principles and framework for life cycle assessment in ISO 14040 and describes requirements and guidelines in ISO 14044. Four phases in LCA study including: (1) Goal and scope definition phase; (2) Life cycle inventory analysis phase (LCI); (3) Life cycle impact assessment phase (LCIA); and (4) Life cycle interpretation phase (ISO, 2006).

.

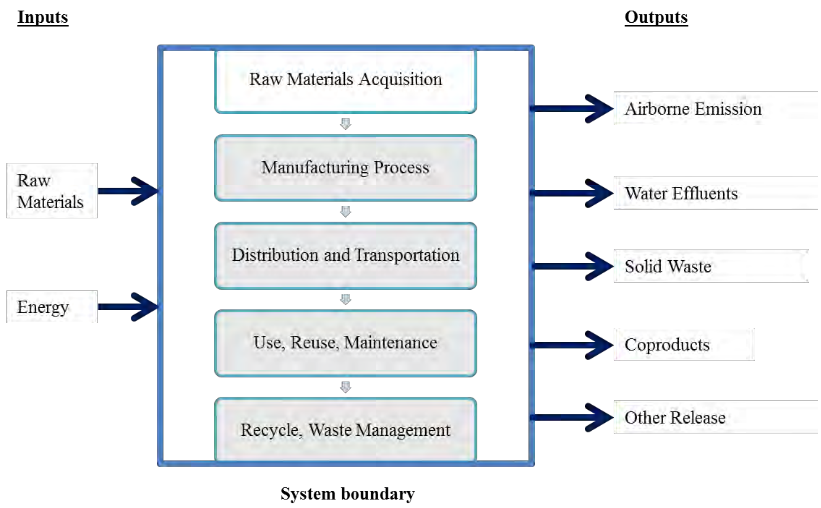

Figure 2.1 Life cycle stages, inputs and outputs for life cycle assessment.

2.1.1 Goal and Scope Definition

The product's life cycle or the LCA models is simplification of the complex reality process which may cause the disguise data. In order to reduce the irrelevant of assessment from simplification, Goal and scope definition is the first step which is very significant part in LCA study.

Goal of LCA can be differently defined in each LCA study depend on the purpose, for example, identifying hotspot for improvement process, retrieving Ecolabel or environmental footprint label, and comparing products in each category.

Scope of LCA can be defined by setting system boundary with corresponding to goal, life cycle stage, and time boundary. Due to the LCA is an iterative process, the scope that set in the first time may be changed later when more information become available. There are four levels of life cycle stage:

2.1.1.1 Cradle to Grave

This boundary covers all life cycle stage, starting from collecting raw material, manufacturing, usage, recycling, and disposal.

2.1.1.2 Cradle to Gate

This boundary covers partial life cycle stage, starting from collecting raw material until entering manufacturing process.

2.1.1.3 Gate to Gate

This boundary covers partial life cycle stage, consider only manufacturing process.

2.1.1.4 Gate to Grave

This boundary covers partial life cycle stage, starting from usage until product disposal.

2.1.2 Life Cycle Inventory Analysis (LCI)

LCI is data collection and calculation phase, all relevant input and output flow in all stage are recorded. The relevant flows such as; resource consumption, emission, waste flows, energy usage, and also economic flow (transportation). LCI result will be used to evaluate the environmental impact in the next phase.

To collect a plenty of data, classify the data is the good way to gathering. Data that performed in LCA can be divided into two groups which are foreground data and background data. Foreground data is the specific data for each process that can be directly gathered from the source, such as, interviews, questionnaire, or stream table from process design. And about the background data is the other support data such as energy, transportation, or waste management depend on the goal and scope of study. This data can be gathered from the database, statics and literature (Curran, 2012). For LCI databases, there have some public available database and also some restricted-access database. Some of online LCI databases from several regions in the world are shown in Table 2.1.

The LCI data are extracted from many processes that connected together. Therefore, LCI phase is also needed the system scheme for calculating the process. There are many methods for calculate LCI such as process flow diagram; Matrix representation of product system; the IO-based hybrid analysis, and the integrated hybrid analysis (Suh and Huppes, 2003). For LCSoft software, Matrix representation is used as calculation method to generated LCI result.

Table 2.1 Available national life cycle inventory databases (Curran *et al.*, 2006)

Name	Website	Availability	Language	Date Focus	No. Datasets	Geograp-hic
Australian Life Cycle Inventory Data Project	http://www.auslci.com.au/	Free	English		100	Australia
BUWAL250	http://svi-Verpackung.ch/de/Services/1&Publikatione/	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
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	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

2.1.2.1 Matrix Representation of Product System

Matrix Representation is the computation structure to calculate LCI result which proposed by Heijungs and Suh (2002). Which calculate by matrix equation 2.1 and 2.2

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

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

Given that matrix "*A*" is referred to "*Technology Matrix*" which composed of economic flow of each process (i.e. feedstock or product for the unit process), "*s*" is referred to "*scaling factor*" that upscale the economic flow to reach the target amount, and "*f*" is referred to "*Final Demand Vector*" which equal to reference flow. "*B*" is referred to "*Intervention Matrix*" which composed of environmental flow (i.e. emission from the unit process), and "g" is referred to "*Total Intervention Matrix*" which contain both economic flow and environmental flow that meet with reference amount.

2.1.2.2 Allocation

LCI data are normally collected for each product system or identify the inputs and outputs per sub-process. However, there have processes which produce more than one product, called *"multifunctional process"*. For example, crude oil refinery process, 1 kg of crude oil can produced multiple of product such as diesel, gasoline, fuel oil and etc. Thus, the emission from these processes should be separated by applying allocation. Allocation is done by dividing environmental load of the inputs and outputs from process among the co-product. Criteria for allocation can be divided into two types, physical allocation and economic allocation. Physical allocation is a relationship of the products that determined from physical property such as mass, volume, energy, or number of units. And economic allocation is a relationship that determined from revenue of products.

.

2.1.3 Life Cycle Impact Assessment (LCIA)

After all inventories input and output from the process are listed, the data will be used to perform LCIA as a next step. LCIA is the process to understand and evaluate the environmental impacts of product and/or process system. With uncountable released substance to the environment, the emission cause many types of environmental impacts, for example, climate change, eutrophication, human toxicity, and resource depletion. ISO has developed the standard for doing LCIA in three mandatory steps which are impact category selection, classification, and characterization. In addition, optional steps for interpreting the results are also developed, such as, normalization, grouping, sensitivity analysis, uncertainty analysis.

2.1.3.1 Selection and Definition of Impact Categories

First step of LCIA is identification types of environmental impacts. There are two types, *Midpoint* and *Endpoint* impacts, which are consist of many potential environmental impact.

Midpoint categories represent effect or mechanism of the release substance. These categories normally used as focus points of environmental policy for example: climate change, photochemical smog, and marine ecotoxicity.

Endpoint categories represent the concern issue at the end of cause effect chain, which may formulated many midpoint environmental impacts into one endpoint impact category. Human health, ecosystem species, and natural resource are example of Endpoint categories. At this level, the extensive knowledge of environmental effect is not required. However, endpoint categories are optional way, due to higher statistical uncertainties from aggregation of data gap and assumption along the cause effect chain. Relation between midpoint and endpoint categories, are shown in Figure 2.2.

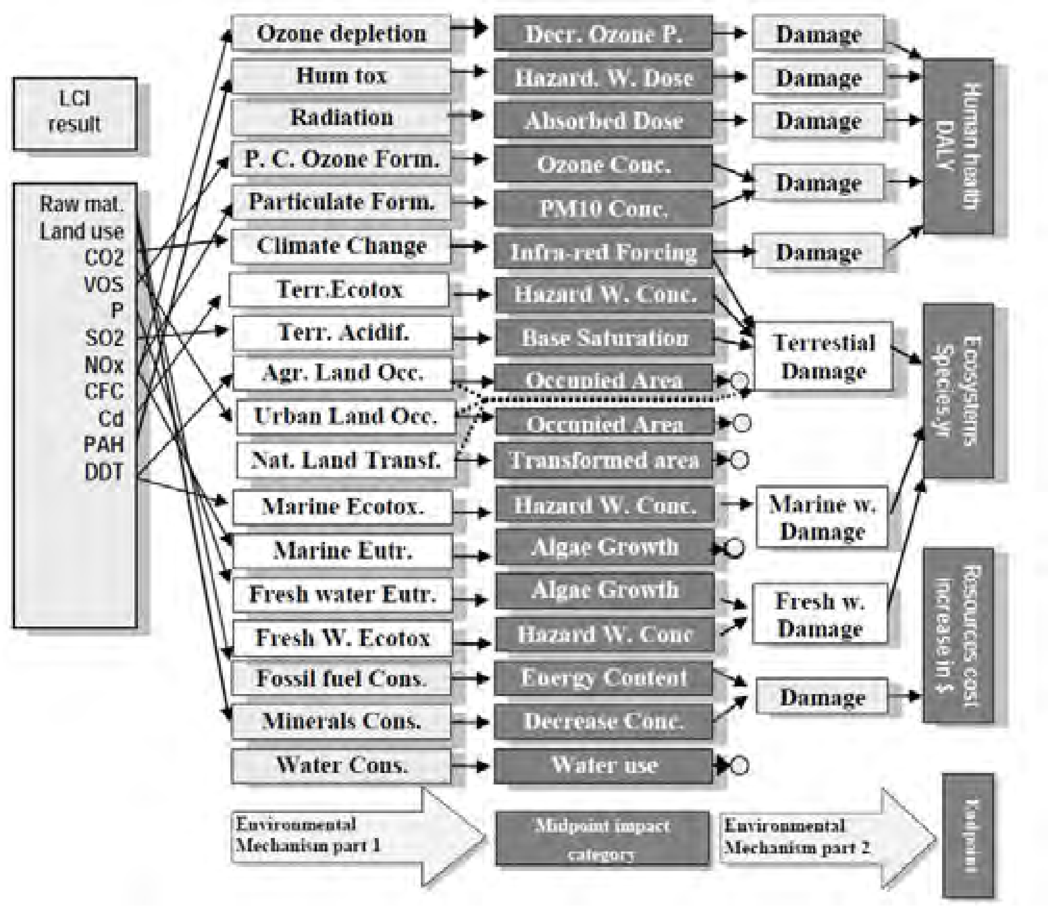

Figure 2.2 Relation between inventory, midpoint categories and endpoint categories, ReCiPe 2008 (Eco-efficiency Action Project, 2010).

2.1.3.2 Classification

Classification is step to distinguish the inventory data from LCI phase into impact categories. For example CO_2 emission will be classified into climate change category. For the inventory data that can be classified in two or more different categories, there need to follow this instruction (ISO, 2006).

- *Partition a representative portion of the LCI results to the impact categories to which they contribute. This is typically allowed in cases when the effects are dependent on each other.*
- *Assign all LCI results to all impact categories to which they contribute. This is typically allowed when the effects are independent of each other.*

2.1.3.3 Characterization

To calculate the LCI results, conversion factors that are called "*characterization factors*" will be used to convert the LCI results into representative indicators on each impact category. Characterization factors are equivalent unit that show the effect of LCI component on each impacts category. Therefore, each impact category (i.e. acidification, climate change, eutrophication, human toxicity, etc.) has different characterization factor such as nitrogen equivalent indicates to the Marine eutrophication. The following equation is commonly used for impact indicator characterization (Curran, 2006):

$$\text{Inventory Data} \times \text{Characterization Factor} = \text{Impact Indicators} \tag{2.3}$$

These three mandatory steps, LCIA methodology, are requirement for doing LCIA. However, there have some methodologies that are commonly used to assess environmental impact. Table 2.2 shows typically LCIA methodology.

Table 2.2 Typically LCIA methodology (Margni 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)	

International Reference Life Cycle Data System (ILCD) Handbook is guidance document for life cycle assessment which developed by Environment and Sustainability in the European Commission Joint Research Centre (JRC). They provided the recommended LCIA methodology that selected the good characterization factor from other methodologies. In addition, ILCD methodology is requirement for evaluating product environment footprint results. Therefore, ILCD methodology was implemented as new calculation pathway for new version of LCSoft. Implemented ILCD methodology is consisted of 15 midpoint impact categories:

Climate change: global warming potential calculating the radiative forcing over 100 years model, developed by the Intergovernmental Panel on Climate Change.

Human toxicity, cancer effects and non-cancer effects: Comparative Toxic Unit for humans (CTUh) expressing the estimated increase in morbidity in the total human population per unit mass of a chemical emitted (cases per kilogram) from USEtox model.

Freshwater ecotoxicity: Comparative Toxic Unit for ecosystems (CTUe) expressing an estimate of the potentially affected fraction of species (PAF) integrated over time and volume per unit mass of a chemical emitted (PAF m3 year/kg) from USEtox model.

Ozone depletion: Ozone Depletion Potential (ODP) calculating the stratospheric ozone depletion over 100 years model.

Particulate matter/respiratory inorganics: calculating intake fractions for fine particles (kg PM2.5-eq/kg).

Ionizing radiation HH (human health): calculating human exposure efficiency in comparison to Uranium.

Photochemical ozone formation: expression of the impact from ozone and other reactive oxygen compound such as NMVOC or NOx.

Acidification: Accumulated Exceedance (AE) characterizing the change in critical load exceedance of terrestrial and main freshwater ecosystems that cause by deposition of acidifying substances.

Terrestrial eutrophication: Accumulated Exceedance (AE) characterizing the change in critical load exceedance of eutrophying substances that cause by deposition of airborne emissions such as nitrogen compound and ammonia.

Freshwater eutrophication: expression of the degree to which the emitted nutrients reaches the freshwater end compartment (phosphorus considered as limiting factor in freshwater) from ReCiPe model.

Marine eutrophication: expression of the degree to which the emitted nutrients reaches the marine end compartment (nitrogen considered as limiting factor in marine water) from ReCiPe model.

Land use: Soil Organic Matter (SOM) which is mass deficit of soil organic carbon (kg C/m2/a).

Water resource depletion: Freshwater scarcity: scarcity-adjusted amount of water used.

Mineral, fossil and renewable resource depletion: scarcity of mineral resource which calculated as 'Reserve base', which refers to size of those parts of resources that had reasonable potential for becoming economic.

2.1.3.4 Optional Elements

2.1.3.4.1 Normalization

Normalization is one of optional LCIA steps to understand the relative contribution for each impact indicator result of the product system to the reference value. The reference information are relate to a community (e.g. domestic, national or the world), person (e.g. Thailand citizen) or other system, over a given period of time (Guinee, 2002). Normalization can be done by converting all indicator results into dimensionless quantities, which divide the impact assessment results with normalization factors.

Normalization factor (NF) is determined by the ratio between the impacts per unit of emission and the total impacts of all substances on the reference. Generally, the normalization factor is in the unit of emission over a year of whole country or average people. In the different community, normalization factor also have a little different for instance, normalization factor for Europe and Slovenia. Eventually, applying the normalization, the results should be documented with all methods and assumptions.

2.1.3.4.2 Grouping

Grouping is optional LCIA steps to minimize number of impact categories by combining the indicator into one set and ranking the important of that category.

2.1.3.4.3 Weighting

Weighting is optional step that adjust the impact result in order to reflect the study goal. Weighting is applied by multiplying each impact categories score by weighting factor.

2.1.4 Interpretation

The final stage of LCA study is life cycle interpretation. In this phase, the results from all previous steps are evaluated and analyzed to get the conclusion and recommendation of the study.

2.1.4.1 Contribution Analysis

The contribution analysis is the function to calculate the contribution of LCI and LCIA results in a product's life cycle. And determine the data which play important role in the environmental impacts or process flows.

2.1.4.2 Sensitivity Analysis

Sensitivity analysis is method to determine the robustness of the results by considering the effect after deliberate changing some assumptions such as system boundary, characterization models, and amount of utility (Goedkoop *et al.*, 2008).

2.1.4.3 Uncertainty Analysis

Another method to determine the robustness is uncertainty analysis. Data in LCA are collected from various sources and different reliability, for example; data has collected on the different day, different place, or different community. The purpose of uncertainty analysis is to assesses the influence on results of variations in process data or model by calculating the total error range of the results (Guinee, 2002). One of the good procedures is Monte Carlo simulation. It empirically varies input data of the calculation according to a given probability distribution or uncertainty ranges, runs the calculation, and stores the outcome. With a large number of iterative run, we can determine the error from function express in following equation (Ciroth *et al.*, 2004):

$$f(x) = f(x_t + \Delta x) = y_t + \Delta \mathrm{y} = \mathrm{y} \qquad (2.4)$$

Where Δx is Error in x

Δy is Error in y

x_t is True value for x

y_t is True value for y

y is Observed/ calculated value for variable y

2.1.5 Data Quality Indicator

Life cycle inventory database contain the various data which are environmental data, system data, performance data, and so on. Sometime there are lacks of some detailed, that cause the significant variations or "data uncertainty". Data quality indicator (DQI) is one technique that often used to estimate the data uncertainty in LCA based on the descriptive metadata and expert knowledge (Wang, and Shen, 2013). DQI may be used to judge the consistency of the actual quality of collected data related to the goal and scope. Generally, DQI often formatted as pedigree matrix (DQPM) as show in Figure 2.3. The quality of data can be estimate by summing the indicator score from individual indicators. The weakest indicator score generally weaken overall quality of the data set (ILCD, 2010).

Indicator score	1	2	3	4	5
Indicators, which are independent of the study in which the data are applied:					
Reliability of the source	Verified data based on measurements	Verified data partly based on assumptions or non-verified data based on measurements	Non-verified data partly based on assumptions	Qualified estimate (e.g. by industrial expert)	Non-qualified estimate or unknown origin
Completeness	Representative data from a sufficient sample of sites over an adequate period to even out normal fluctuations	Representative data from a smaller number of sites but for adequate periods	Representative data from an adequate number of sites but from shorter periods	Representative data but from a smaller number of sites and shorter periods or incomplete data from an adequate number of sites and periods	Representativeness unknown or incomplete data from a smaller number of sites and/or from shorter periods
Indicators relating to the technological and natural production conditions under which the data are valid, and therefore dependent of the data quality goals for the study in which the data are applied:					
Temporal correlation	Less than 3 years of difference to year of study	Less than 6 years of difference	Less than 10 years of difference	Less than 15 years of difference	Age of data unknown or more than 15 years of difference
Geographical correlation	Data from area under study	Average data from larger area in which the area under study is included	Data from area with similar production conditions	Data from area with slightly similar production conditions	Data from unknown area or area with very different production conditions
Further technological correlation	Data from enterprises, processes and materials under study	Data from processes and materials under study but from different enterprises	Data from processes and materials under study but from different technology	Data on related processes or materials but from same technology	Unknown technology or data on related processes or materials, but from different technology

Figure 2.3 Data quality matrix with 5 data quality indicator (Weidema, 1998).

The pedigree matrix approach can be used to calculate uncertainties which represented by a probability distribution or range for each parameter. Generally, the sample of measured values or data often appears as a normal or lognormal distribution.

For lognormal distribution, the distribution can be characterized by square of geometric standard deviation covers the 95% confidence interval. In this approach, an uncertainty factor is assigned to each of data quality indicators and data quality criteria (very good, good, fair, and poor) based on expert judgments (Frischknecht *et al.*, 2007) as shown in Table 2.3, and the basic uncertainty factor (U_b) can be derived from the Table 2.4. The uncertainty factors are used to estimate the GSD^2 (the square of the geometric standard deviation) by Equation 2.5.

$$SD_{g95} = \sigma_g^2 = exp^{\sqrt{[\ln(U_1)]^2+[\ln(U_2)]^2+[\ln(U_3)]^2+[\ln(U_4)]^2+[\ln(U_5)]^2+[\ln(U_b)]^2}} \quad (2.5)$$

Table 2.3 Uncertainty scaling factors based on data quality ratings (Frischknecht *et al.*, 2007)

Indicator score	Very good	Good	Fair	Poor
Precision (U_1)	1.00	1.10	1.20	1.50
Completeness (U_2)	1.00	1.05	1.10	1.20
Temporal representativeness (U_3)	1.00	1.10	1.20	1.50
Geographical representativeness (U_4)	1.00	1.02	1.05	1.10
Technological representativeness (U_5)	1.00	1.20	1.50	2.00

Table 2.4 Basic uncertainty factor (Frischknecht *et al.*, 2007)

Input / output group	U_b	Input / output group	U_b
Demand of:		**Emission to air of:**	
thermal energy	1.05	CO2	1.05
electricity	1.05	SO2	1.05
semi-finished products	1.05	combustion: NOX, NMVOC total, methane, N2O and NH3	1.50
working materials	1.05	combustion: CO	5.00
transport services	2.00	combustion: individual hydrocarbons, TSM	1.50
waste treatment services	1.05	combustion: PM10	2.00
Infrastructure	3.00	combustion: PM2.5	3.00
Resources:		combustion: polycyclic aromatic hydrocarbons (PAH)	3.00
primary energy carriers	1.05	combustion: heavy metals	5.00
metals, salts		process emissions: individual VOCs	2.00
land use, occupation	1.50	process emissions: CO2	1.05
land use, transformation	2.00	process emissions: TSM	1.50
Waste heat:		process emissions: PM10	2.00
emission to air, water, and soil	1.50	process emissions: PM2.5	3.00
Emission to water of:		from agriculture: CH4, NH3	1.20
BOD, COD, DOC, TOC	1.50	from agriculture: N2O, NOX	1.40
inorganic compounds (NH4, PO4, NO3, Cl, Na etc.)	1.50	radio nuclides (e.g., Radon-222)	3.00
individual hydrocarbons, PAH	3.00	process emissions: other inorganic emissions	1.50
heavy metals	5.00	**Emission to soil of:**	
from agriculture: NO3, PO4	1.50	oil, hydrocarbon total	1.50
from agriculture: heavy metals	1.80	pesticides	1.20
from agriculture: pesticides	1.50	heavy metals	1.50
radio nuclides	3.00	radio nuclides	3.00

For normal distribution, the distribution can be characterized by standard deviation which determined by converting the aggregate quality DQI scores (Equation 2.6) into beta functions. The data quality indicator score reflected the reliability of data. In addition, quality score could be transformed into shape parameter (α,β) and determined the minimum and maximum value by using transformation matrix as shown in Table 2.5, which showed shape of distribution and probability of the data, that was helpful information for uncertainty analysis. Equation 2.7 was used for estimate variance of data.

$$DQI = \sum \frac{Quality\ Scale}{Number\ of\ Data\ quality\ indicator} \tag{2.6}$$

$$variance(X) = \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)} \tag{2.7}$$

Table 2.5 Transformation matrix (Endong Wang, 2013)

Aggregated DQI Score	**Beta distribution function**	
	Shape parameters (α,β)	**Range endpoints (+/-%)**
5	(5,5)	10
4.5	(4,4)	15
4	(3,3)	20
3.5	(2,2)	25
3	(1,1)	30
2.5	(1,1)	35
2	(1,1)	40
1.5	(1,1)	45
1	(1,1)	50

2.1.6 Environmental Footprint

Over the last few years, many company concern about the sustainability management and expect to market the product as environmental friendly. However, in several state markets face the problem that there are many indicators or methods to get the green products. Sometime, different markets use different indicators cause the cost for companies and confusion for customers. Therefore, European Commission proposes the Product Environmental Footprint (PEF) and Organization Environmental Footprint (OEF) methods as a common way of measuring environmental performance. Eventually, these two methods may become part of future European policies on sustainable development.

The PEF and OEF method have been developed based on Life Cycle Assessment (LCA) with the existing, tested, and widely use methods, standard, and guideline. For phases of Environmental Footprint study can see in Figure 2.4.

This method can potentially cover 14 impact categories: acidification; particulate matter; global warming; ozone depletion; human toxicity –carcinogenics; human toxicity – noncarcinogenics; ionizing radiation; photochemical ozone formation; terrestrial eutrophication; deposited waste; freshwater ecotoxicity; water resource consumption; mineral extraction. These categories are required to use definition and characterization factor from ILCD Handbook.

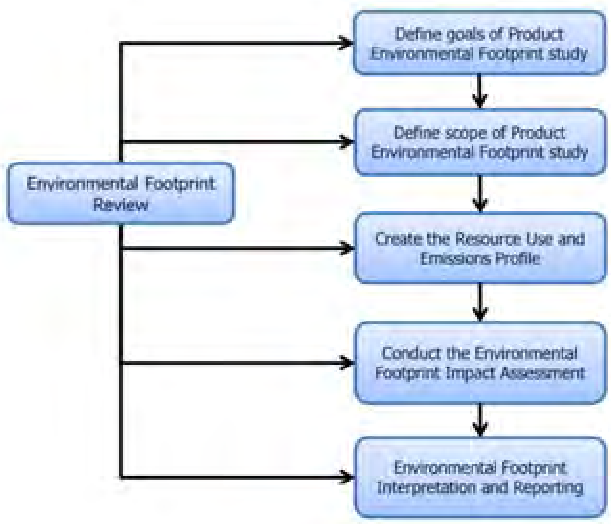

Figure 2.4 Phases of a Product Environmental Footprint study (Manfredi *et al.*, 2012).

2.2 Review of LCSoft Development

LCA software was used to calculate environmental impact from resource and energy usage and emission to the environment. As the important issue, several LCA software tools had been developed such as SimaPro, and GaBi. However, there did not have LCA software that could integrate with the process design tool yet. As a result, the first version of LCSoft was developed by Piyaruk *et al.* (2012). LCSoft was developed by using VBA (Visual Basic Application) in Microsoft Excel with the concept of user-friendly interface as shown in Figure 2.5. This version software could cooperate with PROII simulation program in order to evaluate environmental impacts for chemical and biochemical processes.

The final result of the first version consisted of inventory data cover thirteen substance, energy and fuel consumption, carbon footprint evaluation, and eight environmental impacts categories including: global warming, ozone depletion, photochemical formation, acidification, eutrophication, human toxicity, aquatic toxicity and terrestrial toxicity. LCSoft version 1.0 was easy to understand and very useful for process evaluation, nevertheless, more LCI data and more characterization factors needed to be added into the software in order to cover more process in the chemical industry.

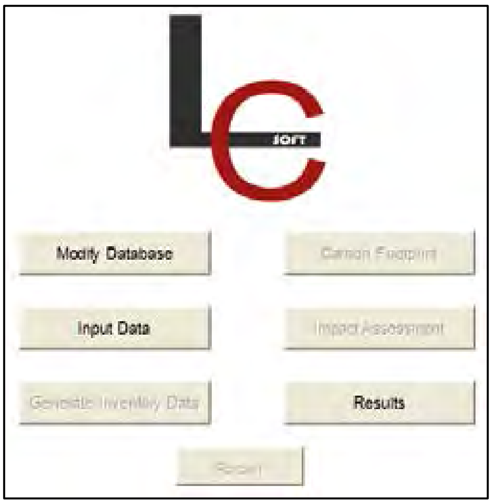

Figure 2.5 LCSoft 1.0's interface (Piyarak, 2012).

For the next version of LCSoft was developed by Kalakul *et al*. (2013). Second version of LCSoft was not only improved the performance from first version, but also had more applicable functions. It could integrate with process design tools including ECON (Saengwirun, 2011)– economic analysis software and SustainPro (Carvalho *et al.*, 2013)– sustainable process design software in order to identify process hotspot. The main user interface of LCSoft version2 and integrated software is shown in Figure 2.6.

Figure 2.6 Main interface of integrated software (Kalakul *et al.*, 2014).

Also this version had extended the LCI data for chemical and biochemical process, and saved as the LCI knowledge base which allow user to manage the database. In addition, three more impact categories such as human toxicity carcinogenic, human toxicity non-carcinogenic, and fresh water eco-toxicity were added.

.

The third version of LCSoft was developed by Supawanich *et al.* (2014). In this version, Life cycle Inventor (LCI) calculation function was developed under the matrix based method (Heijungs and Suh, 2002). Also, extended Life Cycle Inventory database and added more impact categories; water consumption, mineral extraction, deposited waste, and renovated energy consumption. Moreover, the contribution analysis function and uncertainty analysis function which based on Monte Carlo simulation was initial- developed in this version. The calculation method of LCSoft software can be divided into five steps and two optional steps as shown in Figure 2.7.

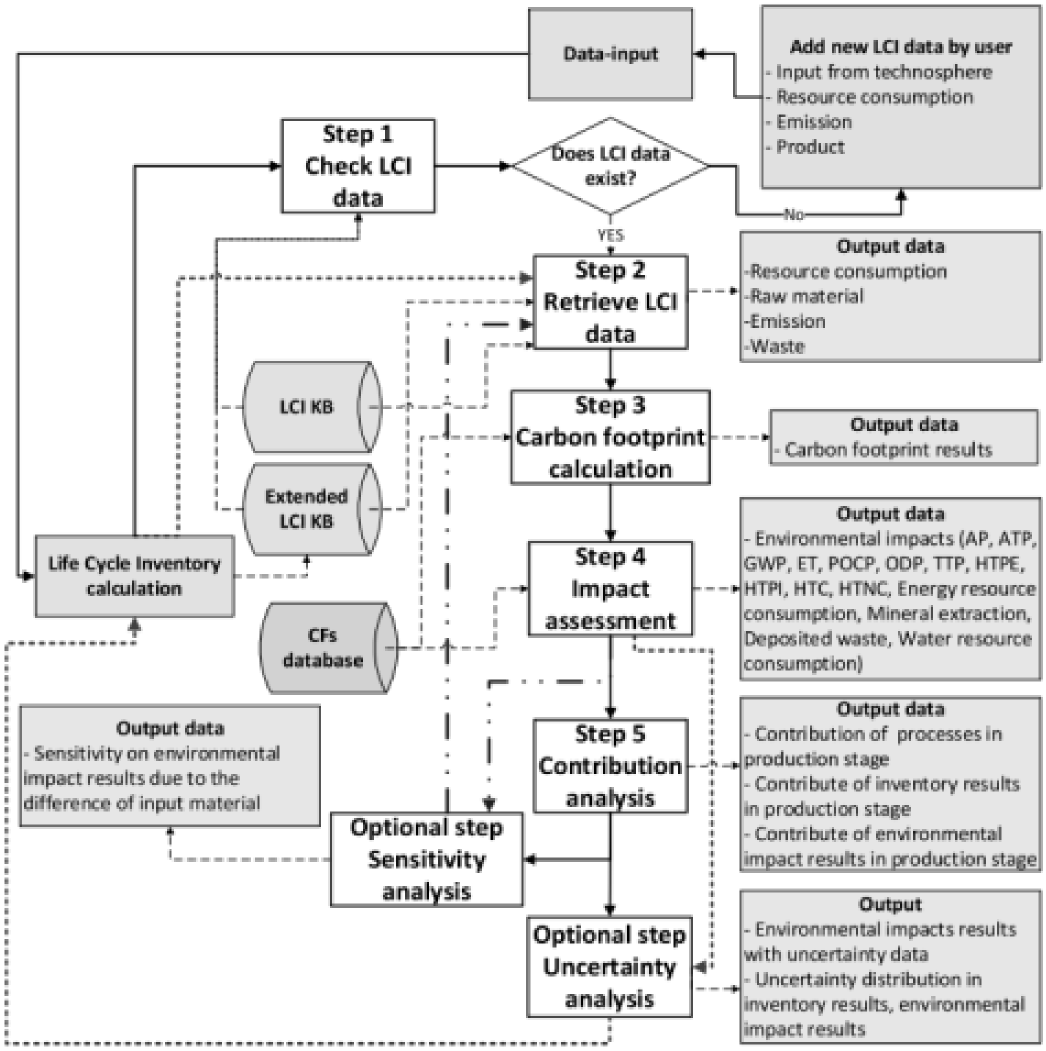

Figure 2.7 LCSoft's Frameworks (Supawanich *et al.*, 2015).

The latest version of LCSoft was developed by Kaesinee *et al.* (2015). For LCsoft version 4.0 had improved the software by extending the LCI database and adding of new impact categories which are photochemical ozone formation, marine eutrophication, freshwater eutrophication, terrestrial eutrophication, ionizing radiation, and particular matter. In addition, this version had developed the evaluation of eco-efficiency function, important indicator for sustainable development, which was calculated in term of value or cost related to the environmental influence of product. The characterization factor for all impact categories and details in LCSoft software are shown in Table 2.6.

Table 2.6 Characterization factors and unit of environmental impacts in LCSoft (Kaesinee *et al.*, 2016; Supawanich *et al.*, 2015)

Impact Category (I^k)	Characterization factor ($CF^k{}_{t,c}$)	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.	
Photochemical oxidation	$CF^{POCP}{}_{t,c}$	kg C_2H_2 eq.	
Ozone depletion	$CF^{ODP}{}_{t,c}$	kg CFC-11 eq.	
Terrestrial toxicity	$CF^{TTP}{}_{t,c}$	$1/LD_{50}$	
Human toxicity by exposure	$CF^{HTPE}{}_{t,c}$	1/TWA	
Human toxicity by ingestion	$CF^{HTPI}{}_{t,c}$	$1/LD_{50}$	
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 resource consumption	$CF^{Energy}{}_{t,c}$	MJ eq.	Cumulative Energy Demand 1.05
Mineral extraction	$CF^{Mineral}{}_{t,c}$	kg Sb eq.	CML-IA
Deposited waste	$CF^{Waste}{}_{t,c}$	UBP	Ecological scarcity 2013
Water resource consumption	$CF^{Water}{}_{t,c}$	UBP	
Photochemical ozone formation	$CF^{PCOF}{}_{t,c}$	kg NMVOC eq.	ILCD2011
Marine eutrophication	$CF^{Marine}{}_{t,c}$	kg N eq.	
Freshwater eutrophication	$CF^{Freshwater}{}_{t,c}$	kg P eq.	
Terrestrial eutrophication	$CF^{Terrestrial}{}_{t,c}$	mol N eq.	
Ionizing radiation	$CF^{IR}{}_{t,c}$	kbq U_{235} eq.	
Particular matter	$CF^{PM}{}_{t,c}$	kg PM2.5 eq.	

CHAPTER III
METHODOLOGY

3.1 Materials and Equipment

3.1.1 Equipment

Notebook, Intel® Core™ i7-6500U CPU 2.5 GHz with Turbo Boost up to 2.9 GHz, 12GB of RAM

3.1.2 Software

- LCSoft
- Visual Basic for Applications
- SimaPro 8.2.3

3.2 Methodology

3.2.1 Improvement of LCI and LCIA Calculation

3.2.1.1 Adding New Pathway for Calculation

LCSoft was performed the environmental impact assessments by using methodology that had twenty-one impact categories, which gathered from variety source and continuously improved over the years. In this version, feature to select the design methodology was added, in order to cover wider range of applications and increase flexibility of software. New methodology that had implement as new choice for calculating LCIA was selected from recommends methodology in ILCD Handbook.

3.2.1.2 Allocation

Allocation was one of technique to deal with multifunctional process (multiple product process) in order to separate emission or load of the process to each product in the product system. Allocation model was added in this version of LCSoft, which user could specify the allocation of the process in the database management section.

3.2.2 Development of LCSoft Features

3.2.2.1 Data Quality Indicator

Data Quality was an important key to analyses uncertainty of environmental impact. Accurate and reliable results start from good quality data input. In this features, Data Quality Matrix (DQM) were provided as the rating indicator where users could estimate the quality of his/her data collection.

3.2.2.2 Normalization

Normalization provided relation between the impact results, and determined the significant of environmental impacts. Normalization was done by converting all indicator results into dimensionless which multiplied the impact assessment results with normalization factors. However, the normalization factors were depended on goal of study. As a result, normalization could reflect the relative emission that associated with the community.

3.2.2.3 Endpoint Impact Categories

In previous version of LCSoft, the impact categories was defined only midpoint level which only focused on the direct effect and mechanism of the emission. In order to be more applicable software, the endpoint level was added for evaluating overall affects or the end of mechanism. The characterization factors for endpoint were retrieved from ILCD and ReCiPe methods. Endpoint level had three impact categories which are Human Health, ecosystem species, and natural resource.

3.2.2.4 Parameter Sensitivity Analysis

The purpose of parameter sensitivity analysis was investigation the effect from changing selected value (design-controlled) on impact assessment results. The sensitivity analysis was introduced in previous version of LCSoft, but there only applicable to change in assumption source (i.e. changing type of fuel from diesel to natural gas for generating the process electricity). In parameter sensitivity analysis function, users were allowed to introduce the changes in selected parameter and determined the influence from that case.

3.2.2.5 Calculation with uncertainty

The calculation with uncertainty in the product system features was added. In this features, user can specify range of uncertainty which associate with his/her data. The uncertainty would be included in every inventory in the product system, therefore the fluctuation from uncertainty could be shown in this features.

3.2.3 Extension of LCI Database for Covering All Impact Categories

LCSoft database was gathered from U.S. LCI (U.S. Life Cycle Inventory Database, 2012), ELCD (European reference Life Cycle Database, 2006) and other open available source. This database was used to calculate most of impact categories; however, there could not evaluate in some categories which only affected from specific substance. In this version, LCSoft database was extended by adopting partial information from available sources in order to cover all of impact categories assessment, "Benzene production, at plant" was used as a case study for checking the impact categories result. The extension framework is shown in Figure 3.1.

3.2.4 Validation and Improvement of LCSoft Software

The validation of LCSoft was performed by comparing the results with commercial LCA software, SimaPro, in order to validate the accuracy, reliability and deficiency of the LCSoft. Production of Para-Xylene by Toleune Methylation (Nateetorn, 2016) and Production of bio-ethanol from cassava rhizome (Mangnimit, 2013) were used as the case study. The process details are show in Appendix A and Appendix B, respectively.

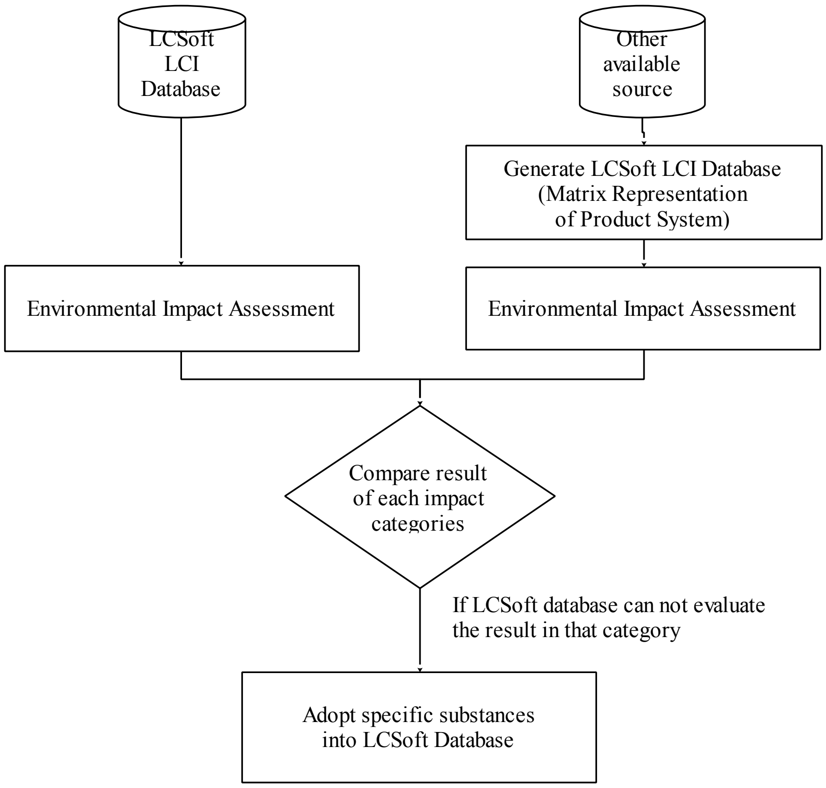

Figure 3.1 The extension framework of LCI database.

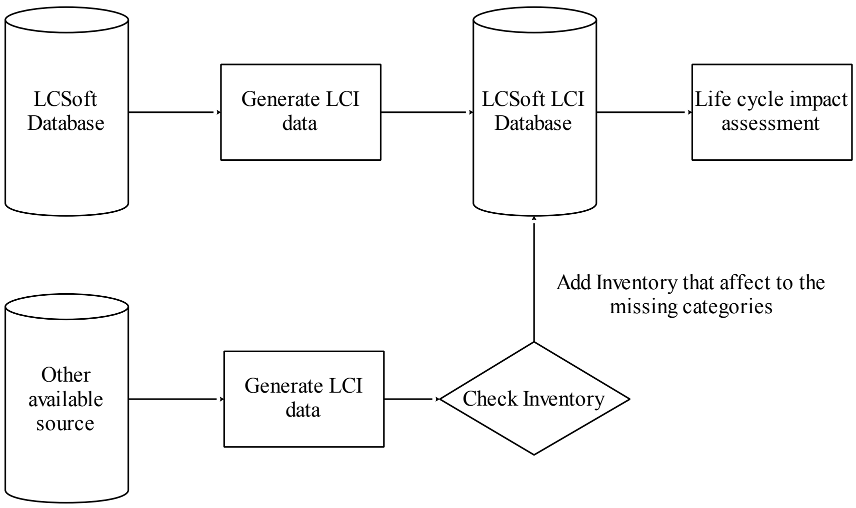

Figure 3.1 The extension framework of LCI database (cont'd).

CHAPTER IV
RESULTS AND DISCUSSION

4.1 Improvements on LCI and LCIA Calculations

4.1.1 Adding New Pathway for Calculation

4.1.1.1 Existing of Calculation Methodology in LCSoft

In the previous version of LCSoft, the calculation method had twenty-one impact categories that collected from various sources; 8 impact categories from U.S. Environmental Protection Agency (EPA), 3 impact categories from USEtox, 6 impact categories from ILCD method, and the rest from other sources as shown in previous section Table 2.5. In addition, 12 impact categories (from U.S.EPA, from USEtox, and Photochemical Ozone Formation category) were applied with 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) to extend range of characterization factors data of organic substances.

4.1.1.2 New Calculation Methodology in LCSoft

In order to enlarge the range of assessments and improve flexibility of LCSoft, new calculation method was introduced as new pathway for calculation, where users were allowed to select the calculation method that related to their goal or requirement. The new calculation method had fifteen impact categories followed the recommendation methodologies from ILCD Handbook, which included; global warming potential, ozone depletion, human toxicity cancer effect, human toxicity non-cancer effect, fresh water ecotoxicity, particular matter, ionizing radiation, photochemical ozone formation, acidification, terrestrial eutrophication, freshwater eutrophication, marine eutrophication, water resource consumption, mineral extraction, and land use. Characterization factors of new impact were based on ILCD 2011 as shown in Table 4.1.

Table 4.1 Characterization factors and unit of new environmental impact categories

Impact Category (I_k)	Characterization factor ($CF^k_{t,c}$)	Unit
Global warming potential	$CF^{GWP}_{t,c}$	kg CO_2 eq.
Ozone depletion	$CF^{ODP}_{t,c}$	kg CFC-11 eq.
Human toxicity, cancer effect	$CF^{HTC}_{t,c}$	CTUh
Human toxicity, non-cancer effect	$CF^{HTNC}_{t,c}$	CTUh
Fresh water ecotoxicity	$CF^{ET}_{t,c}$	CTUe
Particular matter	$CF^{PM}_{t,c}$	kg PM2.5 eq.
Ionizing radiation	$CF^{IR}_{t,c}$	kg U_{235} eq.
Photochemical ozone formation	$CF^{PCOF}_{t,c}$	kg NMVOC eq.
Acidification	$CF^{AP}_{t,c}$	molc H+ eq.
Terrestrial eutrophication	$CF^{Terrestrial}_{t,c}$	molc N eq.
Freshwater eutrophication	$CF^{Freshwater}_{t,c}$	kg P eq.
Marine eutrophication	$CF^{Marine}_{t,c}$	kg N eq.
Water resource consumption	$CF^{Water}_{t,c}$	m^3 water eq.
Mineral extraction	$CF^{Mineral}_{t,c}$	kg Sb eq.
Land use	$CF^{Land}_{t,c}$	kg C deficit

New calculation method in LCSoft was verified by using case study, which was a production of 1 kg of acetic acid by the cradle-to-gate process "acetic acid, 98% in H_2O, at plant/RER" (Althaus *et al.,* 2007), and compared the results with the same process in SimaPro v.8.2.3. The process detail is described in Table C1. The comparative results of new calculation method (Table 4.2) show the very good match and efficiently evaluated the environmental impacts in all categories.

Table 4.2 Comparative results of acetic acid process between SimaPro and LCSoft

Impact Categories	Unit	LCSoft	Simapro	Difference	Percentage Difference
Global warming	kg CO2 eq	1.5763	1.5775	-0.0013	0.08
Ozone depletion	kg CFC-11 eq	2.8E-07	2.8E-07	0.0000	0.00
Human toxicity, cancer effect	CTUh	7.4E-08	7.4E-08	0.0000	0.00
Human toxicity, non-cancer effect	CTUh	1.4E-07	1.4E-07	0.0000	0.00
Fresh water ecotoxicity	CTUe	1.1677	1.1678	-0.0001	0.01
Particulate matter	kg PM2.5 eq	0.0006	0.0006	0.0000	0.00
Ionizing radiation	kg U_{235} eq	0.5902	0.5898	0.0004	0.06
Photochemical ozone formation	kg NMVOC eq	0.0057	0.0053	0.0004	6.51
Acidification	molc H+ eq	0.0075	0.0075	0.0000	0.00
Terrestrial eutrophication	molc N eq	0.0115	0.0114	0.0001	0.69
Freshwater eutrophication	kg P eq	1.9E-05	1.9E-05	0.0000	0.00
Marine eutrophication	kg N eq	0.0010	0.0010	0.0000	0.00
Water resource consumption	m^3 water eq	0.0185	0.0188	-0.0003	1.76
Mineral extraction	kg Sb eq	5.6E-10	5.6E-10	0.0000	0.00
Land use	kg C deficit	6.1114	6.1114	0.0000	0.00

4.1.2 Allocation

Allocation function was added in LCSoft to calculate the processes with multiple products or multifunctional processes. For example, process "Crude oil, in refinery" from US.LCI database as shown in Table 4.3. There had more than one product outputs from the process. Therefore, the emissions and inputs from this process were separated in to sub-process by applying the allocation, such as process, "Diesel, at refinery", or "Gasoline, at refinery". Physical allocation by mass was used in LCSoft LCI database as default for dividing the emission. For new or modify process data, users could specify %allocation that associated with their data collection.

The LCI result of this new LCI calculation in LCSoft and SimaPro 8.2.3 were validated with multifunctional process "Diesel, at refinery – RNA" and shown in Table 4.4 and Figure 4.1. The LCI data of this process was obtained by applying the allocation in "Crude oil, in refinery" process (Table C2).

Table 4.3 Part of LCI data of "Crude oil, in refinery" process from US.LCI database

Name	Amount	Unit	%Allocation
Output to technosphere			
Diesel, at refinery	0.244	L	21.87
Gasoline, at refinery	0.525	L	42.05
Kerosene, at refinery	0.109	L	9.09
Liquefied petroleum gas, at refinery	0.0482	L	2.69
Refinery gas, at refinery	0.0591	m^3	4.49
Residual fuel oil, at refinery	0.0502	L	4.89
Petroleum coke, at refinery	0.058	kg	5.99
Petroleum refining coproduct, unspecified, at refinery	0.0503	kg	5.19
Bitumen, at refinery	0.0358	kg	3.69
Input from technosphere			
Crude oil, at production	4.0984	kg	
Electricity, at grid, US, 2000	0.5492	kWh	
Liquefied petroleum gas, combusted in industrial boiler	0.0038	L	
Natural gas, combusted in industrial boiler	0.0363	m^3	
Residual fuel oil, combusted in industrial boiler	0.0889	L	
Transport, barge, average fuel mix	0.0047	tkm	
Transport, ocean freighter, average fuel mix	18.7705	tkm	
Dummy, Transport, pipeline, unspecified	2.5861	tkm	
Dummy, Disposal, solid waste, unspecified, to sanitary landfill	0.0222	kg	

Table 4.4 Part of LCI result of "Diesel, at refinery" process from US.LCI database

Substance	Compartment	Unit	LCSoft previous database	LCSoft updated database with allocation	SimaPro	Percentage Difference (Updated database/SimaPro)
Acetone	Water	kg	1.91E-06	3.36E-08	3.51E-08	4.56
Ammonia	Air	kg	1.10E-03	1.93E-05	1.92E-05	0.11
Barium	Water	kg	2.35E-01	4.12E-03	4.16E-03	0.78
Benzene	Water	kg	3.21E-04	5.63E-06	5.89E-06	4.51
Copper	Air	kg	9.03E-09	1.58E-10	1.64E-10	3.37
Cumene	Air	kg	3.18E-12	5.57E-14	5.62E-14	0.80
Hexane	Air	kg	4.02E-11	7.04E-13	7.10E-13	0.80
Lead	Air	kg	8.00E-07	1.40E-08	1.41E-08	0.61
Methane	Air	kg	2.06E-01	3.62E-03	3.94E-03	8.61
Sulfur	Water	kg	5.08E-04	8.91E-06	9.31E-06	4.33

For Table 4.4, the LCI calculation results from previous and updated LCSoft database including elementary names and their values were compared with the calculation results from SimaPro database. The LCI calculation results show that LCSoft updated database with allocation model yield the fewer amounts of inventories than previous version of LCSoft database, which the updated database had the calculation results close to the results from SimaPro.

For Figure 4.1, the horizontal axis indicates the elementary flow considered and the vertical axis represents the ratio of LCI results of SimaPro 8.2.3 to LCSoft. The ratio of LCI results of SimaPro to LCSoft, which distribute around 1. These results indicate that updated LCSoft database has the better LCI calculation model which provides the same calculation results as commercial software. However, the ratio results were mostly more than 1, because the SimaPro model had larger sets of combustion fuel emission factors in process "Natural gas, combusted in industrial equipment" compared with those in LCSoft model.

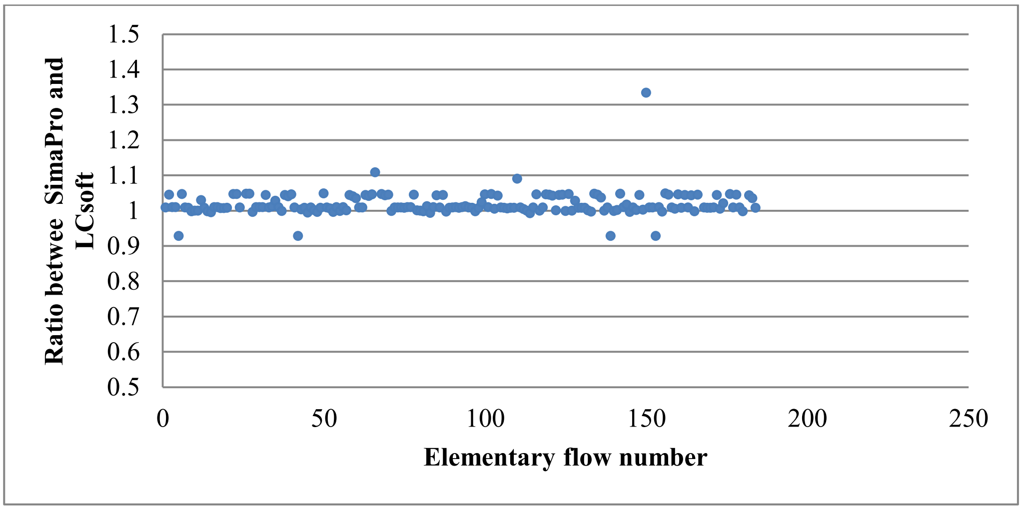

Figure 4.1 Ratio of LCI result from SimaPro 8.2.3 to LCSoft 5.0 (based on process Diesel, at refinery – RNA).

4.2 Development of New LCSoft Features

In order to wider the range of applications, and improve capacity of the software, five new helpful features were introduced to LCSoft.

4.2.1 Data Quality Indicator

The big issue when performing LCA is data quality. The data, which is used in environmental impacts evaluation, are gathered from many sources such as interview, collecting from real process, parameter from process simulation, etc. These indefinite sources caused unreliable and uncertainty results. In order to solve the problem, Data Quality Matrix was introduced into LCSoft where users could check the quality of their data by rating through the guideline as shown in Table 4.5. Seven quality indicators consisted of rule of incursion/exclusion, technological correlation, geographical correlation, supplier independence, acquisition method, age of data, and data representative were provided in LCSoft. After qualifying, aggregated quality score could estimate the distributions of the data regarding to type of distributions.

Table 4.5 LCSoft Data Quality Matrix (Wang and Shen, 2013)

		Quality Scale				
		5	4	3	2	1
		very good	good	fair	poor	very poor
Data quality indicators	**1. Rule of incursion/ exclusion**	Transparent, justified, homogeneous application	Transparent, justified, uneven application	Transparent, not-justified, uneven application	Non-transparent on exclusion but specification of inclusion	Unknown
	2. Technological correlation	Data from process studied of the exact company with exact technology	Data from process studied of company with similar technology	Data from process studied of company with different technology	Data from process related of company with similar technology	Data from process related of company with different technology
	3. Geographical correlation	Data from the exact area	Average data	Data from an area with similar production conditions	Data from an area with slightly similar production conditions	Unknown area
	4. Supplier independence	Verified data from independent source	Verified data from enterprise with interest in the study	Independent source but based on unverified information	Unverified information from irrelevant enterprise	Unverified information from enterprise interested in the study
	5. Acquisition method	Directly measured data	Calculated data based in measurements	Calculated data partly based on assumptions	Qualified estimation by experts	Non-qualified estimation
	6. Age	<3 years old	<6 years old	<10 years old	<15 years old	≥15 years old
	7. Data representative	Representative data from a sufficient sample of sites over an adequate period to even out normal fluctations	Representative data from a smaller number of sites but for an adequate period	Representativ e data from an adequate number of sites but for a shorter period	Data from a smaller number of sites for a shorter period, or incomplete data from an adequate number of sites and periods	Representativ eness unknown or incomplete data from insufficient sample of sites and/or for a shorter period

LCSoft provided three types of distributions for user selection which consisted of range, normal distribution, and lognormal distribution. The range or uniform distribution was characterized by minimum and maximum value. The normal distribution was characterized by standard deviation and best guest value. The lognormal distribution was characterized by geometric variance and best guest value. The default of software was set lognormal distribution as the standard distribution for data qualifying.

The applications of this new feature was validated by comparing geometric variance results that estimate from LCSoft with the results from SimaPro, which the process “acetic acid, 98% in H_2O, at plant/RER” (Althaus et al., 2007) was used as case studied by using both process data and uncertainty data. The comparison result is shown in the Table 4.6. LCSoft results have insignificant percentage difference from SimaPro results which indicate that LCSoft can estimate the uncertainty information same as commercial software.

Table 4.6 Estimated geometric variance of each inventories based on process “acetic acid, 98% in H_2O, at plant/RER” calculated from LCSoft and SimaPro.

Inventories	**Geometric variance**		**Percentage difference**
	LCSoft	**SimaPro**	
Inputs from technosphere			
carbon monoxide, CO, at plant	1.38	1.5	8.51
chemical plant, organics	4.20	4.3	2.39
heat, unspecific, in chemical plant	2.52	2.6	3.14
methanol, at plant	1.38	1.5	8.51
electricity, medium voltage, production UCTE, at grid	2.52	2.6	3.14
transport, lorry >16t, fleet average	3.17	3.2	0.90
transport, freight, rail	3.17	3.2	0.90
water, decarbonised, at plant	1.38	1.5	8.51
Input from nature			
Water, cooling, unspecified natural origin	2.52	2.6	3.14
Emission to air			
Acetic acid	3.17	3.2	0.90
Carbon dioxide, fossil	2.52	2.6	3.14
Carbon monoxide, fossil	2.74	2.8	2.17
Heat, waste	2.52	2.6	3.14
Hydrogen	3.17	3.2	0.90
Methane, fossil	3.17	3.2	0.90
Methanol	3.17	3.2	0.90

4.2.2 Normalization

Normalization is a technique to provide the relative environmental impacts result of the product or process system compare to reference value (i.e. average environmental impacts to domestic people in one year). This method normalizes the indicator results by dividing with a selected reference value or normalization factors to midpoint or endpoint classes. As a result, dimensionless of normalization impact score are obtained which are easy to interpretation. However, it is not indicated the severity of that impact. Since LCSoft calculation method was collected from many models which set of normalization factors were not available. Therefore, normalization function was added in to LCSoft by allow user to specify the normalization factor that compatible with their goal. In addition, normalization factor set from ILCD method was provided as optional selection for supporting ILCD calculation method. The recommended normalization factor (European Commission, 2016) and results for 1 kg acetic acid (98 %), at plant – RER (Althaus *et al.,* 2007) production are shown in Table 4.7.

Table 4.7 Recommended normalization factor and results for ILCD method

Impact Categories	Unit	Normalization Factor per Person	Impacts result	Normalized results
Global warming potential	kg CO_2 eq.	9.22E+03	1.57630	0.00017
Ozone depletion	kg CFC-11 eq.	2.16E-02	2.80E-07	0.00001
Human toxicity, cancer effect	CTUh	3.69E-05	7.40E-08	0.00201
Human toxicity, non-cancer effect	CTUh	5.33E-04	1.40E-07	0.00026
Acidification	mol H+ eq.	4.73E+01	1.16770	0.02469
Particular matter	kg PM2.5 eq.	3.80E+00	0.00060	0.00016
Fresh water ecotoxicity	CTUe	8.74E+03	0.59020	0.00007
Ionizing radiation	kbq U_{235} eq.	1.13E+03	0.00570	0.00001
Photochemical ozone formation	kg NMVOC eq.	3.17E+01	0.00750	0.00024
Terrestrial eutrophication	mol N eq.	1.76E+02	0.01150	0.00007
Freshwater eutrophication	kg N eq.	1.48E+00	0.00002	0.00001
Marine eutrophication	kg P eq.	1.69E+01	0.00100	0.00006
Land use	kg C deficit	7.48E+04	6.11140	0.00006
Water resource consumption	m^3 water eq.	8.14E+01	0.01850	0.00023
Mineral extraction	kg Sb eq.	1.01E-01	5.60E-10	0.00000

4.2.3 Parameter Sensitivity Analysis

Parameter sensitivity analysis is the study how the variation can be apportioned to the change of inputs in the product/process system. LCSoft originally had the sensitivity analysis in term of investigated the effect from different sources such as sort of raw material, and type of utility. In this version, parameter sensitivity analysis was introduced to investigate the effect from changing selected parameter value (design-controlled) by comparing the variation of impact assessment results with other assumptions.

Pretreatment for bioethanol process using cassava rhizome as a feed stock was used as case study. The mass and energy flows were taken from simulation results developed by Mangnimit *et al.* in 2013. The related streams and details of equipment were given as in Appendix A. Amount of input biomass 377 tons per day was set as the base case, and then the increased amount 10% and -10% from the base case was recalculated for investigating the effect from that changed. The sensitivity analysis results show in both table and chart as shown in Table 4.8, Figure 4.2, and Figure 4.3. As a result, this feature could help indicate which environmental impact categories have the effect from the variation of selected parameter. On the other hand, it could determine the contribution of selected parameter to environmental impacts result when compared the effect with other parameters.

From the percentage of environmental impact change in Figure 4.2, global warming potential is the most sensitive environmental impact category whereas fresh water ecotoxicity is the least one when the input biomass has been changed. Deposited waste and mineral extraction are not affected from the variation change. Also, in Figure 4.3, environmental impact categories that are highly affected on the variation of input biomass are terrestrial eutrophication and particular matter. In contrast, terrestrial toxicity is the environmental impact, which has the least effect on the variation of input biomass.

Table 4.8 Parameter sensitivity analysis of bioethanol process in pretreatment section.

Variation Change		Cassava root		
Impact category	Unit	10%	0%	-10%
Human toxicity by ingestion	1/LD 50	3.06E-09	2.89E-09	2.71E-09
Human toxicity by exposure	1/TWA	8.45E-08	7.94E-08	7.42E-08
Aquatic toxicity	1/LC50	1.81E-07	1.67E-07	1.53E-07
Global warming potential	kg CO2 eq.	-0.9590	-0.8713	-0.7836
Ozone depletion	kg CFC-11 eq.	8.95E-12	8.20E-12	7.44E-12
Photochemical oxidation	kg C2H2 eq.	7.72E-04	7.04E-04	6.35E-04
Acidification	mol H+ eq.	0.1147	0.1043	0.0940
Human toxicity-carcinogenics	kg benzene eq	9.05E-05	8.29E-05	7.52E-05
Human toxicity-noncarcinogenics	kg toluene eq	0.2471	0.2263	0.2055
Fresh water ecotoxicity	kg 2,4-D eq	0.0062	0.0057	0.0052
Deposited waste	UBP	0.0000	0.0000	0.0000
Mineral extraction	kg Sb eq	0.0000	0.0000	0.0000
Water consumption	UBP	0.0000	0.0000	0.0000
Non-renewable, fossil	MJ eq	0.5120	0.4699	0.4278
Non-renewable, nuclear	MJ eq	0.0000	0.0000	0.0000
Renewable, biomass	MJ eq	0.0000	0.0000	0.0000
Renewable, wind, solar, geothermal	MJ eq	0.0000	0.0000	0.0000
Renewable water	MJ eq	0.0000	0.0000	0.0000
Terrestrial toxicity	1/LD 50	3.06E-09	2.89E-09	2.71E-09
Photochemical ozone formation	kg NMVOC eq	6.71E-04	6.12E-04	5.53E-04
Marine eutrophication	kg N eq	3.18E-04	2.90E-04	2.62E-04
Freshwater eutrophication	kg P eq	0.0000	0.0000	0.0000
Terrestrial eutrophication	mol N eq	0.0143	0.0130	0.0117
Ionizing radiation	kg U_{235} eq	0.0000	0.0000	0.0000
Particulate matter	kg PM2.5 eq	6.48E-05	5.89E-05	5.30E-05

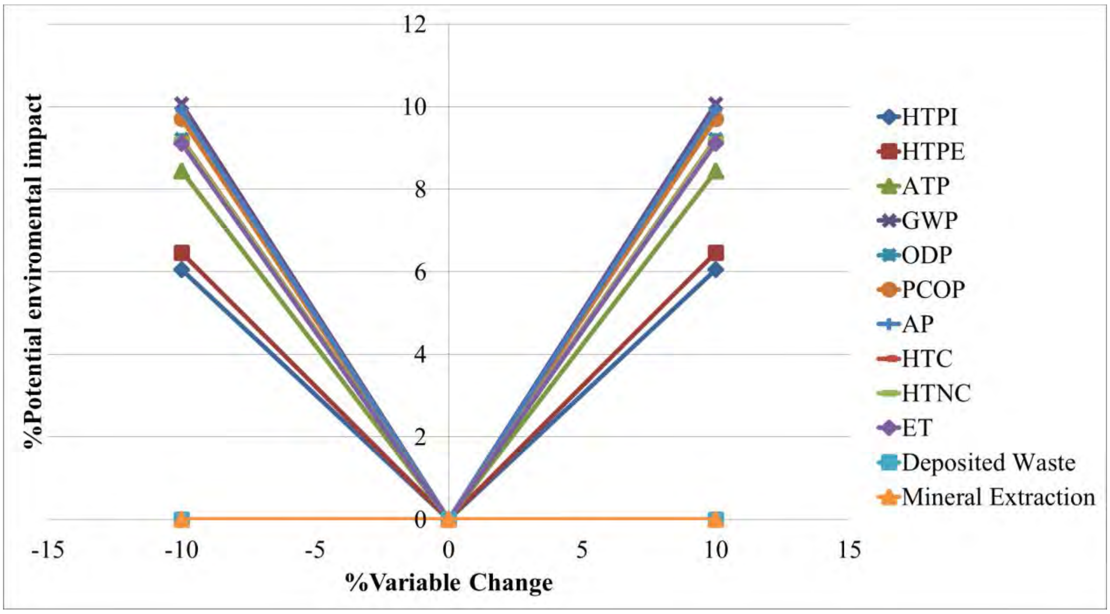

Figure 4.2 Percentage of the first group of environmental impact change when the amount of cassava root has been changed.

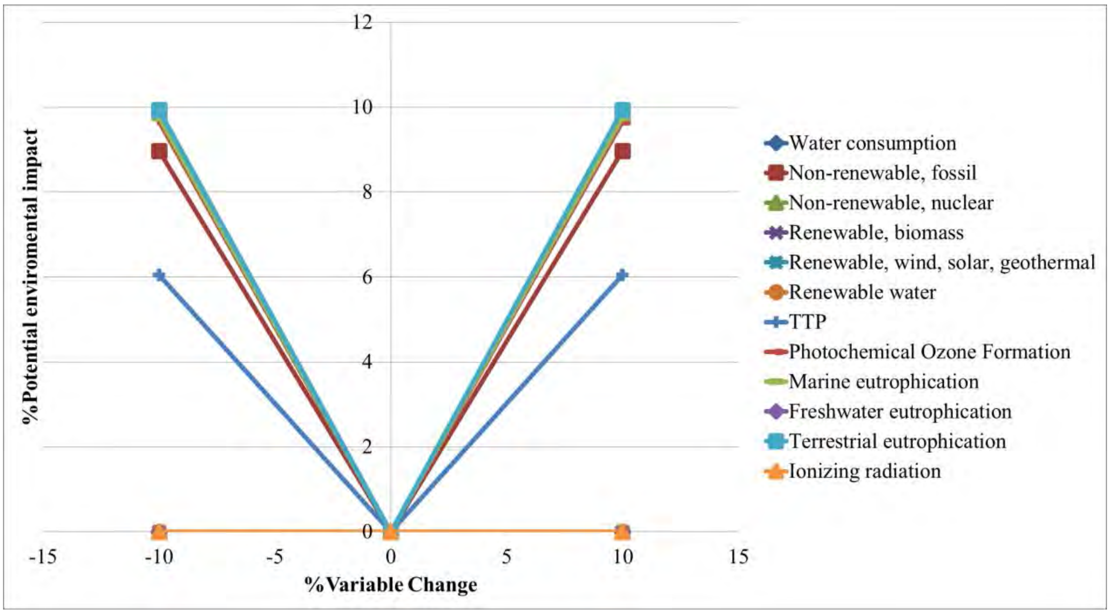

Figure 4.3 Percentage of the second group of environmental impact change when the amount of cassava root has been changed.

4.2.4 Endpoint Impact Categories

Endpoint categories are represented the impact at the end of cause-effect chain, for example, the extinction of a species. Which are the accumulate effect from many midpoint impacts categories. These are helpful for easy understanding the environmental impact from the process. Therefore, endpoint impact categories were added in to LCSoft as optional calculation. The calculation model for endpoint categories was same as midpoint impact categories which characterization factor for endpoint categories were collected from ILCD handbook and ReCiPe methods. Both methods provided endpoint impact categories in three types which are Human health, Ecosystem species, and Natural resource.

Human health indicator is described by Disability Adjusted Life Years (DALY) quantifying the impact of premature death or disability that environmental impacts have on the population. Ecosystem species is described by Potentially Disappeared Fraction of species (PDF) expressing the loss of species in terrestrial ecosystems caused by environmental impacts. Natural resource is described by Surplus costs which was expression of the marginal increase of costs ($/kg) due to extraction/production (kg).

In order to validate this feature, production of bio-ethanol from cassava rhizome (Mangnimit *et al.*, 2013) was also a case study for performing this feature in LCSoft. The endpoint impact indicator results, calculating by ReCiPe method from LCSoft were compared with the results from SimaPro v.8.2.3. The results are shown in the Table 4.9, which LCSoft provided the endpoint impact categories result close to the results from SimaPro. However, the differences are affected from the inventory data of combustions process in SimaPro that yield larger set of emission than LCSoft.

Table 4.9 Comparative endpoint indicator results between LCSoft and SimaPro

Endpoint Categories	Unit	LCSoft	SimaPro	Percent Differrence
Human health	DALY	1.11E-06	1.38E-06	10.98
Ecosystem species	species.yr	3.59E-09	4.08E-09	6.33
Natural resource	$	0.043862	0.0522	8.68

4.2.5 Calculation with Uncertainty

Uncertainty is normally included in every part of LCA study, which brings the question, that the results are included uncertainty or not. Therefore, the calculation with uncertainty in the product system features was added for essential providing the result with uncertainty. In this features, user could specify range of uncertainty which should associate with their data. The specify value was used as range of random LCI (Life cycle inventory) data, that result to fluctuation of environmental impact result.

A case study, bio-ethanol production from cassava rhizome (Mangnimit *et al.*, 2013) was used to give more clearly explanation by setting ten percent uncertainty range in the LCI data. Part of LCI data and the environmental impacts results are shown in Table 4.10 and Table 4.11 respectively. The inventories data from the process were random in the uncertainty range, minus ten percent to plus ten percent. Thus, the environmental impacts, which were directly affected from LCI data, also changed from the original process as percentage difference that shown in Table 4.11.

Table 4.10 Comparison of LCI data between original process and process with 10% uncertainty range

Substance	Compartment	Sub Compartment	Unit	Original process	With 10% Uncertainty range	Percentage Difference
1,4-Butanediol	water	river	kg	1.84E-12	1.79E-12	2.30
2,4-D	soil	agricultural	kg	3.86E-11	3.75E-11	2.77
2-Chloro acetophenone	air	unspecified	kg	2.48E-15	2.47E-15	0.42
2-Hexanone	water	unspecified	kg	7.51E-10	7.31E-10	2.64
2-Propanol	air	high population	kg	8.58E-08	8.45E-08	1.57
4-Methyl-2-pentanone	water	unspecified	kg	2.01E-10	2.03E-10	1.15
Acenaphthene	air	high population	kg	7.86E-14	7.68E-14	2.19
Acetic acid	air	unspecified	kg	2.45E-08	2.49E-08	1.61
Acetone	water	unspecified	kg	9.03E-10	9.02E-10	0.19
Aluminum	air	unspecified	kg	9.75E-06	9.78E-06	0.37
Antimony	water	unspecified	kg	6.30E-09	6.27E-09	0.58
Barite	water	ocean	kg	3.76E-05	3.77E-05	0.28
Barium	air	unspecified	kg	1.31E-13	1.31E-13	0.13
Barium	water	ground-	kg	3.51E-08	3.38E-08	3.70
Benzene	air	unspecified	kg	2.53E-05	2.49E-05	1.54

Table 4.11 Comparison of LCIA data between original process and process with 10% uncertainty range

Impact Categories	Unit	Original process	With 10% Uncertainty range	Percentage Difference
Human toxicity by ingestion	1/LD 50	2.34E-07	2.33E-07	0.30
Human toxicity by exposure	1/TWA	1.74E-06	1.73E-06	0.68
Aquatic toxicity	1/LC50	1.17E-05	1.17E-05	0.04
Global warming potential	kg CO2 eq.	0.4416247	0.47146	6.76
Ozone depletion	kg CFC-11 eq.	4.23E-07	4.12E-07	2.47
Photochemical oxidation	kg C2H2 eq.	0.0020296	0.00203	0.07
Acidification	mol H+ eq.	0.2122397	0.21446	1.04
Human toxicity-carcinogenics	kg benzene eq	0.0048792	0.00487	0.12
Human toxicity-noncarcinogenics	kg toluene eq	5.47110	5.61219	2.58
Fresh water ecotoxicity	kg 2,4-D eq	0.2266203	0.22755	0.41
Deposited waste	UBP	46.09924	46.7913	1.50
Mineral extraction	kg Sb eq	3.91E-09	3.90E-09	0.32
Water consumption	UBP	4.1199689	4.10784	0.29
Non-renewable, fossil	MJ eq	14.432837	14.30456	0.89
Non-renewable, nuclear	MJ eq	0.00	0.00	0.00
Renewable, biomass	MJ eq	0.0178816	0.01770	1.00
Renewable, wind, solar, geothermal	MJ eq	0.0063429	0.00615	3.00
Renewable water	MJ eq	0.3433622	0.33546	2.30
Terrestrial toxicity	1/LD 50	2.339E-07	2.33E-07	0.30
Photochemical ozone formation	kg NMVOC eq	0.00220	0.00220717	0.44
Marine eutrophication	kg N eq	0.0007126	0.00071	0.66
Freshwater eutrophication	kg P eq	7.744E-06	7.5808E-06	2.11
Terrestrial eutrophication	mol N eq	0.01787	0.01822	1.94
Ionizing radiation	kg U_{235} eq	0.15633	0.15253	2.43
Particulate matter	kg PM2.5 eq	0.00017	0.00017	0.55

4.3 Extension of LCI Database for Covering All Impact Categories

Originally, LCSoft LCI database was obtained from US LCI (U.S. Life Cycle Inventory Database, 2014), ELCD (European reference Life Cycle Database, 2006) and other literatures. The database were organized through LCI knowledge base (LCI KB) management tool which divided into two level, LCI KB's first level and LCI KB's second level as shown in Figure 4.4.

LCI KB's first level was organized into 3 main categories depend on type of products or processes: (1) Material, (2) Utility, and (3) Transportation. Which each category was divided into 5 sub-categories.

LCI KB's second level was LCI data of each unit process, which consisted of 2 categories: (1) input type, there were two type of input, input from technosphere (activities and/or material required from other unit processes) and input from resources (energy, mineral, water, and other natural resources); (2) output type, such as emission (air, soil, and water), by-product or waste, and others.

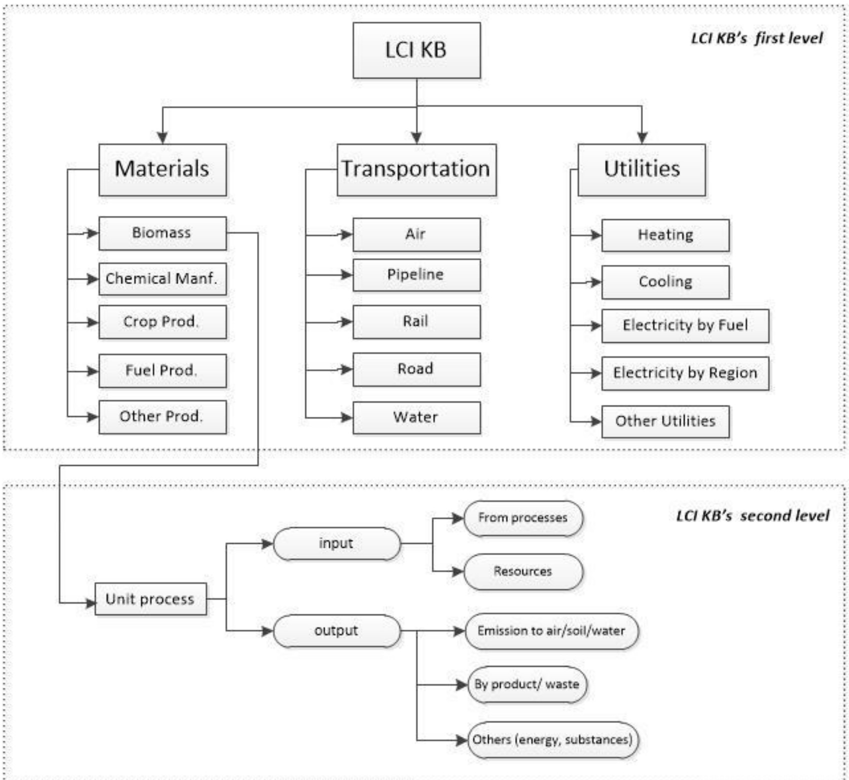

Figure 4.4 LCSoft LCI database structure.

LCSoft LCI database could cover the most of impact categories calculation; however, there could not evaluate in some categories which only affected from specific substance. In this version, LCSoft LCI database was extended by adopting partial inventory from other available sources in order to cover the missing impact categories assessment. Production of 1 kg benzene, at plant – RNA from US.LCI database was used as case study for checking the missing impact categories result. Table C3 shows detail of benzene production process.

As a result, nine impact categories result were missing, which were deposited waste, mineral extraction, water consumption, non-renewable energy from nuclear consumption, renewable energy from biomass consumption, renewable energy from wind, solar, geothermal consumption, renewable water, freshwater eutrophication, and ionizing radiation as shown in grey area in Table 4.12.

Table 4.12 Environmental impact results of benzene production US. LCI database

Impact Categories	Benzene - US. LCI	Unit
Human toxicity by ingestion	6.22E-08	1/LD 50
Human toxicity by exposure	1.17E-06	1/TWA
Aquatic toxicity	1.96E-06	1/LC50
Global warming potential	0.5756	kg CO2 eq.
Ozone depletion	1.31E-07	kg CFC-11 eq.
Photochemical oxidation	0.0011	kg C2H2 eq.
Acidification	0.0499	mol H+ eq.
Human toxicity-carcinogenics	0.0004	kg benzene eq.
Human toxicity-noncarcinogenics	1.1172	kg toluene eq.
Fresh water ecotoxicity	0.0277	kg 2,4-D eq.
Deposited waste	0	UBP
Mineral extraction	0	kg Sb eq.
Water consumption	0	UBP
Non-renewable, fossil	5.3938	MJ eq.
Non-renewable, nuclear	0	MJ eq.
Renewable, biomass	0	MJ eq.
Renewable, wind, solar, geothermal	0	MJ eq.
Renewable water	0	MJ eq.
Terrestrial toxicity	6.22E-08	1/LD 50
Photochemical Ozone Formation	0.0011	kg NMVOC eq.
Marine eutrophication	0.0004	kg N eq.
Freshwater eutrophication	0	kg P eq.
Terrestrial eutrophication	0.0044	mol N eq.
Ionizing radiation	0	kg U_{235} eq.
Particulate matter	2.79E-05	kg PM2.5 eq.

In order to calculate the missing impact categories, LCI database should be extended to covers the relative substances. The lists of substances were obtained from characterization factor of missing impact categories. Table 4.13 shows some of relative substances for each missing impact categories. These substances had been checked with LCSoft LCI database, and adopted the deficient inventory in LCSoft from other available sources.

Table 4.13 Example of relative substances in missing categories

Impact Categories	Emissions Source	Substances
Nonrenewable, fossil	resource	Coal, 18 MJ per kg, in ground Coal, hard, 26.4 MJ per kg, in ground Coal, brown, 10 MJ per kg, in ground Coal, brown, in ground Coal, feedstock, 26.4 MJ per kg, in ground Coal, bituminous, 24.8 MJ per kg Coal, hard, unspecified, in ground Energy, from coal Energy, from coal, brown Energy, from gas, natural Energy, from oil Energy, from peat Energy, from sulfur Energy, unspecified
Nonrenewable, nuclear	resource	Energy, from uranium Uranium ore, 1.11 GJ per kg, in ground Uranium, 2291 GJ per kg, in ground Uranium, 560 GJ per kg, in ground Uranium, in ground
Renewable, biomass	resource	Biomass, feedstock Energy, from biomass Energy, from wood Energy, gross calorific value, in biomass Energy, gross calorific value, in biomass, primary forest
Renewable, wind, solar, geothermal	resource	Energy, geothermal Energy, geothermal, converted Energy, kinetic (in wind), converted Energy, solar Energy, solar, converted
Renewable, water	resource	Energy, from hydro power Energy, from hydrogen Energy, potential (in hydropower reservoir), converted Water, barrage

Table 4.13 Example of relative substances in missing categories (cont'd)

Impact Categories	Emissions Source	Substances
Deposited waste	waste	TOC, Total Organic Carbon Volume occupied, underground deposit Volume occupied, final repository for low-active radioactive waste Volume occupied, final repository for radioactive waste
Water resource consumption	resource	Water, cooling, unspecified natural origin Water Water, salt, ocean Water, salt, sole
Freshwater eutrophication	soil	Phosphate Phosphoric acid Phosphorus, total
	water	Phosphate Phosphoric acid Phosphorus, total
Ionizing radiation Human Health	unspecified	Carbon-14 Cesium-134 Cesium-137 Cobalt-58 Cobalt-60 Hydrogen-3, Tritium Iodine-129 Iodine-131 Iodine-133 Krypton-85 Lead-210 Plutonium-238 Plutonium-alpha Polonium-210 Radium-226 Radon-222 Thorium-230 Uranium-234 Uranium-235 Uranium-238 Xenon-133 Americium-241 Antimony-124 Antimony-125 Curium alpha Manganese-54 Ruthenium-106 Silver-110 Strontium-90

The LCI data of available databases were generated by LCSoft calculation method (Matrix Inversion), which total inventories of the products and processes were retrieved. The products or processes inventories were compared with original inventories with similar products or processes in LCSoft. The relative inventories with missing impact categories were adopted into the LCSoft LCI database. Table 4.14 shows some part LCI of 1 kilogram of Benzene production which greys area shows the adopted inventories.

With the extended LCSoft LCI database, the missing impact categories could calculate as shown in Table 4.15. Although these extended data may aggregated and/or reduced some of environmental impact results, the effect from all impact could investigate and was very helpful for process design and optimization.

Table 4.14 Some part of LCI of 1 kilogram benzene production

Substance	Compartment	Sub compartment	Unit	Total
Acrolein	air	unspecified	kg	6.30E-09
Ammonia, as N	water	unspecified	kg	2.88E-12
Ammonia	air	unspecified	kg	8.52E-07
Acetophenone	air	unspecified	kg	1.64E-14
Cobalt-60	air	low population density	kBq	9.161E-12
Cobalt-60	water	river	kBq	3.83E-08
Copper, ion	water	unspecified	kg	4.80E-08
Isophorone	air	unspecified	kg	6.32E-13
Isoprene	air	unspecified	kg	8.94E-06
Kerosene	air	unspecified	kg	1.17E-08
Krypton-85	air	low population density	kBq	1.46E-06
Lead	air	unspecified	kg	7.41E-09
Lead	water	unspecified	kg	9.47E-08
Lead-210	air	high population density	kBq	4.21E-09
Phenols, unspecified	air	unspecified	kg	1.46E-08
Phenols, unspecified	water	unspecified	kg	1.40E-08
Phosphate	water	ground-	kg	4.81E-11
Propanal	air	unspecified	kg	4.14E-13
Propene	air	unspecified	kg	1.50E-07
Propylene oxide	air	unspecified	kg	2.13E-09
p-Xylene	water	unspecified	kg	1.86E-10
Strontium-90	water	river	kBq	4.64E-06
Styrene	air	unspecified	kg	2.72E-14
Sulfide	water	unspecified	kg	1.01E-06
Sulfur dioxide	air	unspecified	kg	0.0001

Table 4.15 Environmental impact results of benzene production of extended database

Impact Categories	Benzene	Unit
Human toxicity by ingestion	6.22E-08	1/LD 50
Human toxicity by exposure	1.17E-06	1/TWA
Aquatic toxicity	1.96E-06	1/LC50
Global warming potential	0.5756	kg CO2 eq.
Ozone depletion	1.31E-07	kg CFC-11 eq.
Photochemical oxidation	0.0011	kg C2H2 eq.
Acidification	0.0499	mol H+ eq.
Human toxicity-carcinogenics	0.0004	kg benzene eq.
Human toxicity-noncarcinogenics	1.1172	kg toluene eq.
Fresh water ecotoxicity	0.0277	kg 2,4-D eq.
Deposited waste	61.6732	UBP
Mineral extraction	4.91E-09	kg Sb eq.
Water consumption	19.5281	UBP
Non-renewable, fossil	6.4862	MJ eq.
Non-renewable, nuclear	0.0000	MJ eq.
Renewable, biomass	0.1069	MJ eq.
Renewable, wind, solar, geothermal	1.65E-05	MJ eq.
Renewable water	0.0837	MJ eq.
Terrestrial toxicity	6.22E-08	1/LD 50
Photochemical ozone formation	0.0011	kg NMVOC eq.
Marine eutrophication	0.0004	kg N eq.
Freshwater eutrophication	9.30E-06	kg P eq.
Terrestrial eutrophication	0.0044	mol N eq.
Ionizing radiation	0.0002	kg U_{235} eq.
Particulate matter	2.79E-05	kg PM2.5 eq.

4.4 Validation of LCSoft using Case Studies

In this version, LCSoft was updated with new features and improvement of the existing functions. For further improvement, the performance of LCSoft was validated for efficiency, reliability, and deficiency by comparing the environmental impact assessment results from case studies with latest version of commercial LCA software, SimaPro v.8.2.3. The validations by performing LCA calculation through general method in LCSoft (21 impact categories) and ILCD method (15 impact categories) were conducted using LCSoft and SimaPro v.8.2.3 with two case studies: (1) bioethanol production from cassava rhizome; (2) para-xylene production from toluene methylation.

4.4.1 Bioethanol Production from Cassava Rhizome

In parameter sensitivity analysis part, bioethanol production from cassava rhizome case study was introduced. The boundary system of LCA study focused on cradle-to-gate which included production of cassava phase, transportation, and manufacturing. The process data were taken from the simulation results (Mangnimit *et al.*, 2013) as shown in Figure A1, Table A1 and Table A2 for flowsheet, stream table, and equipment table, respectively. Input biomass was 377 tons/day and ethanol product was 119 tons/day. For LCA study, 1 kg of pure ethanol was considered as the functional unit. The contribution of this process is shown in Table 4.16

Table 4.16 Process contribution of bioethanol production from cassava rhizome

Process Contribution	Amount	Unit
Material		
Ammonia, steam reforming, liquid, at plant	3.31	kg
Cassava root	15008.13	kg
Enzyme, Cellulase, Novozyme Celluclast	8.32	kg
Corn steep liquor	147.47	kg
Sulfuric acid, at plant	258.34	kg
Utility		
Natural gas, combusted in industrial equipment	60584.60	MJ
Cooling energy, natural gas, at cogen unit with absorption chiller 100 kW	47938.30	MJ
Electricity, natural gas, at power plant	5.70	kWh

4.4.1.1 LCSoft Consideration Model

In order to analyze the environmental impacts result, the contained process and material in LCSoft LCI database, which obtained from US.LCI database and other literature, were used to calculate. The materials were: Cassava rhizome, Ammonia, Sulfuric acid, Corn steep liquor, and cellulose enzyme. The utility process were: electricity using natural gas, Natural gas, combusted in industrial equipment, and Cooling energy, natural gas, at cogen unit with absorption chiller 100 kW. Therefore, the impacts associated with these materials and processes were included in the assessment which calculated by either general LCSoft method with 21 impact categories or new pathway for calculation with 15 impact categories.

4.4.1.2 SimaPro Consideration Model

The material and process were used from SimaPro database which were selected from the similar process as LCSoft. However, some materials that not existed in Simapro, such as, Cassava rhizome, Corn steep liquor, and Cellulose enzyme, were modeled by using LCI data from literature. Since the calculation methodologies in LCSoft were gathered from many sources, the variety methods were selected in order to compare with all environmental impact categories in LCSoft. Characterization factor from TRACI method was used to calculate acidification, aquatic toxicity, global warming potential, human toxicity by exposure, human toxicity by ingestion, ozone depletion, photochemical oxidation, and fresh water ecotoxicity. CML-IA was used to calculate mineral extraction. Ecological Scarcity 2013 was used to calculate water consumption and deposited waste. Cumulative Energy Demand was used to calculate energy consumption. And the rest categories were calculated by ILCD method.

4.4.1.3 Validation of Environmental Impact Assessment Calculation

Comparison of environmental impact result for fifteen impact categories were calculated by ILCD 2011 midpoint method from both software, as shown in Table 4.17. The validation results from new version of LCSoft and SimaPro provided the same trend of calculations for the most environmental impact categories, which LCSoft gave a slightly different result than SimaPro, the percentage difference of these categories are not more than ten percent. However, SimaPro yield higher environmental impact than LCSoft in fresh water ecotoxicity category, human toxicity, cancer effect and non-cancer effect, particulate matter, photochemical ozone formation, acidification mineral extraction and other relative categories with combustion fuel emissions. The differences were come from the different set of emission factors between both software, such as combustion fuel emission factor, US.LCI database in SimaPro model had larger sets of emission factors, compared with those in the LCSoft model.

Table 4.17 Comparative result of bioethanol process between Simapro and LCSoft using ILCD method

Impact Categories	Unit	LCSoft	SimaPro 8.2.3	Difference	Percentage Difference
Global Warming	kg CO2 eq	0.44907	0.48502	-0.03595	7.70
Ozone Depletion	kg CFC-11 eq	8.1E-08	8.1E-08	-1.2E-10	0.15
Human toxicity, cancer effect	CTUh	2.2E-08	2.4E-08	-2.2E-09	9.51
Human toxicity, non-cancer effect	CTUh	4.2E-08	7.5E-08	-3.24E-08	55.10
Fresh water ecotoxicity	CTUe	0.54346	1.39449	-0.85103	87.83
Particulate matter	kg PM2.5 eq	0.00017	0.00053	-0.00036	103.10
Ionizing radiation	kg U_{235} eq	0.15633	0.15624	0.00009	0.06
Photochemical Ozone Formation	kg NMVOC eq	0.00220	0.00259	-0.00039	16.38
Acidification	molc H+ eq	0.00528	0.01302	-0.00774	84.58
Terrestrial eutrophication	molc N eq	0.01788	0.01769	0.00019	1.09
Freshwater eutrophication	kg P eq	7.7E-06	7.7E-	0.00000	0.00
Marine eutrophication	kg N eq	0.00071	0.00071	0.00000	0.04
Water resource consumption	m^3 water eq	0.00284	0.00288	-0.00004	1.46
Mineral Extraction	kg Sb eq	4.78E-09	1.29E-07	-1.25E-07	-185.74
Land use	kg C deficit	9.44269	9.44710	-0.00441	0.05

In addition, the validation by general calculation method in LCSoft (21 impact categories) was done in order to consistency verified the software. Comparison of environmental impact results for twenty-one impact categories were calculated, as shown in Table 4.18. There were different LCIA results in some environmental impact categories obtained from LCSoft and SimaPro. Global warming potential, ozone depletion, and human toxicity-carcinogenics environmental impact results from LCSoft were greater than SimaPro, because characterization factors of environmental impact categories contained in LCSoft were extended by Group Contribution method (Hukkerikar *et al*., 2012), which could estimate characterization factor of substance that not exist in SimaPro. On the contrary, environmental impact results on acidification, human toxicity-noncarcinogenics, fresh water ecotixcity, photochemical ozone formation, and particulate matter, SimaPro yield higher result than LCSoft, because SimaPro model had larger sets of emission factors associated with the combustion fuels compared with those in LCSoft model.

Table 4.18 Comparative result of bioethanol process between Simapro and LCSoft

Impact Categories	Unit	LCSoft	SimaPro 8.2.3	Difference	Percentage Difference
Human toxicity by ingestion	1/LD 50	2.34E-07	x	x	x
Human toxicity by exposure	1/TWA	1.74E-06	x	x	x
Aquatic toxicity	1/LC50	1.17E-05	x	x	x
Global warming potential	kg CO2 eq.	0.44162	0.40799	0.03363	7.92
Ozone depletion	kg CFC-11 eq.	4.23E-07	8.12E-08	3.41E-07	135.51
Photochemical oxidation	kg C2H2 eq.	0.00203	0.00044	0.00159	128.77
Acidification	mol H+ eq.	0.21224	0.50622	-0.29398	81.84
Human toxicity-carcinogenics	kg benzene eq	0.00488	0.00165	0.00322	98.70
Human toxicity-noncarcinogenics	kg toluene eq	5.47110	7.30708	-1.83598	28.74
Fresh water ecotoxicity	kg 2,4-D eq	0.22662	1.78883	-1.56221	155.02
Deposited Waste	UBP	46.09924	46.09931	-0.00007	0.00
Mineral Extraction	kg Sb eq	3.91E-09	x	x	x
Water consumption	UBP	1.09243	1.08536	0.00707	0.65
Non-renewable, fossil	MJ eq	14.13138	14.66581	-0.53443	3.71
Non-renewable, nuclear	MJ eq	x	x	x	x
Renewable, biomass	MJ eq	0.01788	0.01787	0.00001	0.07
Renewable, wind, solar, geothermal	MJ eq	0.00634	0.00634	0.00000	0.00
Renewable water	MJ eq	0.34336	0.34336	0.00000	0.00
Terrestrial toxicity	1/LD 50	2.34E-07	x	x	x
Photochemical ozone formation	kg NMVOC eq	2.20E-03	0.00259	-0.00039	16.38
Marine eutrophication	kg N eq	0.00071	0.00071	0.00000	0.04
Freshwater eutrophication	kg P eq	7.74E-06	7.74E-06	0.00000	0.00
Terrestrial eutrophication	mol N eq	0.01788	0.01769	0.00019	1.09
Ionizing radiation	kg U_{235} eq	0.15633	0.15624	0.00009	0.06
Particulate matter	kg PM2.5 eq	0.00017	0.00053	-0.00036	103.10

4.4.2 Para-xylene Production from Toluene Methylation

Production of para-xylene from toluene methylation was taken to validate the new version of LCSoft with SimaPro8.2.3. The process was cradle-to-gate, which was analyzed in production of feedstock, transportation, and manufacturing. The data were taken from the simulation results (Nateetorn *et al.*, 2016) as shown in flowsheet (Figure B1), stream table (Table B1), and equipment table (Table B2). Input toluene, methanol, and product para-xylene were 569, 318, and 513 tons/day, respectively. For LCA study, 1 kg of pure para-xylene was considered as the functional unit. The contribution of this process is shown in Table 4.19.

Table 4.19 Process contribution of para-xylene production process

Process Contribution	Amount	Unit
Material		
Toluene, at plant/RNA	23707.57	kg
Methanol, at plant/RNA	13255.07	kg
Utility		
Electricity, natural gas, at power plant/US	34.39	kWh
Cooling energy, natural gas, at cogen unit with absorption chiller 100 kW	344838.32	MJ
Natural gas, combusted in industrial equipment/RNA	333134.73	MJ

4.4.2.1 LCSoft Consideration Model

LCSoft LCI database, which obtained from US.LCI and other literature, were used to calculate. The materials were: Toluene and Methanol. The utility process were electricity using natural gas, natural gas, combusted in industrial equipment, and cooling energy, natural gas, at cogen unit with absorption chiller 100 kW. Therefore, the impacts associated with these materials and processes were included in the assessment which calculated by either general LCSoft method with 21 impact categories or new pathway for calculation with 15 impact categories.

4.4.2.2 SimaPro Consideration Model

The material and process were used from Simapro database which are selected from the similar process as LCSoft. However, material “Toluene, at plant” was not existed in SimaPro then the model was used LCI data from literature. Since the calculation methodologies in LCSoft were gathered from many sources, the variety methods were selected in order to compare with all environmental impact categories in LCSoft. Characterization factor from TRACI method was used to calculate environmental impact on acidification, aquatic toxicity, global warming potential, human toxicity by exposure, human toxicity by ingestion, ozone depletion, photochemical oxidation, and fresh water ecotoxicity categories. CML-IA was used to calculate mineral extraction. Ecological Scarcity 2013, was used to calculate water consumption and deposited waste. Cumulative Energy Demand (CED) was used to calculate energy consumption. And the rest categories were calculated by ILCD method.

4.4.2.3 Validation of Environmental Impact Assessment Calculation

Para-xylene production from toluene methylation case study was conducted to validate LCSoft by perform LCIA through general LCSoft method (21 impacts) and ILCD method (15 impacts). Comparisons of environmental impact results from both methods are shown in Table 4.18 and Table 4.19.

For Table 4.20, environmental impacts results were estimated by ILCD method, and compared the results between LCSoft and SimaPro. The major differences were fresh water ecotoxicity, human toxicity, cancer effect and non-cancer effect, particulate matter, photochemical ozone formation, acidification mineral extraction impact categories, which were the same impact categories that are different in previous case study. The values from SimaPro were greater than LCSoft. These differences were also occurred from the different emission factor data set in the USLCI database between both software. For example, although material from both software was the same such as toluene, but the feedstock for toluene which was "Petroleum refining for olefin product" did not have the same dataset. SimaPro model yields larger set of metal and sulfur compound more than LCSoft which affected to the environmental impact results in categories that mentioned above. Also, the emission factor associated with combustion fuels in SimaPro had larger set of emissions compared to those in LCSoft. For global warming categories LCSoft yield this impact more than SimaPro, because in SimaPro dataset did not have carbon monoxide emission for methanol production. Although, both software used the dataset from USLCI database, SimaPro may use adapted dataset from USLCI, while LCSoft used exact dataset from USLCI database. For this reason LCIA results from LCSoft and SimaPro were different.

For Table 4.21, environmental impacts results were estimated by general LCSoft method with 21 impact categories, the problem from database was same as previous method and previous case study. SimaPro had higher impact score in acidification, human toxicity, fresh water ecotoxicity, photochemical ozone formation, and particulate matter categories. And LCSoft had higher impact score in global warming potential, ozone depletion, and human toxicity-carcinogenics categories. These differences are also caused from differences in database and the Group Contribution method that implemented on this method.

Table 4.20 Comparative result of para-xylene process between SimaPro and LCSoft using ILCD method

Impact Categories	Unit	LCSoft	Simapro	Difference	Percentage Difference
Global Warming	kg CO2 eq	3.5031	3.2400	0.2631	7.80
Ozone Depletion	kg CFC-11 eq	1.35E-07	1.36E-07	-5.79E-10	0.43
Human toxicity, cancer effect	CTUh	4.65E-08	1.08E-07	-6.15E-08	79.65
Human toxicity, non-cancer effect	CTUh	1.69E-07	7.95E-07	-6.26E-07	129.78
Fresh water ecotoxicity	CTUe	2.7988	15.5000	-12.7011	138.82
Particulate matter	kg PM2.5 eq	0.0011	0.0016	-0.0005	37.39
Ionizing radiation	kg U_{235} eq	0.2610	0.2610	0.0000	0.00
Photochemical Ozone Formation	kg NMVOC eq	0.0105	0.0151	-0.0046	36.01
Acidification	molc H+ eq	0.0081	0.0381	-0.0300	129.76
Terrestrial eutrophication	molc N eq	0.0277	0.0282	-0.0005	1.82
Freshwater eutrophication	kg P eq	4.28E-06	4.28E-06	0.0000	0.00
Marine eutrophication	kg N eq	0.00246	0.00263	-0.00017	6.79
Water resource consumption	m^3 water eq	0.0048	0.0048	0.0000	0.00
Mineral extraction	kg Sb eq	4.64E-08	1.05E-06	-1.00E-06	183.08
Land use	kg C deficit	1.0447	1.0400	0.0047	0.45

Table 4.21 Comparative result of para-xylene process between SimaPro and LCSoft

Impact Categories	Unit	LCSoft	Simapro	Difference	Percentage Difference
Human toxicity by ingestion	1/LD 50	7.29E-07	x	x	x
Human toxicity by exposure	1/TWA	7.83E-06	x	x	x
Aquatic toxicity	1/LC50	2.92E-05	x	x	x
Global warming potential	kg CO2 eq.	3.4328	3.0700	0.3628	11.16
Ozone depletion	kg CFC-11 eq.	7.32E-07	1.36E-07	5.96E-07	137.31
Photochemical oxidation	kg C2H2 eq.	0.0072	0.0020	0.0052	113.85
Acidification	mol H+ eq.	0.3906	1.5500	-1.1594	119.49
Human toxicity-carcinogenics	kg benzene eq	0.0100	0.0047	0.0053	72.23
Human toxicity-noncarcinogenics	kg toluene eq	14.1237	49.8746	-35.7509	111.72
Fresh water ecotoxicity	kg 2,4-D eq	0.5095	1.1200	-0.6105	74.92
Deposited Waste	UBP	76.9470	77.0000	-0.0530	0.07
Mineral Extraction	kg Sb eq	6.53E-09	x	x	x
Water consumption	UBP	1.8046	1.8000	0.0046	0.25
Non-renewable, fossil	MJ eq	102.4165	106.0000	-3.5835	3.44
Non-renewable, nuclear	MJ eq	x	x	x	x
Renewable, biomass	MJ eq	0.0298	0.0298	0.0000	0.00
Renewable, wind, solar, geothermal	MJ eq	0.0106	0.0106	0.0000	0.00
Renewable water	MJ eq	0.5731	0.5730	0.0001	0.02
Terrestrial toxicity	1/LD 50	7.29E-07	x	x	x

Table 4.21 Comparative result of para-xylene process between SimaPro and LCSoft (cont'd)

Impact Categories	Unit	LCSoft	Simapro	Difference	Percentage Difference
Photochemical Ozone Formation	kg NMVOC eq	0.0105	0.0151	-0.0046	35.97
Marine eutrophication	kg N eq	0.0025	0.0026	-0.0002	6.79
Freshwater eutrophication	kg P eq	4.28E-06	4.28E-06	0.0000	0.00
Terrestrial eutrophication	mol N eq	0.0277	0.0282	-0.0005	1.82
Ionizing radiation	kg U_{235} eq	0.2609	0.2610	-0.0001	0.02
Particulate matter	kg PM2.5 eq	0.0011	0.0017	-0.0005	37.39

4.5 LCSoft New Version Framework

Figure 4.5 shows new LCSoft version framework which grey area represents improvement of source codes on this version. There is five main steps and various optional steps in order to analyze LCA. Five main steps including: (1) existence of LCI data checking; (2) retrieve LCI data; (3) impact assessment; (4) environmental (4) contribution analysis; and (5) interpretation. Six optional steps including: (1) carbon footprint calculation; (2) endpoint impact categories calculation; (3) normalization; (4) parameter and source sensitivity analysis; (5) uncertainty analysis; (6) alternative comparison; and (6) eco-efficiency evaluation. The detail is summarized in Table 4.22 and described as follow:

4.5.1 Step 1: LCI Data Checking

LCI data of products or processes will be checked from all set of data that contained in LCSoft database. All data will be shown to users which users can add or modify. After finished adding or modifying data, the LCI result will be recalculated by LCI calculation function and save in software directory.

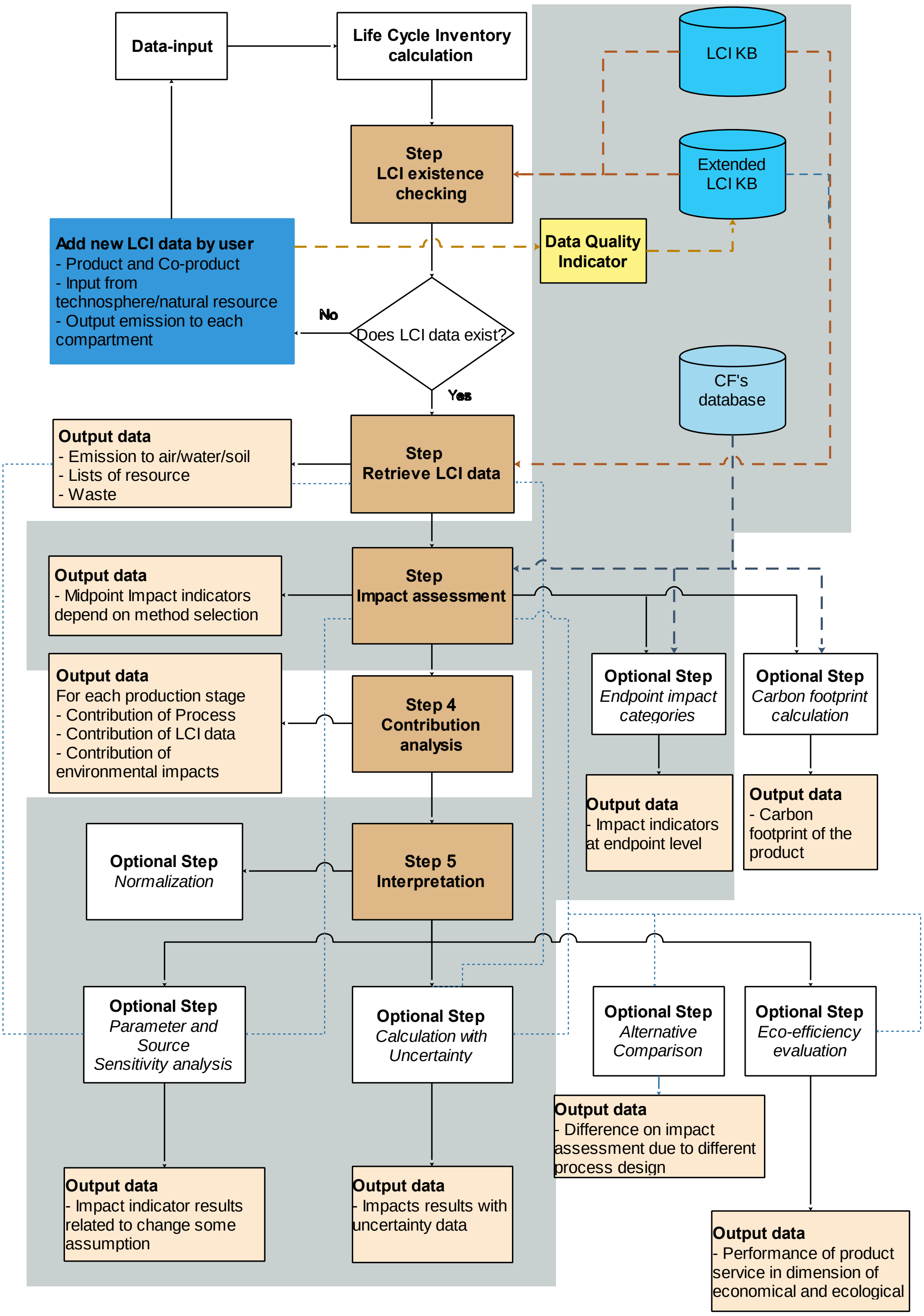

Figure 4.5 LCSoft version 5 framework.

4.5.2 Step 2: Retrieve LCI Data

LCI data which relate to products and/or processes are retrieved from LCI KB and Extended LCI KB, for example, raw materials, natural resources, and emissions from the processes.

4.5.3 Step 3: Impact Assessment

Environmental impact is calculated by using equation 2.3 and impact categories are depend on selected methodology, 21 midpoint impact categories contain in LCSoft methodology as shown in Table 2.4, 15 midpoint impact categories contain in ILCD methodology as shown in Table 4.2, and also endpoint impact categories. In addition, LCSoft also has feature to determine the specific footprint such as Carbon Footprint.

4.5.3.1 Carbon Footprint

Carbon footprint is amount of carbon dioxide and greenhouse gas associated with one kilogram of product. Carbon footprint is estimated by using global warming potential (GWP) indicator as equation 4.3-4.4. LCSoft will use characterization factor according to selected calculation method.

$$\mathrm{CO2_{eq}} = (\mathrm{m^{PRO}_{GHG,air}} \times \mathrm{CF^{GWP}_{GHG,air}})/\mathrm{m_{product}} \quad (4.3)$$

$$\text{Carbon footprint} = \sum \mathrm{CO2_{eq}} \quad (4.4)$$

Where GHG is Greenhouse gas, $\mathrm{m^{PRO}_{GHG,air}}$ is mass flow rate of greenhouse gas (GHG), $\mathrm{CF^{GWP}_{GHG,air}}$ is characterization factor of global warming potential, and $\mathrm{CO2_{eq}}$ is carbon dioxide equivalent per 1 kg of product (Kalakul *et al.*, 2013).

4.5.3.2 Endpoint Impact Categories

Endpoint categories represent the impact at the end of cause effect chain, which may formulated many midpoint environmental impacts into one endpoint impact category. Human health, ecosystem species, and natural resource are example of endpoint categories. In this version, two endpoint calculation methods are available, ILCD endpoint and ReCiPe.

4.5.4 Step 4: Contribution Analysis

Contribution analysis will show the contribution of productions or process system which is helpful information for further development. This step is distinguished into 3 parts which are processes contribution, LCI contribution, and LCIA contribution.

4.5.4.1 Processes Contribution

Material or utility that used in the unit or processes are recorded and shown in order to identify the contribution in each production stage.

4.5.4.2 LCI Contribution

LCI contribution will show the information about elementary in each production stage, which very useful for improving the processes and/or product design.

4.5.4.3 LCIA Contribution

Environmental impact result will be analyzed in each impact categories. LCIA contribution will show the effect from each process which helpful for determining the hotspot or the significant contribution.

4.5.5 Step 5: Interpretation

Interpretation is included with many optional steps which are helpful feature for analyzing the result and archiving the goal of study.

4.5.5.1 Optional Step: Normalization

In order to make an easier comparison between impacts score of different impact categories. LCSoft allow users to perform normalization by adding set of normalization factor that relate to their goal.

4.5.5.2 Optional Step: Parameter and Source Sensitivity Analysis

For study the effect of different assumption on environmental impacts, LCSoft allow users to perform sensitivity analysis which user can either change the type or amount of substances and/or utilities in order to see the variation of impact assessment and find the optimal process.

4.5.5.3 Optional Step: Calculation with Uncertainty

For assess the influence of variations in process data and data quality on impact result. In order to calculate the precision uncertainty, data quality should be provided clearly. In this version, the data quality did not include in LCSoft database. However, LCSoft can perform LCA based on uncertainty value where users can specify estimate amount of disturbance to process.

4.5.5.4 Optional Step: Alternative Comparison

For compare the different process/product design and get more information for decision making based on environmental impacts results.

4.5.5.5 Optional Step: Eco-efficiency Evaluation

Eco-efficiency can be evaluated through indicators based on the ratio of economic and environment. More eco-efficiency value is obtained, the more sustainable process is.

Table 4.22 Calculation steps and new features in LCSoft

Calculation step	Previous development	New features in LCSoft
Step1: Check LCI data	The LCI data of related products or processes are checked with permission to add or modify LCI data. LCI results could be obtained by the LCI calculation function that contained in the software. Calculation model: Heijungs and Suh (2002).	- Allocation is used to calculate LCI results for multifunction process. - Data Quality Matrix is available to qualify the quality of LCI data.
Step2: Retrieve LCI data	Resource and raw material consumption, and emission of related products or processes are received from LCI KB for calculations in step3.	
Step3: Impact assessment	The LCI results are classified and characterized for each impact category based on effect on environment. LCSoft provides data on 21 midpoint environmental impact categories.	New pathway for calculation, 15 midpoint impact categories from ILCD method are available to calculate.
Step4: Contribution analysis	The process, LCI results, and impact assessment results are shown for each production stage.	
Step5: Interpretation	Optional steps which are helpful features for analyzing the results and archiving the goal of study are provided. - Carbon footprint calculation - Source Sensitivity analysis - Alternative comparison - Eco-efficiency evaluation	New optional steps are added. - Normalization - Parameter Sensitivity analysis - Calculation with uncertainty

CHAPTER V
CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

Environmental awareness and assessment are become significant issues because of the increasing in demands of people and the growth of industries, pressure on the chemical process industries to improve their environmental performance, and demand for assessment software that can be integrated with process design tools. Life Cycle Assessment (LCA) software, LCSoft has been developed for this purpose considering the user-friendly concept. Regarding to development framework of this new version, LCSoft was further developed with four main task includes: (1) improvement on LCI and LCIA calculation by adding new pathway for calculation and allocation; (2) development of new features, which normalization, data quality indicator, endpoint categories indicator, parameter sensitivity analysis, and calculation with uncertainty features were developed; (3) extension of LCI database to cover on all impact categories calculation, (4) validation of the software through case studies, bio-ethanol from cassava rhizome and para-xylene from toluene methylation. The assessment results of LCSoft were compared with latest version of commercial software, SimaPro 8.2.3. LCSoft based on the framework allows a consistency and systematic calculation of inventories and emissions, and has ability to interface with other important tools such as process simulation, process economics and sustainability analysis. Therefore, LCSoft has become a reliable and very efficient tool to analyze either new, existing and/or intensified processes.

5.2 Recommendations

Although new version of LCSoft was greatly improved and implemented with new helpful features, the software could develop for further improvement as following recommendations:

5.2.1 Water Footprint Calculation

A water footprint is the fraction of environmental impacts generated by a human activity on a wide range of environmental issues which are related to water. They include impacts associated with water use, and the subsequent effect on water availability for humans and ecosystems, as well as direct impacts on the water resource from emissions to air, soil and water. To enlarge the calculation feature in LCSoft, more applicable indicator like this should be carried on.

5.2.2 LCI Calculation Function

LCI calculation function is an important part, because the completeness of LCI calculation affect directly to quality of LCA results. In this version, LCI calculation function was further developed by applying the multifunctional process and allocation which can give accurate results compared to commercial LCA software, SimaPro. However, this function need to be further developed for other advance calculation such as process with cut-off, or closed- loop recycling.

5.2.3 LCI Database

LCI database is also significant part in LCA. It should be enlarging with good quality and completeness dataset, in order to wider range of applications and provide reliable assessment results.

5.2.4 Uncertainty Analysis

Although the function to calculate LCA with uncertainty and data quality indicator was available in this version, uncertainty analysis still very useful function in order to understand LCA clearly and quantify the effect of uncertainty in LCI data or in impact category model.

Finally, future works are focused on more impact indicator together with improvement of LCI calculation, and extension of LCI database for supporting on various process calculations, especially for chemical and biochemical processes. Besides, uncertainty analysis needs to be further developed.

REFERENCES

Althaus, H.J., Chudacoff, M., Hischier, R., Jungbluth, N., Osses, M., and Primas, A. (2007) Life Cycle Inventories of Chemicals - Ecoinvent Report v2.0 Dübendorf: Swiss Centre for Life Cycle Inventories.

Carvalho, A., Matos, H. A., and Gani, R. (2013) SustainPro - A tool for systematic process analysis, generation and evaluation of sustainable design alternatives. Computers and Chemical Engineering, 50, 8-27.

Ciroth, A., Fleischer, G., and Steinbach, J. (2004) Uncertainty calculation in life cycle assessments. The International Journal of Life Cycle Assessment, 9(4), 216-226.

Curran, M.A., Notten, P., Chayer, J.-A., and Cicas, G. (2006) Report on activity of task force 1 in the life cycle inventory programme: Data registry - Global life cycle inventory data resources. The International Journal of Life Cycle Assessment, 11(4), 284-289.

Curran, M.A. (2012) Sourcing life cycle inventory data. In M.A. Curran (Eds.), Life Cycle Assessment Handbook: A Guide for Environmentally Sustainable Products (pp. 105-141). Hoboken, NJ: John Wiley & Sons.

European Commission, Joint Research Centre (2010) International Reference Life Cycle Data System (ILCD) Handbook - General Guide for Life Cycle Assessment - Detailed Guidance. Luxembourg: Publications Office of the European Union.

European Commission, Joint Research Centre (2011) International Reference Life Cycle Data System (ILCD) Handbook - Recommendations for Life Cycle Assessment in the European Context. Luxembourg: Publications Office of the European Union.

European Commission, Joint Research Centre (2012) Characterisation Factors of the ILCD Recommended Life Cycle Impact Assessment Methods - Database and Supporting Information. Luxembourg: Publications Office of the European Union.

Franklin Associates. (2010) Revised Final Report - Cradle-to-gate life cycle inventory of nine plastic resins and four polyurethane precursors. Kansas: Prairie Village.

Frischknecht, R., Jungbluth, N., Althaus, H., Doka, G., Heck, T., Hellweg, S., Hischier, R., Nemecek, T., Rebitzer, G., and Spielmann, M. (2007) Overview and Methodology - Ecoinvent Report No. 1. Dübendorf: Swiss Centre for Life Cycle Invenrtories.

Goedkoop, M., De Schryver, A., Oele, M., Durksz, S., and de Roest, D. (2008) Introduction to LCA with SimaPro 7. Netherlands: PRé Consultants.

Guinee, J. B. (2002) Handbook on life cycle assessment operational guide to the ISO standards. The International Journal of Life Cycle Assessment, 7(5), 311-313.

Heijungs, R. (1994) A generic method for the identification of options for cleaner product. Ecological Economics, 10, 69-81.

Heijungs, R. and Suh, S. (2002) The Computational Structure of Life Cycle Assessment. Dordrecht, the Netherlands: Kluwer Academic.

Heijungs, R. and Guineév, J.B. (2012) An overview of the life cycle assessment method – past, present, and future. In M.A. Curran (Eds.), Life Cycle Assessment Handbook, (pp.15-41). Hoboken, NJ: John Wiley & Sons.

International Organization for Standardization (2006a) Environmental Management - Life Cycle Assessment - Principles and Framework (ISO Standard No. 14040). Brussels, Belgium.

International Organization for Standardization (2006b) Environmental Management - Life Cycle Assessment - Requirements and Guidelines (ISO Standard No. 14044). Brussels, Belgium.

Kaesinee, P., Pomthong, M., and Gani, R. (2016) Systematic, efficient and consistent LCA calculations for chemical and biochemical processes. Computer Aided Chemical Engineering, 38, 1249-1254.

Kalakul, S., Malakul, P., Siemanond, K., and Gani, R. (2014) Integration of life cycle assessment software with tools for economic and sustainability analyses and process simulation for sustainable process design. Journal of Cleaner Production, 71, 98-109.

Margni, M. and Curran, M.A. (2012) Life cycle impact assessment. In M.A. Curran (Eds.), Life Cycle Assessment Handbook: A Guide for Environmentally Sustainable Products (pp. 67-103). Hoboken, NJ: John Wiley & Sons.

Nateetorn, A., Babi, D.K., Uthaiporn, S., and Gani, R. (2016) Phenomena based process intensification of toluene methylation for sustainable para-xylene production. Computer Aided Chemical Engineering, 38, 1093-1098.

Piyarak, S. (2012) Development of software for life cycle assessment. M.S. Thesis, The Petroleum and Petrochemical College, Chulalongkorn University, Bangkok, Thailand.

Saengwirun, P. (2011) ECON: a software for cost calculation and economic analysis. M.S. Thesis, The Petroleum and Petrochemical College, Chulalongkorn University, Bangkok, Thailand.

Suh, S., and Huppes, G. (2003) Methods for life cycle inventory of a product. Journal of Cleaner Production, 13(7), 687-697.

Supawanich, P., Malakul, P., and Gani, R. (2015) Life cycle assessment studies of chemical and biochemical processes through the new LCSoft Software-tool. Computer Aided Chemical Engineering, 37, 2549-2554.

Wang, E., and Shen, Z. (2013) A hybrid data quality indicator and statistical method for improving uncertainty analysis in LCA of complex system – application to the whole-building embodied energy analysis. Journal of Cleaner Production, 43, 166-173.

Weidema, B. P. (1998) Multi-user test of the data quality matrix for product life cycle inventory data. The International Journal of Life Cycle Assessment, 3(5), 259-265.

Eco-efficiency Action Project. "Impact Assessment Methodologies – What is the State of the Art?" Eco-efficiency Action Project. 22 Feb 2010. 27 June 2016 <http://eco-efficiency-action-project.com/tag/recipe-2008>

Manfredi, S., Allacker, K., Chomkhamsri, K., Pelletier, N., and Souza, D. M. d. (2012) "Product Environmental Footprint (PEF) guide." European Commission, Joint Research Centre. 17 July 2012. 8 April 2016 <http://ec.europa.eu/environment/eussd/pdf/footprint/PEF%20methodology%20final%20draft.pdf>

National Renewable Energy Laboratory (2012) "U.S. Life Cycle Inventory Database." National Renewable Energy Laboratory (NREL). 19 November 2012. 16 May 2016 <https://www.lcacommons.gov/nrel/search>

APPENDICES

Appendix A Production of Bio-ethanol from Cassava Rhizome Process Details

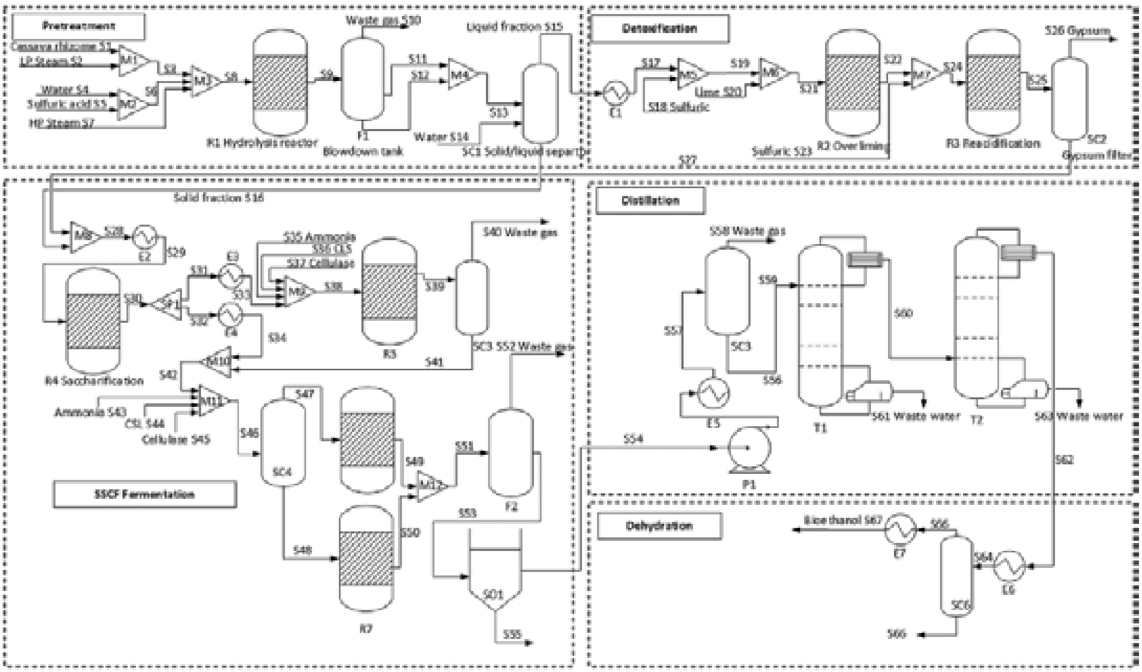

Figure A1 Production of bio-ethanol from cassava rhizome process flowsheet.

Table A1 Stream table of bio-ethanol from cassava rhizome process

Stream Name		S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15
Stream Description																
Stream Phase		Mixed	Vapor	Mixed	Liquid	Liquid	Liquid	Vapor	Mixed	Mixed	Vapor	Liquid	Solid	Mixed	Liquid	Mixed
Temperature	C	30.000	160.000	100.018	25.000	25.000	25.000	268.000	188.002	190.000	103.854	103.854	103.854	103.854	25.000	62.663
Pressure	ATM	1.000	6.000	1.000	1.000	1.000	1.000	13.000	12.100	12.100	1.000	1.000	1.000	1.000	1.000	1.000
Total Molecular Weight		103.896	18.015	84.688	18.015	98.079	18.308	18.015	38.223	40.920	18.725	35.367	94.665	47.174	18.015	23.111
Total Weight Comp. Rates	kg/hr															
Cellulose		4680.592	0.000	4680.592	0.000	0.000	0.000	0.000	4680.592	4320.186	0.000	0.000	4320.186	4320.186	0.000	21.601
Hemicellulose		6674.090	0.000	6674.090	0.000	0.000	0.000	0.000	6674.090	333.705	0.000	0.000	333.705	333.705	0.000	1.669
Lignin		3653.449	0.000	3653.449	0.000	0.000	0.000	0.000	3653.449	3653.449	0.000	0.000	3653.449	3653.449	0.000	18.267
Glucose		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	364.047	0.000	364.047	0.000	364.047	0.000	287.597
Xylose		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	6825.731	0.000	6825.731	0.000	6825.731	0.000	4436.725
Cellobiose		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	34.584	0.000	34.584	0.000	34.584	0.000	27.321
Ethanol		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Water		129.522	785.091	914.613	4972.114	0.000	4972.114	3153.382	9040.110	8273.831	2371.593	5902.238	0.000	5902.238	12898.248	14852.384
Sulfuric Acid		0.000	0.000	0.000	0.000	99.441	99.441	0.000	99.441	99.441	0.000	99.441	0.000	99.441	0.000	78.559
Furfural		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	242.695	115.985	126.711	0.000	126.711	0.000	100.101
Ammonia		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Oxygen		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Carbon Dioxide		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Glycerol		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Succinic Acid		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Lactic Acid		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
HMF		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Xylitol		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Acetic Acid		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CornSteep Liquor		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ZM		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Cellulase		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Lime		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CASO4		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ash		578.255	0.000	578.255	0.000	0.000	0.000	0.000	578.255	578.255	0.000	0.000	578.255	578.255	0.000	0.000

Table A1 Stream table of bio-ethanol from cassava rhizome process (cont'd)

Stream Name		S16	S17	S18	S19	S20	S21	S22	S23	S24	S25	S26	S27	S28	S29	S30	S31	S32	S33	S34	S35
Stream Description																					
Stream Phase		Mixed	Mixed	Liquid	Mixed	Solid	Mixed	Mixed	Liquid	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Vapor
Temperature	C	62.663	50.000	25.000	49.941	25.000	49.861	49.861	25.000	49.836	49.836	49.836	49.836	54.135	65.000	65.000	65.000	65.000	41.562	40.858	25.000
Pressure	ATM	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Total Molecular Weight		46.462	23.111	98.079	23.210	74.093	23.353	23.301	98.079	23.342	23.329	137.765	22.980	29.476	29.476	30.087	30.087	30.087	30.087	30.087	17.031
Total Weight Comp. Rates	kg/hr																				
Cellulose		4298.585	21.601	0.000	21.601	0.000	21.601	21.601	0.000	21.601	21.601	21.601	0.000	4298.585	4298.585	378.275	37.828	340.448	37.828	340.448	0.000
Hemicellulose		332.036	1.669	0.000	1.669	0.000	1.669	1.669	0.000	1.669	1.669	1.669	0.000	332.036	332.036	332.036	33.204	298.832	33.204	298.832	0.000
Lignin		3635.182	18.267	0.000	18.267	0.000	18.267	18.267	0.000	18.267	18.267	0.000	18.267	3653.449	3653.449	3653.449	365.345	3288.104	365.345	3288.104	0.000
Glucose		76.450	287.597	0.000	287.597	0.000	287.597	287.597	0.000	287.597	287.597	0.575	287.022	363.472	363.472	4698.472	469.847	4228.625	469.847	4228.625	0.000
Xylose		2389.006	4436.725	0.000	4436.725	0.000	4436.725	4436.725	0.000	4436.725	4436.725	8.873	4427.852	6816.857	6816.857	6816.857	681.686	6135.172	681.686	6135.172	0.000
Cellobiose		7.263	27.321	0.000	27.321	0.000	27.321	27.321	0.000	27.321	27.321	0.000	27.321	34.584	34.584	54.448	5.445	49.003	5.445	49.003	0.000
Ethanol		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Water		3948.102	14852.384	0.000	14852.384	0.000	14852.384	14922.474	0.000	14922.474	14939.617	0.000	14939.617	18887.719	18887.719	18453.191	1845.319	16607.872	1845.319	16607.872	0.000
Sulfuric Acid		20.883	78.559	112.236	190.795	0.000	190.795	0.000	46.664	46.664	0.000	0.000	0.000	20.883	20.883	20.883	2.088	18.794	2.088	18.794	0.000
Furfural		26.609	100.101	0.000	100.101	0.000	100.101	100.101	0.000	100.101	100.101	0.200	99.901	126.510	126.510	126.510	12.651	113.859	12.651	113.859	0.000
Ammonia		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.832
Oxygen		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Carbon Dioxide		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Glycerol		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Succinic Acid		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Lactic Acid		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
HMF		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Xylitol		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Acetic Acid		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CornSteep Liquor		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ZM		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Cellulase		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Lime		0.000	0.000	0.000	0.000	179.415	179.415	35.282	0.000	35.282	0.031	0.031	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CASO4		0.000	0.000	0.000	0.000	0.000	0.000	264.838	0.000	264.838	329.610	329.610	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ash		578.255	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	578.255	578.255	578.255	57.825	520.429	57.825	520.429	0.000

Table A1 Stream table of bio-ethanol from cassava rhizome process (cont'd)

Stream Name		S36	S37	S38	S39	S40	S41	S42	S43	S44	S45	S46	S47	S48	S49	S50
Stream Description																
Stream Phase		Liquid	Mixed	Mixed	Mixed	Vapor	Mixed	Mixed	Vapor	Liquid	Solid	Mixed	Mixed	Liquid	Mixed	Liquid
Temperature	C	25.000	25.000	41.000	41.000	42.531	42.531	41.033	25.000	25.000	25.000	41.000	41.000	41.000	41.000	41.000
Pressure	ATM	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Total Molecular Weight		18.015	18.090	29.546	26.166	43.990	24.607	29.497	17.031	18.015	22.840	29.446	29.227	161.023	25.907	90.079
Total Weight Comp. Rates	kg/hr															
Cellulose		0.000	0.000	37.828	37.828	0.000	37.828	378.275	0.000	0.000	0.000	378.275	378.275	0.000	37.374	0.000
Hemicellulose		0.000	0.000	33.204	33.204	0.000	33.204	332.036	0.000	0.000	0.000	332.036	332.036	0.000	332.036	0.000
Lignin		0.000	0.000	365.345	365.345	0.000	365.345	3653.449	0.000	0.000	0.000	3653.449	3653.449	0.000	3653.449	0.000
Glucose		0.000	0.000	469.847	43.898	0.000	43.898	4272.523	0.000	0.000	0.000	4272.523	4144.347	128.176	218.432	0.000
Xylose		0.000	0.000	681.686	121.398	0.000	121.398	6256.569	0.000	0.000	0.000	6256.569	6068.872	187.697	828.310	0.000
Cellobiose		0.000	0.000	5.445	5.445	0.000	5.445	54.448	0.000	0.000	0.000	54.448	54.448	0.000	0.000	0.000
Ethanol		0.000	0.000	0.000	495.168	37.138	458.031	458.031	0.000	0.000	0.000	458.031	458.031	0.000	5321.673	0.000
Water		0.000	37.743	1883.062	1883.987	0.942	1883.045	18490.917	0.000	0.000	0.000	18490.917	18490.917	0.000	18449.795	0.000
Sulfuric Acid		0.000	0.000	2.088	2.088	0.000	2.088	20.883	0.000	0.000	0.000	20.883	20.883	0.000	20.883	0.000
Furfural		0.000	0.000	12.651	12.651	0.000	12.651	126.510	0.000	0.000	0.000	126.510	126.510	0.000	126.510	0.000
Ammonia		0.000	0.000	0.832	0.000	0.000	0.000	0.000	2.481	0.000	0.000	2.481	2.481	0.000	0.000	0.000
Oxygen		0.000	0.000	0.000	1.379	1.379	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	7.762	0.000
Carbon Dioxide		0.000	0.000	0.000	472.356	448.738	23.618	23.618	0.000	0.000	0.000	23.618	23.618	0.000	4665.470	0.000
Glycerol		0.000	0.000	0.000	0.586	0.000	0.586	0.586	0.000	0.000	0.000	0.586	0.586	0.000	4.243	0.000
Succinic Acid		0.000	0.000	0.000	1.822	0.000	1.822	1.822	0.000	0.000	0.000	1.822	1.822	0.000	13.602	0.000
Lactic Acid		0.000	0.000	0.000	0.331	0.000	0.331	0.331	0.000	0.000	0.000	0.331	0.331	0.000	2.429	315.870
HMF		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Xylitol		0.000	0.000	0.000	6.083	0.000	6.083	6.083	0.000	0.000	0.000	6.083	6.083	0.000	47.590	0.000
Acetic Acid		0.000	0.000	0.000	2.397	0.000	2.397	2.397	0.000	0.000	0.000	2.397	2.397	0.000	17.514	0.000
CornSteep Liquor		59.691	0.000	59.691	59.691	0.000	59.691	59.691	0.000	87.781	0.000	147.472	147.472	0.000	147.472	0.000
ZM		0.000	0.000	0.000	6.014	0.000	6.014	6.014	0.000	0.000	0.000	6.014	6.014	0.000	23.956	0.000
Cellulase		0.000	0.757	0.757	0.757	0.000	0.757	0.757	0.000	0.000	7.566	8.322	8.322	0.000	8.322	0.000
Lime		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CASO4		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ash		0.000	0.000	57.825	57.825	0.000	57.825	578.255	0.000	0.000	0.000	578.255	578.255	0.000	578.255	0.000

Table A1 Stream table of bio-ethanol from cassava rhizome process (cont'd)

Stream Name		S51	S52	S53	S54	S55	S56	S57	S58	S59	S60	S61	S62	S63	S64	S65	S66	S67
Stream Description																		
Stream Phase		Mixed	Vapor	Mixed	Liquid	Solid	Liquid	Liquid	Vapor	Liquid	Vapor	Liquid	Liquid	Liquid	Vapor	Vapor	Vapor	Liquid
Temperature	C	41.021	41.021	41.021	41.021	41.021	41.240	100.510	100.000	100.000	93.831	116.676	93.343	109.986	100.000	100.018	100.018	40.000
Pressure	ATM	1.000	1.000	1.000	1.000	1.000	4.760	4.760	4.760	4.760	1.770	1.770	1.770	1.770	1.770	1.000	1.000	1.000
Total Molecular Weight		26.075	42.297	24.681	22.152	67.371	22.152	22.152	42.462	21.890	38.742	19.419	42.121	18.746	42.121	46.033	18.015	46.033
Total Weight Comp. Rates	kg/hr																	
Cellulose		37.374	0.000	37.374	0.000	37.374	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Hemicellulose		332.036	0.000	332.036	0.000	332.036	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Lignin		3653.449	0.000	3653.449	0.000	3653.449	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Glucose		218.432	0.000	218.432	218.432	0.000	218.432	218.432	0.000	218.432	0.000	218.432	0.000	0.000	0.000	0.000	0.000	0.000
Xylose		828.310	0.000	828.310	828.310	0.000	828.310	828.310	0.000	828.310	0.000	828.310	0.000	0.000	0.000	0.000	0.000	0.000
Cellobiose		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ethanol		5321.673	258.596	5063.077	5063.077	0.000	5063.077	5063.077	15.189	5047.887	4987.130	60.757	4962.195	24.935	4962.195	4962.195	0.000	4962.195
Water		18449.795	131.714	18318.081	18318.081	0.000	18318.081	18318.081	16.486	18301.595	689.608	17611.987	317.856	371.752	317.856	2.479	315.376	2.479
Sulfuric Acid		20.883	0.000	20.883	20.883	0.000	20.883	20.883	0.000	20.883	0.000	20.883	0.000	0.000	0.000	0.000	0.000	0.000
Furfural		126.510	2.189	124.321	124.321	0.000	124.321	124.321	0.739	123.582	0.356	123.226	0.000	0.356	0.000	0.000	0.000	0.000
Ammonia		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Oxygen		7.762	7.650	0.112	0.112	0.000	0.112	0.112	0.112	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Carbon Dioxide		4665.470	4068.938	596.532	596.532	0.000	596.532	596.532	596.532	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Glycerol		4.243	0.000	4.243	4.243	0.000	4.243	4.243	0.000	4.243	0.000	4.243	0.000	0.000	0.000	0.000	0.000	0.000
Succinic Acid		13.602	0.000	13.602	13.602	0.000	13.602	13.602	0.000	13.602	0.000	13.602	0.000	0.000	0.000	0.000	0.000	0.000
Lactic Acid		318.299	0.001	318.299	318.299	0.000	318.299	318.299	0.000	318.299	0.000	318.299	0.000	0.000	0.000	0.000	0.000	0.000
HMF		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Xylitol		47.590	0.000	47.590	47.590	0.000	47.590	47.590	0.000	47.590	0.000	47.590	0.000	0.000	0.000	0.000	0.000	0.000
Acetic Acid		17.514	0.152	17.363	17.363	0.000	17.363	17.363	0.007	17.356	0.012	17.344	0.000	0.012	0.000	0.000	0.000	0.000
CornSteep Liquor		147.472	0.566	146.906	146.906	0.000	146.906	146.906	0.126	146.780	0.042	146.738	0.000	0.042	0.000	0.000	0.000	0.000
ZM		23.956	0.000	23.956	0.000	23.956	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Cellulase		8.322	0.000	8.322	0.000	8.322	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Lime		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CASO4		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ash		578.255	0.000	578.255	0.000	578.255	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Table A2 Equipment table of bio-ethanol from cassava rhizome process

Pump		
Pump Name		**P1**
Work	KWH	5.698

Reactor								
ConReactor Name		**R1**	**R2**	**R3**	**R4**	**R5**	**R6**	**R7**
Temperature	C	190	50	50	65	41	41	41
Pressure	ATM	12.100	1.000	1.000	1.000	1.000	1.000	1.000
Duty	MJ/HR	0.000	-399.600	-97.700	1613.200	-843.300	-8214.400	-322.900
Heat Of Reaction	MJ/HR	-1.288	-0.381	-0.093	-0.878	-0.011	-0.380	0.092
Product Enthalpy	KJ/KG	-227.731	1309.967	1335.907	821.194	-36.536	-272.505	8.343
Feed Enthalpy	KJ/KG	-4142.821	1205.755	1310.420	-1562.669	19.703	39.694	31.737
ΔEnthalpy	KJ/KG	3915.090	104.212	25.488	2383.863	-56.239	-312.199	-23.393
	GJ/KG	3.915	0.104	0.025	2.384	-0.056	-0.312	-0.023

Flash			
Flash Name		**F1**	**F2**
Temperature	C	103.854	41.021
Pressure	ATM	1.000	1.000
DP	ATM	11.100	0.000
Duty	MJ/HR	0.000	0.000

Stream Calculator							
Stream Calculator Name		**SC1**	**SC2**	**SC3**	**SC4**	**SC5**	**SC6**
Duty	MJ/HR	0.000	0.000	0.000	0.000	0.000	0.000
Overhead Product Temperature	C	62.663	49.837	42.531	41.000	100.000	100.018
Bottoms Product Temperature	C	62.663	49.837	42.531	41.000	100.000	100.018

Table A2 Equipment table bio-ethanol from cassava rhizome process (cont'd)

Heat Exchanger								
Hx Name		**E1**	**E2**	**E3**	**E4**	**E5**	**E6**	**E7**
Duty	MJ/HR	859.300	1113.000	235.200	2180.000	5678.500	4804.000	4840.400

Column			
Column Name		**T1**	**T2**
Condenser Duty	MJ/HR	-18089.200	-19971.200
Reboiler Duty	MJ/HR	24889.600	14371.400
Column Total Molar Feed	KG-MOL/DAY	27507.280	3517.017
Column Total Wt. Feed	KG/DAY	602124.669	136253.109
Column Condenser Pres	ATM	1.770	1.770
Column Condenser Temp	C	93.831	93.344
Column Reflux Rate	KG-MOL/DAY	0.000	9628.490
Column Reflux Ratio		3.200	3.200

Appendix B Production of Para-xylene by Toluene Methylation Process Details

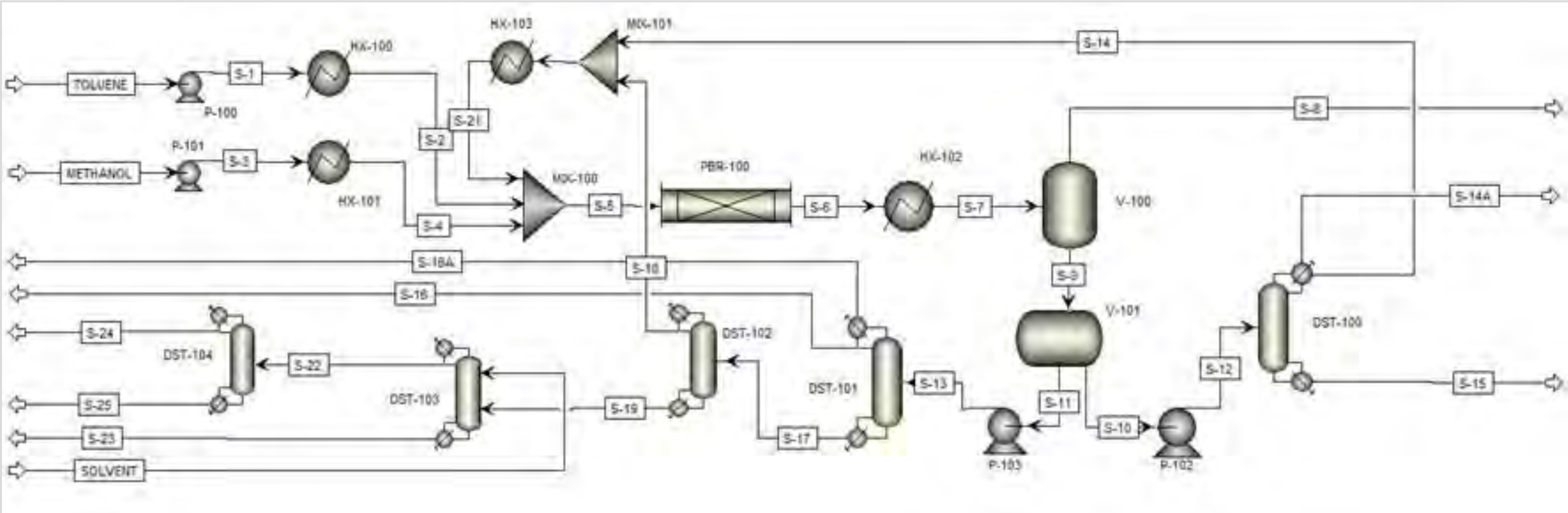

Figure B1 Production of para-xylene by toluene methylation process flowsheet.

Table B1 Stream table of para-xylene by toluene methylation process

	METHANOL	S-1	S-2	S-3	S-4	S-5	S-6	S-7	S-8	S-9	S-10	S-11	S-12	S-13	S-14	S-14A
Temperature K	298.1	298.2	673.1	298.2	673.1	673.1	673.1	323.1	323.1	323.1	323.1	323.1	332.7	321.7	359.5	359.5
Pressure atm	1	2.96	2.96	2.96	2.96	2.96	2.96	1	1	1	1	1	4.44	8.39	3.95	3.95
Vapor Frac	0	0	1	0	1	1	1	0.06	1	0	0	0	0	0	0	1
Solid Frac	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow kmol/hr	413.676	257.298	257.298	413.676	413.676	1559.72	1623.14	1623.14	96.775	1526.36	454.927	1071.44	454.927	1071.44	127.575	4.354
Mass Flow kg/hr	13255.073	23707.6	23707.6	13255.1	13255.1	110958	110958	110958	2933.92	108024	9685.33	98338.3	9685.33	98338.3	3731.25	129.678
Volume Flow l/min	278.613	456.977	78495.3	278.624	128035	478765	498435	44414.2	42331.9	2082.32	183.31	1947.88	185.513	1944.7	84.067	523.541
Enthalpy MMBtu/hr	-94.609	3.171	27.134	-94.605	-70.253	14.314	-2.504	-120.77	-4.46	-116.31	-117.01	-4.431	-117.01	-4.334	-29.255	-0.309
Mass Flow kg/hr																
TOLUENE	0	23707.6	23707.6	0	0	93091.8	70801.9	70801.9	586.464	70215.4	97.963	70117.5	97.963	70117.5	95.302	2.661
METHANOL	13255.073	0	0	13255.1	13255.1	16318.3	4826.14	4826.14	199.322	4626.82	3138.59	1488.23	3138.59	1488.23	3063.26	62.771
WATER	0	0	0	0	0	547.062	7008.39	7008.39	506.557	6501.84	6363.1	138.742	6363.1	138.742	547.06	4.187
BENZENE	0	0	0	0	0	1.191	395.005	395.005	9.233	385.772	0.709	385.064	0.709	385.064	0.683	0.025
P-XYL-01	0	0	0	0	0	973.926	25542.2	25542.2	83.487	25458.7	11.079	25447.6	11.079	25447.6	10.837	0.242
M-XYL-01	0	0	0	0	0	9.79	299.634	299.634	0.927	298.707	0.301	298.406	0.301	298.406	0.295	0.006
O-XYL-01	0	0	0	0	0	2.831	292.676	292.676	0.726	291.95	1.251	290.699	1.251	290.699	1.235	0.016
ETHYLENE	0	0	0	0	0	12.573	1791.59	1791.59	1547.21	244.381	72.343	172.037	72.343	172.037	12.573	59.77
TERT--01	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1:4-D-01	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5-TER-01	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table B1 Stream table of para-xylene by toluene methylation process (cont'd)

	S-15	S-16	S-16A	S-17	S-18	S-19	S-20	S-21	S-22	S-23	S-24	S-25	SOLVENT	TOLUENE
Temperature K	417.6	368.7	368.7	485.6	429.3	457.4	407.9	673.1	410.1	416.1	359.7	387.1	343.1	298.1
Pressure atm	3.95	7.9	7.9	7.9	2.96	2.96	2.96	2.96	0.99	0.99	0.49	0.49	1.48	1
Vapor Frac	0	0	1	0	0	0	0.063	1	0	0	0	0	0	0
Solid Frac	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow kmol/hr	322.998	66.481	7.387	997.568	761.175	236.393	888.75	888.75	208.272	31.121	6.248	202.024	3	257.298
Mass Flow kg/hr	5824.4	2751.94	230.011	95356.3	70263.7	25092.7	73994.9	73994.9	22056.6	3550.97	611.06	21445.5	514.879	23707.6
Volume Flow l/min	111.721	60.505	445.957	2408.23	1604.16	593.685	11498	271875	486.38	78.695	12.704	458.635	10.365	456.948
Enthalpy MMBtu/hr	-85.044	-11.139	-0.179	37.684	25.314	2.069	-3.941	57.433	-0.239	-0.449	0.051	-1.302	-0.405	3.165
Mass Flow kg/hr														
TOLUENE	0	785.176	13.186	69319.1	69289	30.123	69384.3	69384.3	30.123	0	13.307	16.816	0	23707.6
METHANOL	12.553	1421.4	66.832	0	0	0	3063.26	3063.26	0	0	0	0	0	0
WATER	5811.847	134.246	4.496	0	0	0	547.062	547.062	0	0	0	0	0	0
BENZENE	0	372.387	12.169	0.508	0.508	0	1.191	1.191	140.813	0	139.959	0.854	0	0
P-XYL-01	0	0.022	0	25447.6	963.11	24484.5	973.926	973.926	21842.3	2642.2	457.331	21384.98	0	0
M-XYL-01	0	0	0	298.406	9.494	288.911	9.79	9.79	1.32	2.209	0.025	1.295	0	0
O-XYL-01	0	0	0	290.699	1.596	289.102	2.831	2.831	41.875	247.227	0.439	41.437	0	0
ETHYLENE	0	38.71	133.328	0	0	0	12.573	12.573	0	0	0	0	0	0
TERT--01	0	0	0	0	0	0	0	0	0.119	10.983	0	0.118	134.221	0
1:4-D-01	0	0	0	0	0	0	0	0	0	212.145	0	0	380.657	0
5-TER-01	0	0	0	0	0	0	0	0	0	436.201	0	0	0	0

Table B2 Equipment table of para-xylene by toluene methylation process

Unit	Type of unit	Duty/Work	Unit		Activity
			Energy	time	
P-100	Pump	1.874	kW	hr	Electric usage
P-101	Pump	1.142	kW	hr	Electric usage
P-102	Pump	1.335	kW	hr	Electric usage
P-103	Pump	30.043	kW	hr	Electric usage
PBR-100	Reactor	-17,743.939	MJ	hr	Cooling
HX-100	Heat Exchanger	25,282.555	MJ	hr	Heating
HX-101	Heat Exchanger	25,692.864	MJ	hr	Heating
HX-102	Heat Exchanger	-124,775.676	MJ	hr	Cooling
HX-103	Heat Exchanger	64,752.574	MJ	hr	Heating
V-100	Flash	0.000	MJ	hr	Heating
V-101	Decanter	-5,418.241	MJ	hr	Cooling
DST-100-cond	Column-Condenser	-10,838.828	MJ	hr	Cooling
DST-100-reb	Column-Reboiler	13,372.707	MJ	hr	Heating
DST-101-cond	Column-Condenser	-41,323.805	MJ	hr	Cooling
DST-101-reb	Column-Reboiler	73,714.597	MJ	hr	Heating
DST-102-cond	Column-Condenser	-70,437.681	MJ	hr	Cooling
DST-102-reb	Column-Reboiler	59,569.089	MJ	hr	Heating
DST-103-cond	Column-Condenser	-67,957.030	MJ	hr	Cooling
DST-103-reb	Column-Reboiler	65,474.876	MJ	hr	Heating
DST-104-cond	Column-Condenser	-6,343.117	MJ	hr	Cooling
DST-104-reb	Column-Reboiler	5,275.464	MJ	hr	Heating

Appendix C Other case-studies process details

Table C1 Input/output inventories from process Acetic acid, 98 % in H2O, at plant – RER (Althaus *et al.*, 2007)

Name	Amount	Unit	Uncertainty data based on DQI
Input from technosphere			
carbon monoxide, CO, at plant	4.81E-1	kg	(4,2,4,2,3,5)
chemical plant, organics	4.00E-10	unit	(5,5,5,5,5,5)
heat, unspecific, in chemical plant	1.45E+0	MJ	(5,5,5,5,5,5)
methanol, at plant	5.05E-1	kg	(4,2,4,2,3,5)
electricity, medium voltage, production UCTE, at grid	5.70E-2	kWh	(5,5,5,5,5,5)
transport, lorry >16t, fleet average	9.86E-2	tkm	(5,5,5,5,5,5)
transport, freight, rail	5.92E-1	tkm	(5,5,5,5,5,5)
treatment, sewage, unpolluted, to wastewater treatment, class 3	6.14E-5	m3	(5,5,5,5,5,5)
water, decarbonised, at plant	1.54E-1	kg	(4,2,4,2,3,5)
Input from nature (resources)			
Water, cooling, unspecified natural origin	7.80E-2	m3	(5,5,5,5,5,5)
Emission to air			
Acetic acid	5.00E-3	kg	(5,5,5,5,5,5)
Carbon dioxide, fossil	3.71E-2	kg	(5,5,5,5,5,5)
Carbon monoxide, fossil	6.32E-3	kg	(5,5,5,5,5,5)
Heat, waste	1.09E-3	MJ	(5,5,5,5,5,5)
Hydrogen	2.96E-4	kg	(5,5,5,5,5,5)
Methane, fossil	4.99E-3	kg	(5,5,5,5,5,5)
Methanol	2.52E-3	kg	(5,5,5,5,5,5)

Table C2 Input/output inventories from process Diesel, at refinery – RNA (NREL, 2012)

Name	Amount	Unit
Input from technosphere		
carbon monoxide, CO, at plant	4.81E-1	kg
chemical plant, organics	4.00E-10	unit
heat, unspecific, in chemical plant	1.45E+0	MJ
methanol, at plant	5.05E-1	kg
electricity, medium voltage, production UCTE, at grid	5.70E-2	kWh
transport, lorry >16t, fleet average	9.86E-2	tkm
transport, freight, rail	5.92E-1	tkm
treatment, sewage, unpolluted, to wastewater treatment, class 3	6.14E-5	m3
water, decarbonised, at plant	1.54E-1	kg
Emission to air		
Crude oil, at production	8.98E-1	kg
Electricity, at grid, US, 2000	1.20E-1	kWh
Liquefied petroleum gas, combusted in industrial boiler	8.22E-4	L
Natural gas, combusted in industrial boiler	7.94E-3	m3
Residual fuel oil, combusted in industrial boiler	1.95E-2	L
Transport, barge, average fuel mix	1.03E-3	tkm
Transport, ocean freighter, average fuel mix	4.11E+0	tkm
Dummy, Transport, pipeline, unspecified	5.66E-1	tkm
Dummy, Disposal, solid waste, unspecified, to sanitary landfill	0.0049	kg
Emission to water		
Ammonia	1.30E-05	kg
BOD5, Biological Oxygen Demand	2.95E-05	kg
Chromium VI	3.21E-08	kg
Chromium, ion	4.95E-07	kg
COD, Chemical Oxygen Demand	1.99E-04	kg
Oils, unspecified	9.51E-06	kg
Phenols, unspecified	1.99E-07	kg
Sulfide	1.65E-07	kg
Suspended solids, unspecified	2.43E-05	kg

Table C3 Input/output inventories from process Benzene, at plant – RNA (Franklin Associates, 2010)

Name	Amount	Unit
Input from technosphere		
carbon monoxide, CO, at plant	4.81E-1	kg
chemical plant, organics	4.00E-10	unit
heat, unspecific, in chemical plant	1.45E+0	MJ
methanol, at plant	5.05E-1	kg
electricity, medium voltage, production UCTE, at grid	5.70E-2	kWh
transport, lorry >16t, fleet average	9.86E-2	tkm
transport, freight, rail	5.92E-1	tkm
treatment, sewage, unpolluted, to wastewater treatment, class 3	6.14E-5	m3
water, decarbonised, at plant	1.54E-1	kg
Emission to air		
Carbon dioxide, fossil	4.52E-2	kg
Carbon monoxide	1.00E-5	kg
Chlorine	1.00E-7	kg
NMVOC, non-methane volatile organic compounds, unspecified	1.00E-5	kg
Hydrogen	1.00E-9	kg
Nitrogen oxides	6.23E-5	kg
Particulates, unspecified	1.89E-5	kg
Particulates, < 2.5 um	1.00E-5	kg
Particulates, > 2.5 um, and < 10um	1.00E-6	kg
Sulfur oxides	4.43E-4	kg
Emission to water		
Benzene	1.00E-9	kg
BOD5, Biological Oxygen Demand	4.67E-4	kg
COD, Chemical Oxygen Demand	1.08E-3	kg
Dissolved solids	1.05E-4	kg
Oil and grease, unspecified	1.78E-5	kg
Sulfide	1.00E-6	kg
Suspended solids, unspecified	1.00E-6	kg
TOC, Total Organic Carbon	1.00E-8	kg

Appendix D Development of LCI Calculation Function

Table D1 LCI results from LCI calculation of Diesel, at refinery – RNA, US.LCI database (NREL, 2012)

Substance	Compartment	Unit	LCSoft previous database	LCSoft updated database with allocation	SimaPro	Percentage Difference (Updated database/SimaPro)
2-Chloroacetophenone	Air	kg	4.20E-12	7.36E-14	7.42E-14	0.80
2-Hexanone	Water	kg	1.25E-06	2.19E-08	2.29E-08	4.38
Acenaphthene	Air	kg	6.34E-10	1.11E-11	1.12E-11	0.88
Acenaphthylene	Air	kg	3.11E-10	5.45E-12	5.50E-12	0.88
Acetaldehyde	Air	kg	5.03E-07	8.82E-09	8.18E-09	7.48
Acetone	Water	kg	1.91E-06	3.36E-08	3.51E-08	4.56
Acetophenone	Air	kg	8.99E-12	1.58E-13	1.59E-13	0.80
Acids, unspecified	Water	kg	2.03E-09	3.56E-11	3.59E-11	0.70
Acrolein	Air	kg	4.21E-07	7.38E-09	7.36E-09	0.28
Aldehydes, unspecified	Air	kg	2.18E-03	3.83E-05	3.83E-05	0.11
Ammonia	Air	kg	1.10E-03	1.93E-05	1.92E-05	0.11
Ammonia	Water	kg	3.65E-03	6.40E-05	6.58E-05	2.85
Ammonia, as N	Water	kg	1.02E-09	1.79E-11	1.80E-11	0.70
Ammonium chloride	Air	kg	3.62E-06	6.35E-08	6.34E-08	0.23
Ammonium, ion	Water	kg	7.77E-07	1.36E-08	1.36E-08	0.57
Anthracene	Air	kg	2.61E-10	4.58E-12	4.62E-12	0.88
Antimony	Air	kg	2.24E-08	3.92E-10	3.96E-10	0.88
Antimony	Water	kg	1.07E-05	1.88E-07	1.89E-07	0.63
Arsenic	Air	kg	7.29E-07	1.28E-08	1.29E-08	0.62
Barium	Water	kg	2.35E-01	4.12E-03	4.16E-03	0.78
Benzene	Air	kg	2.06E-04	3.62E-06	4.18E-08	195.43
Benzene	Water	kg	3.21E-04	5.63E-06	5.89E-06	4.51
Benzene, 1-methyl-4-(1-methylethyl)-	Water	kg	1.91E-08	3.36E-10	3.51E-10	4.49
Benzene, chloro-	Air	kg	1.32E-11	2.31E-13	2.33E-13	0.80
Benzene, ethyl-	Air	kg	2.55E-05	4.47E-07	9.96E-13	200.00
Benzene, ethyl-	Water	kg	1.80E-05	3.17E-07	3.31E-07	4.59
Benzene, pentamethyl-	Water	kg	1.43E-08	2.51E-10	2.63E-10	4.59
Benzenes, alkylated, unspecified	Water	kg	9.51E-06	1.67E-07	1.66E-07	0.40
Benzo(a)anthracene	Air	kg	9.94E-11	1.74E-12	1.76E-12	0.88
Benzo(a)pyrene	Air	kg	4.72E-11	8.28E-13	8.36E-13	0.88
Benzo(b,j,k)fluoranthene	Air	kg	1.37E-10	2.40E-12	2.42E-12	0.88
Benzoic acid	Water	kg	1.95E-04	3.42E-06	3.56E-06	4.23

Table D1 LCI results from LCI calculation of Diesel, at refinery – RNA, US.LCI database (NREL, 2012) (cont'd)

Substance	Compartment	Unit	LCSoft previous database	LCSoft updated database with allocation	SimaPro	Percentage Difference (Updated database/SimaPro)
Benzyl chloride	Air	kg	4.20E-10	7.36E-12	7.42E-12	0.80
Beryllium	Air	kg	3.55E-08	6.22E-10	6.29E-10	1.07
Beryllium	Water	kg	2.98E-06	5.22E-08	5.36E-08	2.68
Biphenyl	Air	kg	2.11E-09	3.71E-11	3.74E-11	0.88
Biphenyl	Water	kg	6.14E-07	1.08E-08	1.08E-08	0.14
BOD5, Biological Oxygen Demand	Water	kg	3.51E-02	6.16E-04	6.43E-04	4.23
Boron	Water	kg	6.04E-04	1.06E-05	1.10E-05	3.96
Bromide	Water	kg	4.10E-02	7.20E-04	7.52E-04	4.42
Bromoform	Air	kg	2.34E-11	4.10E-13	4.13E-13	0.80
Butadiene	Air	kg	2.56E-08	4.49E-10	4.17E-10	7.49
Cadmium	Air	kg	1.80E-07	3.16E-09	3.17E-09	0.30
Carbon dioxide, biogenic	Air	kg	1.26E-01	2.21E-03	2.23E-03	0.70
Carbon dioxide, fossil	Air	kg	1.98E+01	3.48E-01	3.46E-01	0.61
Carbon disulfide	Air	kg	7.79E-11	1.37E-12	1.38E-12	0.80
Carbon monoxide	Air	kg	3.27E-05	5.73E-07	5.73E-07	0.13
Carbon monoxide, fossil	Air	kg	7.15E-01	1.25E-02	1.25E-02	0.44
Chloride	Air	kg	9.67E-11	1.70E-12	1.71E-12	0.70
Chloride	Water	kg	6.90E+00	1.21E-01	1.27E-01	4.73
Chloroform	Air	kg	3.54E-11	6.20E-13	6.25E-13	0.80
Chromium	Air	kg	5.23E-07	9.18E-09	9.22E-09	0.52
Chromium	Water	kg	4.59E-04	8.04E-06	8.01E-06	0.39
Chromium VI	Air	kg	9.82E-08	1.72E-09	1.74E-09	0.88
Chromium VI	Water	kg	1.93E-06	3.38E-08	3.37E-08	0.20
Chrysene	Air	kg	1.24E-10	2.18E-12	2.20E-12	0.88
Cobalt	Air	kg	1.06E-06	1.86E-08	1.86E-08	0.04
Cobalt	Water	kg	4.25E-06	7.45E-08	7.78E-08	4.28
COD, Chemical Oxygen Demand	Water	kg	6.69E-02	1.17E-03	1.22E-03	3.90
Copper	Air	kg	9.03E-09	1.58E-10	1.64E-10	3.37
Cumene	Air	kg	3.18E-12	5.57E-14	5.62E-14	0.80
Cyanide	Air	kg	1.50E-09	2.63E-11	2.65E-11	0.80
Cyanide	Water	kg	1.39E-08	2.43E-10	2.54E-10	4.25
Decane	Water	kg	5.61E-06	9.84E-08	1.02E-07	3.98
Dibenzofuran	Water	kg	3.64E-08	6.39E-10	6.68E-10	4.42
Dibenzothiophene	Water	kg	2.96E-08	5.18E-10	5.74E-10	10.24
Dinitrogen monoxide	Air	kg	3.54E-04	6.20E-06	2.36E-06	89.63

Table D1 LCI results from LCI calculation of Diesel, at refinery – RNA, US.LCI database (NREL, 2012) (cont'd)

Substance	Compartment	Unit	LCSoft previous database	LCSoft updated database with allocation	SimaPro	Percentage Difference (Updated database/SimaPro)
Docosane	Water	kg	2.05E-07	3.59E-09	3.76E-09	4.53
Dodecane	Water	kg	1.06E-05	1.86E-07	1.94E-07	4.14
Eicosane	Water	kg	2.92E-06	5.12E-08	5.35E-08	4.40
Ethane, 1,1,1-trichloro-, HCFC-140	Air	kg	5.06E-09	8.87E-11	8.86E-11	0.14
Ethane, 1,2-dibromo-	Air	kg	7.19E-13	1.26E-14	1.27E-14	0.80
Ethane, 1,2-dichloro-	Air	kg	2.40E-11	4.21E-13	4.24E-13	0.80
Ethane, chloro-	Air	kg	2.52E-11	4.42E-13	4.45E-13	0.80
Ethene, tetrachloro-	Air	kg	6.52E-08	1.14E-09	1.15E-09	0.75
Fluoranthene	Air	kg	8.82E-10	1.55E-11	1.56E-11	0.88
Fluorene	Air	kg	1.13E-09	1.98E-11	2.00E-11	0.88
Fluorene, 1-methyl-	Water	kg	2.18E-08	3.83E-10	4.00E-10	4.32
Fluorenes, alkylated, unspecified	Water	kg	5.49E-07	9.63E-09	9.63E-09	0.00
Fluoride	Air	kg	1.08E-07	1.89E-09	1.89E-09	0.06
Fluoride	Water	kg	1.26E-05	2.21E-07	2.20E-07	0.23
Fluorine	Water	kg	2.68E-07	4.70E-09	4.75E-09	1.15
Formaldehyde	Air	kg	9.65E-06	1.69E-07	1.68E-07	0.69
Furan	Air	kg	5.65E-12	9.92E-14	1.00E-13	0.95
Hexadecane	Water	kg	1.16E-05	2.03E-07	2.12E-07	4.15
Hexane	Air	kg	4.02E-11	7.04E-13	7.10E-13	0.80
Hexanoic acid	Water	kg	4.03E-05	7.07E-07	7.38E-07	4.31
Hydrocarbons, unspecified	Air	kg	2.09E-05	3.67E-07	3.66E-07	0.35
Hydrocarbons, unspecified	Water	kg	7.80E-12	1.37E-13	1.38E-13	0.70
Hydrogen chloride	Air	kg	1.61E-03	2.82E-05	2.84E-05	0.83
Hydrogen fluoride	Air	kg	1.86E-04	3.27E-06	3.30E-06	0.88
Hydrogen sulfide	Air	kg	3.13E-12	5.48E-14	5.52E-14	0.70
Indeno(1,2,3-cd)pyrene	Air	kg	7.58E-11	1.33E-12	1.34E-12	0.88
Iron	Water	kg	3.41E-02	5.98E-04	6.05E-04	1.20
Isophorone	Air	kg	3.48E-10	6.10E-12	6.15E-12	0.80
Isoprene	Air	kg	3.17E-03	5.56E-05	5.60E-05	0.70
Kerosene	Air	kg	1.74E-06	3.04E-08	3.04E-08	0.30
Lead	Air	kg	8.00E-07	1.40E-08	1.41E-08	0.61
Lead	Water	kg	1.13E-04	1.98E-06	2.02E-06	2.28
Lead-210/kg	Water	kg	1.99E-14	3.49E-16	3.65E-16	4.44
Magnesium	Air	kg	1.37E-05	2.40E-07	2.42E-07	0.88

Table D1 LCI results from LCI calculation of Diesel, at refinery – RNA, US.LCI database (NREL, 2012) (cont'd)

Substance	Compartment	Unit	LCSoft previous database	LCSoft updated database with allocation	SimaPro	Percentage Difference (Updated database/SimaPro)
Magnesium	Water	kg	1.20E-01	2.11E-03	2.21E-03	4.55
Manganese	Air	kg	1.10E-06	1.93E-08	1.94E-08	0.48
Manganese	Water	kg	2.14E-04	3.75E-06	3.90E-06	4.07
Mercaptans, unspecified	Air	kg	1.22E-07	2.13E-09	2.15E-09	0.84
Mercury	Air	kg	1.38E-07	2.42E-09	2.44E-09	0.74
Mercury	Water	kg	1.89E-07	3.32E-09	3.34E-09	0.57
Metallic ions, unspecified	Water	kg	9.53E-11	1.67E-12	1.68E-12	0.70
Metals, unspecified	Air	kg	3.59E-13	6.29E-15	6.33E-15	0.70
Methane	Air	kg	2.06E-01	3.62E-03	3.94E-03	8.61
Methane, bromo-, Halon 1001	Air	kg	9.59E-11	1.68E-12	1.70E-12	0.80
Methane, dichloro-, HCC-30	Air	kg	1.16E-06	2.03E-08	2.04E-08	0.37
Methane, dichlorodifluoro-, CFC-12	Air	kg	6.24E-09	1.09E-10	1.09E-10	0.11
Methane, fossil	Air	kg	8.51E-03	1.49E-04	1.48E-04	0.77
Methane, monochloro-, R-40	Air	kg	3.18E-10	5.57E-12	5.62E-12	0.80
Methane, monochloro-, R-40	Water	kg	7.71E-09	1.35E-10	1.41E-10	4.49
Methane, tetrachloro-, CFC-10	Air	kg	6.24E-10	1.09E-11	1.09E-11	0.11
Methyl ethyl ketone	Air	kg	2.34E-10	4.10E-12	4.13E-12	0.80
Methyl ethyl ketone	Water	kg	1.54E-08	2.70E-10	2.83E-10	4.48
Molybdenum	Water	kg	4.41E-06	7.73E-08	8.07E-08	4.36
m-Xylene	Water	kg	5.83E-06	1.02E-07	1.06E-07	4.07
Naphthalene	Air	kg	2.19E-07	3.85E-09	3.85E-09	0.02
Naphthalene	Water	kg	3.50E-06	6.13E-08	6.40E-08	4.29
Naphthalene, 2-methyl-	Water	kg	3.04E-06	5.33E-08	5.56E-08	4.36
Naphthalenes, alkylated, unspecified	Water	kg	1.55E-07	2.73E-09	2.72E-09	0.14
n-Hexacosane	Water	kg	1.28E-07	2.24E-09	2.34E-09	4.56
Nickel	Air	kg	1.35E-05	2.38E-07	2.37E-07	0.04
Nickel	Water	kg	5.27E-05	9.24E-07	9.49E-07	2.70
Nitrate	Water	kg	6.84E-13	1.20E-14	1.21E-14	0.70
Nitrate compounds	Water	kg	2.75E-11	4.83E-13	4.86E-13	0.70
Nitric acid	Water	kg	6.17E-08	1.08E-09	1.09E-09	0.70
Nitrogen oxides	Air	kg	1.55E-01	2.72E-03	2.73E-03	0.04
Nitrogen, total	Water	kg	1.93E-06	3.39E-08	3.37E-08	0.35

Table D1 LCI results from LCI calculation of Diesel, at refinery – RNA, US.LCI database (NREL, 2012) (cont'd)

Substance	Compartment	Unit	LCSoft previous database	LCSoft updated database with allocation	SimaPro	Percentage Difference (Updated database/SimaPro)
o-Cresol	Water	kg	5.50E-06	9.65E-08	1.01E-07	4.60
Octadecane	Water	kg	2.86E-06	5.01E-08	5.24E-08	4.37
Oils, unspecified	Water	kg	4.46E-03	7.82E-05	8.11E-05	3.60
Organic acids	Air	kg	1.33E-08	2.33E-10	2.33E-10	0.05
Organic substances, unspecified	Air	kg	7.72E-06	1.35E-07	1.37E-07	0.87
PAH, polycyclic aromatic hydrocarbons	Air	kg	1.10E-07	1.93E-09	1.79E-09	7.49
Particulates, > 2.5 um, and < 10um	Air	kg	3.58E-03	6.28E-05	6.27E-05	0.17
Particulates, unspecified	Air	kg	1.66E-02	2.91E-04	2.92E-04	0.09
p-Cresol	Water	kg	5.93E-06	1.04E-07	1.09E-07	4.64
Phenanthrene	Air	kg	3.36E-09	5.89E-11	5.94E-11	0.88
Phenanthrene	Water	kg	5.48E-08	9.60E-10	9.76E-10	1.63
Phenanthrenes, alkylated, unspecified	Water	kg	6.47E-08	1.13E-09	1.13E-09	0.48
Phenol	Air	kg	9.59E-12	1.68E-13	1.70E-13	0.80
Phenol	Water	kg	8.50E-05	1.49E-06	1.49E-06	0.07
Phenol, 2,4-dimethyl-	Water	kg	5.37E-06	9.42E-08	9.84E-08	4.31
Phenols, unspecified	Air	kg	6.19E-07	1.09E-08	1.09E-08	0.17
Phenols, unspecified	Water	kg	1.21E-05	2.12E-07	2.83E-07	28.57
Phthalate, dioctyl-	Air	kg	4.38E-11	7.68E-13	7.74E-13	0.80
Propanal	Air	kg	2.28E-10	4.00E-12	4.03E-12	0.80
Propene	Air	kg	1.69E-06	2.96E-08	2.75E-08	7.49
Pyrene	Air	kg	4.10E-10	7.19E-12	7.26E-12	0.88
Radionuclides (Including Radon)	Air	kg	9.71E-05	1.70E-06	1.70E-06	0.36
Radium-226/kg	Water	kg	6.90E-12	1.21E-13	1.27E-13	4.73
Radium-228/kg	Water	kg	3.54E-14	6.22E-16	6.49E-16	4.39
Selenium	Air	kg	1.75E-06	3.06E-08	3.09E-08	0.85
Selenium	Water	kg	2.35E-06	4.13E-08	4.15E-08	0.50
Silver	Water	kg	4.02E-04	7.06E-06	7.38E-06	4.42
Solids, inorganic	Water	kg	1.57E-10	2.75E-12	2.77E-12	0.70
Strontium	Water	kg	1.05E-02	1.84E-04	1.91E-04	4.23
Styrene	Air	kg	1.50E-11	2.63E-13	2.65E-13	0.80
Sulfate	Water	kg	1.55E-02	2.71E-04	2.83E-04	4.20
Sulfide	Water	kg	9.90E-06	1.74E-07	1.73E-07	0.29
Sulfur	Water	kg	5.08E-04	8.91E-06	9.31E-06	4.33
Sulfur dioxide	Air	kg	4.07E-02	7.13E-04	1.55E-03	73.99

Table D1 LCI results from LCI calculation of Diesel, at refinery – RNA, US.LCI database (NREL, 2012) (cont'd)

Substance	Compartment	Unit	LCSoft previous database	LCSoft updated database with allocation	SimaPro	Percentage Difference (Updated database/SimaPro)
Sulfuric acid, dimethyl ester	Air	kg	2.88E-11	5.05E-13	5.09E-13	0.80
Tar	Air	kg	1.09E-10	1.91E-12	1.92E-12	0.70
Tar	Water	kg	1.56E-12	2.73E-14	2.75E-14	0.70
t-Butyl methyl ether	Air	kg	2.10E-11	3.68E-13	3.71E-13	0.80
Tetradecane	Water	kg	4.65E-06	8.15E-08	8.51E-08	4.30
Thallium	Water	kg	2.27E-06	3.97E-08	3.99E-08	0.46
Tin	Water	kg	4.31E-05	7.56E-07	7.71E-07	1.96
Toluene	Air	kg	3.19E-04	5.59E-06	4.36E-09	199.69
Toluene	Water	kg	3.03E-04	5.32E-06	5.57E-06	4.53
Toluene, 2,4-dinitro-	Air	kg	1.68E-13	2.94E-15	2.97E-15	0.80
Vanadium	Water	kg	5.20E-06	9.13E-08	9.54E-08	4.38
Vinyl acetate	Air	kg	4.56E-12	7.99E-14	8.05E-14	0.80
VOC, volatile organic compounds	Air	kg	6.07E-03	1.06E-04	1.06E-04	0.29
Xylene	Air	kg	1.85E-04	3.24E-06	3.04E-09	199.63
Yttrium	Water	kg	1.29E-06	2.27E-08	2.37E-08	4.16
Zinc	Air	kg	6.02E-09	1.06E-10	1.09E-10	3.37
Zinc	Water	kg	3.97E-04	6.97E-06	7.02E-06	0.76

CURRICULUM VITAE

Name: Mr. Yodsathorn Chavewanmas

Date of Birth: May 12, 1993

Nationality: Thai

University Education:

2011–2015 Bachelor Degree of Chemical Engineering, Faculty of Engineering, King Mongkut's University of Technology Thonburi, Bangkok, Thailand

Work Experience:

July-August 2013	Position:	Student Internship in Production Division
	Company name:	Thai Plaspac Company Limited

Proceedings:

1. Chavewanmas, Y., Malakul, P., and Gani, R. (2017, Oct 1-5) LCSoft – the life cycle assessment software: new developments and status. Proceedings of The 27th European Symposium on Computer-Aided Process Engineering, Barcelona, Spain.
2. Chavewanmas, Y., Malakul, P., and Gani, R. (2017, May 23) Improvement of life cycle assessment software and its application. Proceedings of The 23th PPC Symposium on Petroleum, Petrochemicals, and Polymers and The 8th Research Symposium on Petrochemicals and Materials Technology, Bangkok, Thailand.