



# Integration of life cycle assessment software with tools for economic and sustainability analyses and process simulation for sustainable process design



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## ABSTRACT

The sustainable future of the world challenges engineers to develop chemical process designs that are not only technically and economically feasible but also environmental friendly. Life cycle assessment (LCA) is a tool for identifying and quantifying environmental impacts of the chemical product and/or the process that makes it. It can be used in conjunction with process simulation and economic analysis tools to evaluate the design of any existing and/or new chemical-biochemical process and to propose improvement options in order to arrive at the best design among various alternatives. Although there are several commercial LCA tools, there is still a need for a simple LCA software that can be integrated with process design tools. In this paper, a new LCA software, LCSOFT, is developed for evaluation of chemical, petrochemical, and biochemical processes with options for integration with other process design tools such as sustainable design (SustainPro), economic analysis (ECON) and process simulation. The software framework contains four main tools: Tool-1 is for life cycle inventory (LCI) knowledge management that enables easy maintenance and future expansion of the LCI database; Tool-2 is for estimation of environmental impact characterization factors using group contribution<sup>+</sup> method (GC)<sup>+</sup> in order to calculate environmental impacts for a wide range of chemicals; Tool-3 performs LCA calculations based on a library of models; and, Tool-4 provides interfaces for integration with other tools. To test the software, a bioethanol production process using cassava rhizome is employed as a case study. Results from LCSOFT highlight the estimated environmental performance in terms of various aspects such as carbon footprint, resource and energy consumptions, and various environmental impacts.

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## 1. Introduction

Recently, the modern society has become more concerned about issues such as the depletion of natural resource and environmental impact of its activities. Many industries and businesses these days pay more attention to those activities that affect the environment, indicating that environmental assessment has become a key factor for them in their search for more sustainable options. However, as the development of new chemical processes and the introduction of new advanced technologies continue every day, identification of more sustainable process design options by considering process needs together with economic and environmental factors becomes necessary (De Benedetto and Klemes, 2009; Cucek and Klemes, 2012). Therefore, environmental assessment of the chemical

process must be done, preferably in the early stages of design and/or retrofit for existing processes. One effective tool for environmental assessment is LCA, a tool that helps to quantify the potential environmental impacts throughout the chemical product or process life cycle and to evaluate improvement options in order to select the best design among various alternatives (Carvalho et al., 2008).

The LCA methodologies comprise of a set of methods for impact assessment in a particular chemical process. The technical framework for conducting LCA, according to the International Standardization Organization (ISO) directive, ISO 14040 (Guinée et al., 2002), involves a systematic process consisting of four main steps.

- (1) Goal and scope definition: the intention for the use of LCA and the system boundaries are defined, together with the functional unit for evaluation, for example, 1 kg of product.
- (2) Life cycle inventory (LCI) calculation: all the necessary input and output data for the processes corresponding to the

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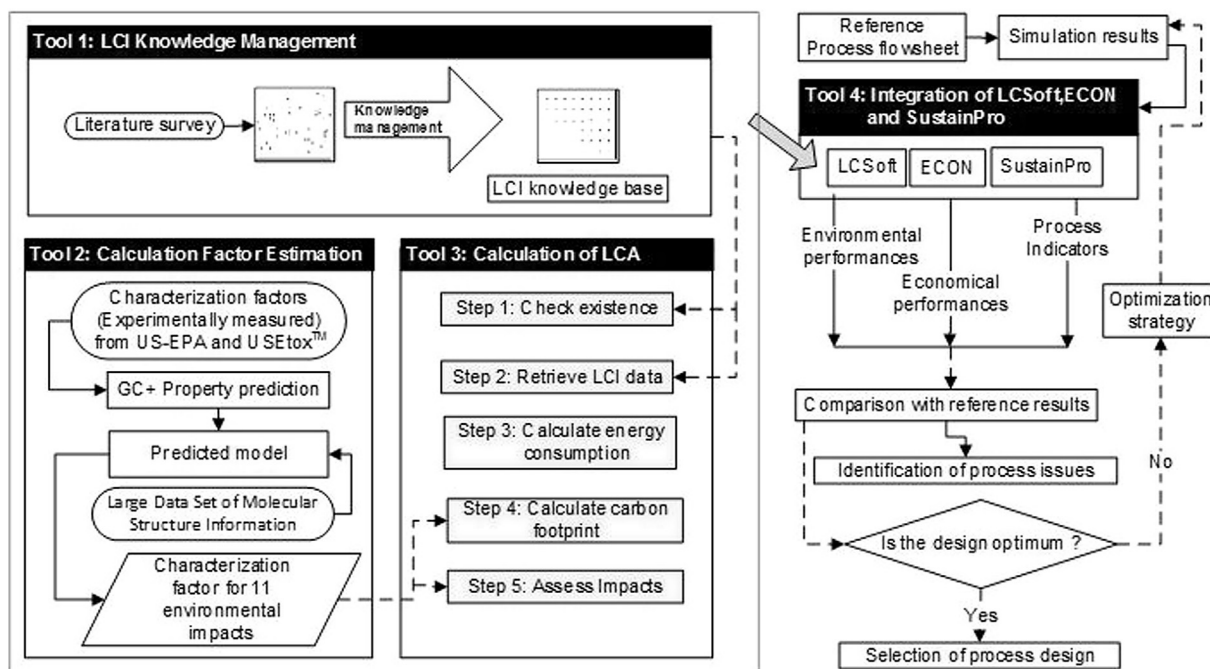


Fig. 1. Systematic framework for LCSofT and tools integration.

product system are collected in terms of the defined functional unit. The emission data for different sub-processes are estimated, combined and presented as the total emissions of the corresponding chemicals.

- (3) Life cycle impact assessment (LCIA): the inventory data on input (material and resources) and output (waste and emissions) are translated into information related to the impacts, such as global warming or ozone depletion, that the operation of the process causes on the environment, human health, and resources. Note that the impact assessment calculations require emission data from the LCI step in terms of a list of chemicals that are released from the process and the chemical-specific characterization factors (CFs) that represent their potency.
- (4) Interpretation: the results from the previous steps are presented for analysis with respect to the goals of the study. In order to quantify the analysis results, the sensitivity and uncertainty of the calculated impacts may also be considered in this step.

Although, various LCA methodologies have been developed (Vigon and Jensen, 1995; Wiloso et al., 2012), it is still difficult to perform the LCA because of the most time-consuming step, which is LCI data collection for relevant feedstock, emission, etc., and the corresponding substance CFs. Therefore, in this work, emphasis has been put on the development of a LCI database and models for the generation of the CFs. Various LCA software such as BOUSTED (Boustead user manual, 2012), SimaPro (SimaPro user manual, 2012), Umberto (ifu Hamburg GmbH, 2012), and GaBi (PE International, 2012) provide different degrees of sustainability analysis (Carvalho et al., 2013). However, the existing software is not directly linked to process synthesis-design tools that generate sustainable design alternatives. Thus, there is still a need for a simple LCA software that can be integrated with process design tools in order to perform multi-objective process evaluation (Cucek and Klemes, 2012). Therefore, the objectives of this work are to develop the new LCA software, LCSofT (Piyarak, 2012), which is exclusively developed for evaluation of chemical–biochemical

processes and its integration with other tools used in sustainable product-process design. LCSofT is therefore integrated with ECON (Saengwirun, 2011) – economic analysis software; SustainPro (Carvalho et al., 2013) – sustainable process design software; and CAPEC DB (Hukkerikar et al., 2012) – property database tool. In this way, LCSofT together with its integrated tools can help the product-process developer to search for more sustainable design options efficiently and reliably.

## 2. Framework

The framework (architecture) of LCSofT is divided into two sections: a section to perform LCA related calculations and a section to integrate LCSofT with other tools. As shown in Fig. 1, the framework of LCSofT contains four main tools: knowledge management (tool-1); calculation factor estimation (tool-2); calculation of LCA (tool-3); integration of LCSofT with ECON, process simulation and SustainPro (tool-4).

### 2.1. Tool-1: knowledge management

The objective of this tool is to organize the LCI data, to enable their easy maintenance, and to allow future expansion of the tool. To manage the data and its transfer to the various calculation steps, a knowledge base (LCI KB) is created by representing the knowledge (collected data) through an especially developed ontology as shown in Fig. 2. LCI data from US LCI (U.S. Life Cycle Inventory Database, 2012) and from other open sources are processed through LCI KB at two levels. LCI KB's first level classifies LCI data into 3 main categories (material, utility and transport) which are further divided into sub-categories (such as plants, biomass, fuels for material as the main category), each of which is linked to unit processes (such as rice straw, cassava root, and wheat straw for plants as the sub-category). LCI KB's second level stores LCI data of each unit process, which is divided into 2 parts: (1) inputs – which accounts for raw material and resource consumptions; (2) outputs – which accounts for emissions related to the compartments (emissions to air, emissions to water, and emissions to soil). In the

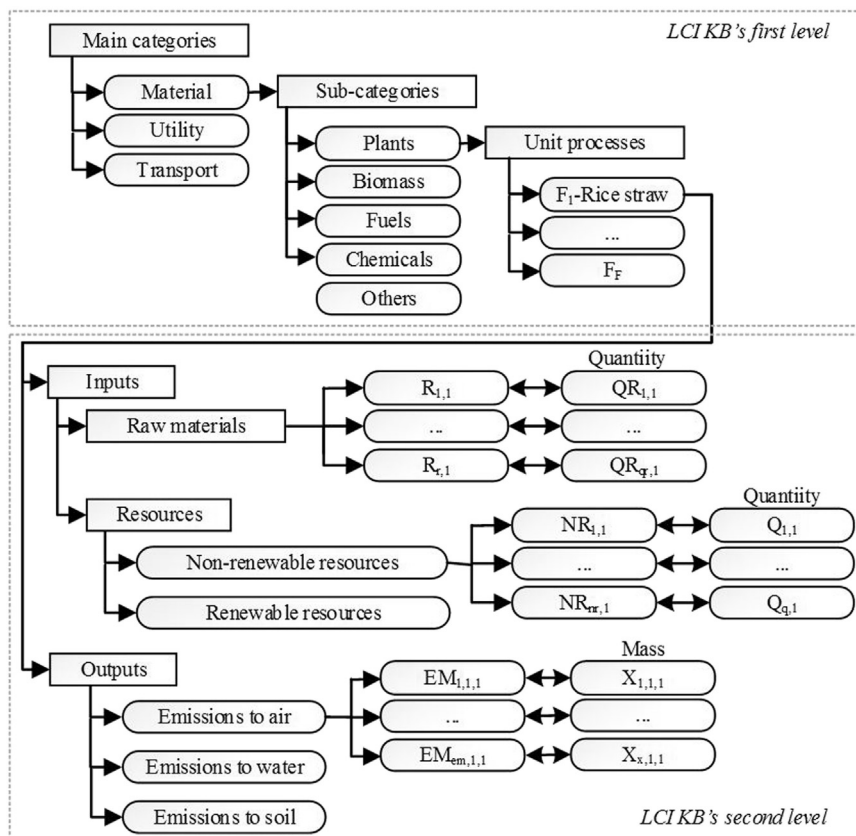


Fig. 2. Structure of LCI KB.

current version of LCSoft, LCI data for 224 unit processes is stored in LCI KB that cover applications in chemical and biochemical process design. Also, LCSoft provides options for users to create their own data base, which can be managed through Tool-1 and stored in the extended LCI KB.

## 2.2. Tool-2: characterization factor estimation

To characterize the emissions that occur in the life cycle of a product or process in terms of their potential environmental impacts, for each category of impact (such as global warming or ozone depletion), the impact assessment applies to substance-specific characterization factors (CFs) that represent the substance's potency. An emission inventory for the life cycle of a product or process often contains hundreds of substances, and many of them have the potential to damage the environment. These potential damages are quantified using characterization factors for different categories of environmental impact. Although a number of different models have been developed for this purpose (Rosenbaum et al., 2008), they cover, however, a limited number of chemicals (substances). Thus, for many chemicals, the characterization factors needed for LCI calculation may not be available. Therefore, within tool-2, the CFs are estimated. The LCSoft database contains data from the USEtox™ database (Rosenbaum et al., 2008) and the US Environmental Protection Agency (EPA) and especially developed predictive property models with high accuracy (Hukkerikar et al., 2012), enabling therefore, the calculation of environmental impacts (human toxicity by ingestion, human toxicity by exposure, aquatic toxicity, terrestrial toxicity, global warming, ozone depletion, photochemical oxidation, acidification, human toxicity-carcinogenics, human toxicity-non carcinogenics,

and fresh water ecotoxicity) for a very wide range of organic chemicals.

## 2.3. Tool-3: calculation of LCA

The calculation of LCA involves five main steps (see Fig. 3).

- Step 1: checks existence of LCI data for the chemical process under investigation using tool-1;
- Step 2: retrieves LCI data from LCI knowledge base to prepare for the calculations in the next step using tool-2;
- Step 3: calculates energy consumption based on heat of combustion of resources consumed in the systems using lists of resource consumptions retrieved from tool-1;
- Step 4: calculates the carbon footprint using LCI data of utility consumed in the system retrieved from tool-1 and global warming characterization factors retrieved from tool-2;
- Step 5: assesses impacts with respect to substances emitted from the life cycle of product or process and their characterization factors for each impact category using LCI data retrieved from tool-1 and characterization factors retrieved from tool-2;

Table 1 provides the calculation details related to steps 1–5, while, more details for characterization factors for specific environmental impacts and their corresponding compartments are given in Table 2.

## 2.4. Tool-4: integration of LCSoft, ECON and SustainPro

The objective of this tool is to integrate ECON, SustainPro, and LCSoft through one generic interface in order to provide efficient

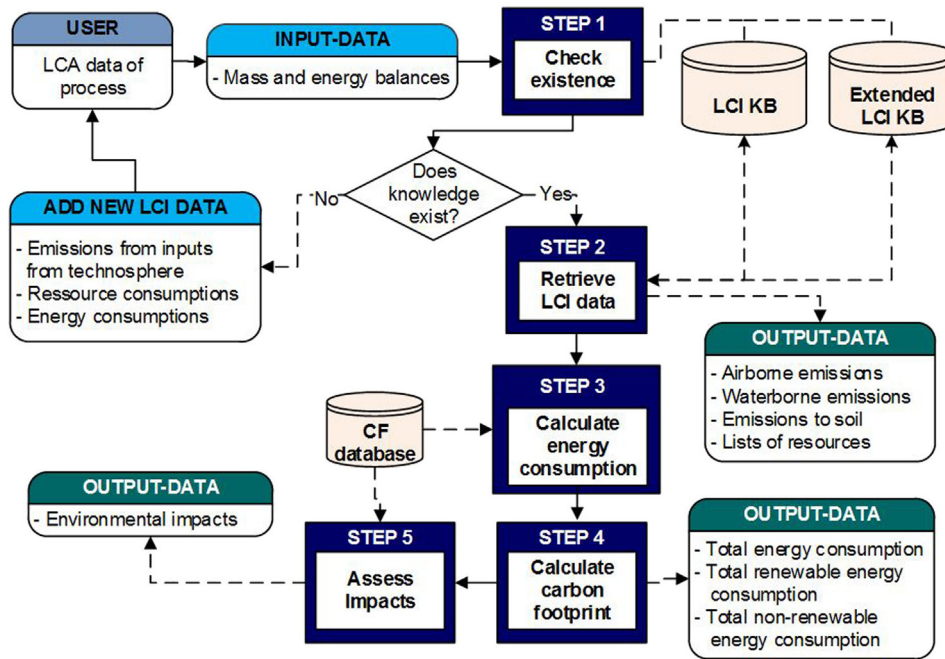


Fig. 3. Activity diagram of LCSOFT.

data communication that makes it a multi-criteria evaluation tool, which can evaluate economic performances using ECON, process sustainability using SustainPro, and environmental impacts using LCSOFT (see Fig. 1). The advantages of this tool are that it makes the data transfer from one software-tool to another very smooth, efficient and consistent, thereby, reducing time spent in performing the calculations. Through Tool-4, the user can easily enter the necessary prerequisites for the integrated software in the main interface in one step. The prerequisites for all software-components are mass and energy balances from the process stream and the corresponding equipment tables. The additional prerequisites for LCSOFT are the definitions of the system boundaries. The additional prerequisites for ECON are equipment sizing parameters, and price of materials. The additional

prerequisites for SustainPro are component properties, and reaction data. Mass and energy balance data from stream and equipment tables are used to generate open paths (OP, path through which a chemical enters and leaves the process) and closed paths (CP, path, such as recycle loops, where chemicals and energy go round and round without going out of the process), and based on these, the performances of each path are calculated in terms of sustainability indicators. The main sustainability indicators are: material value added (MVA), indicator that reflects the value added between the entrance and exit of a given compound in OPs; energy and waste cost (EWC), the sum of the energy cost and waste cost; total value added (TVA), the difference of MVA and EWC. The calculation models used (Uerdinger et al., 2003) are given in Table 3.

**Table 1**  
Calculation steps in LCSOFT.

Calculation step	Description	Input data/output data/calculation models
Step 1: check existence	This step checks the existence of LCI data for the related products or processes, enabling the user opportunity to add or modify LCI data and enable the complete LCA conduction.	Input data: - Mass balance (stream table) - Energy balance or duty of unit operations (equipment table)
Step 2: retrieve LCI data	Input processes, resource consumption, and emissions are retrieved from LCI KB to be stored in the systematic worksheet and be calculated in the next step. The names and amount of input process, resource, and emissions are listed in the separated specific worksheet.	Output data: - Airborne emissions - Waterborne emissions - Emissions to soil - Lists of resources
Step 3: calculate resource and energy consumption	Energy consumption is the amount of energy (MJ) consumed by the resources per functional unit of product (such as 1 kg of product, 1 L of product, or 1 MJ of product) over the life cycle. Resources used in production of raw material phase, energy production phase and manufacturing phase are converted to total energy consumption and % renewable energy.	Calculation models: (Xunmin et al., 2009) $R_{total} = R_{renew} + R_{non-re}$ $R_{renew} = (\sum_{r,i} m_i \times x_{r,i} \times HV_r) / m_{product}$ $R_{non-re} = (\sum_{nr,i} m_i \times x_{nr,i} \times HV_{nr}) / m_{product}$
Step 4: calculate carbon footprint	Carbon footprint (CF) is the overall amount of carbon dioxide and other greenhouse gas emissions per functional unit of product (such as 1 kg of product). The carbon footprint is quantified using indicators such as the global warming potential (GWP).	Calculation models: (Guinée et al., 2002) $CO_{2eq} = (m_{GHC, air}^{PRO} \times CF_{GHC, air}^{GWP}) / m_{product}$ Carbon footprint = $\sum CO_{2eq}$
Step 5: assess impacts	Environmental impacts are calculated from mass of emitted substance multiply by its characterization factors for a specific compartment per functional unit of product (such as 1 kg of product, 1 L of product, or 1 MJ of product). In LCSOFT, 11 impact categories are calculated.	Calculation models: (Guinée et al., 2002) $I^k = \sum_{t,c} EM_{t,c} \times CF_{t,c}^k$



**Table 2**  
Characterization factors and compartments of environmental impacts.

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

**Table 3**  
Sustainability indicator calculation models in SustainPro.

Sustainability indicator	Calculation model
MVA	$MVA_o^{sc} = m_o^{sc} \cdot \left( PP_o^{sc} - CA_o^{sc} \cdot \left( \sum_{rm=1}^{RM} \frac{V_o^{(rm)} \cdot M_o^{(rm)}}{V_o^{sc} \cdot M_o^{(rm)}} \cdot PR_o^{(rm)} \right) \right)$
EWC	$EWC_k^{sc} = \sum_{u=1}^U PE_u \cdot Q_u \cdot \frac{m_k^{sc} \cdot A_{u,k}^{sc}(T,p)}{\sum_{uk=1}^{m_{uk}^{sc}} m_{uk} \cdot A_{u,uk}(T,p)}$
TVA	$TVA_k^{sc} = MVA_k^{sc} - EWC_k^{sc}$

2.5. Implementation details

The VBA (visual basic for applications) programming language with Excel interface is used in developing LCSofT. It has been designed to provide a user-friendly interface (see Fig. 4), especially for product and process design, for which, various simulation results (mass and energy balances) from each design alternative are used. LCSofT has options to import simulation results from process simulators, where, component mass balance data is imported as a stream table and energy balance data is

imported as equipment tables. LCA calculation steps start from defining the stream components, defining equipment utility to check the existence of LCI data in LCI knowledge base, then defining the LCA sections and their system boundaries, and then calculating the environmental impacts by following the five main steps as illustrated in Table 1.

3. Case study

This case study involves a cradle-to-gate investigation of bio-ethanol production from cassava rhizome in Thailand. The mass and energy flows are taken from simulation results, which have been developed separately (Mangnimit, 2013). The raw material (cassava rhizome) enters the process as wet biomass at the rate of 377 tons/day and 119 tons/day of bioethanol product is produced with the addition of cellulose enzyme as the biocatalyst. The functional unit of this study is 1 kg of pure ethanol produced from cassava rhizome. The flowsheet of the process is illustrated in Fig. 5. In order to evaluate the process performance in terms of environmental impacts, the process is divided into different sections with their corresponding sub-system boundaries and life cycle stages: (1) Pretreatment – lignocellulosic material is treated so that it can be hydrolyzed; (2) Detoxification – the compounds that are toxic for the fermentation microorganisms are treated; (3) SSCF – glucose and other sugars are converted to ethanol; (4) Distillation – the outlet from SSCF is distilled until a mixture of nearly azeotropic ethanol-water is obtained; and (5) Dehydration – the ethanol from the distillation section is purified using vapor-phase molecular sieves in order to obtain to obtain dehydrated ethanol.

3.1. Step-1 check for existence of LCI data

First, tool-4 is used to enter the process data in terms of mass balance (Fig. 6) and energy balance (Fig. 7). Using this information and searching for the LCI related data for the upstream process (production of raw material) within the LCSofT database (tool-1), it is found that data for the following substances are available:

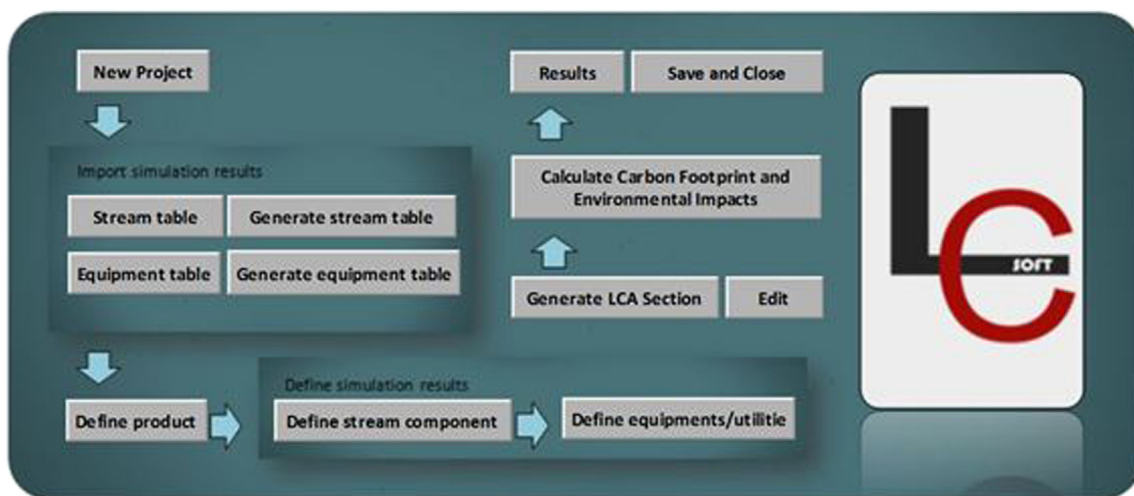


Fig. 4. LCSofT main interface.

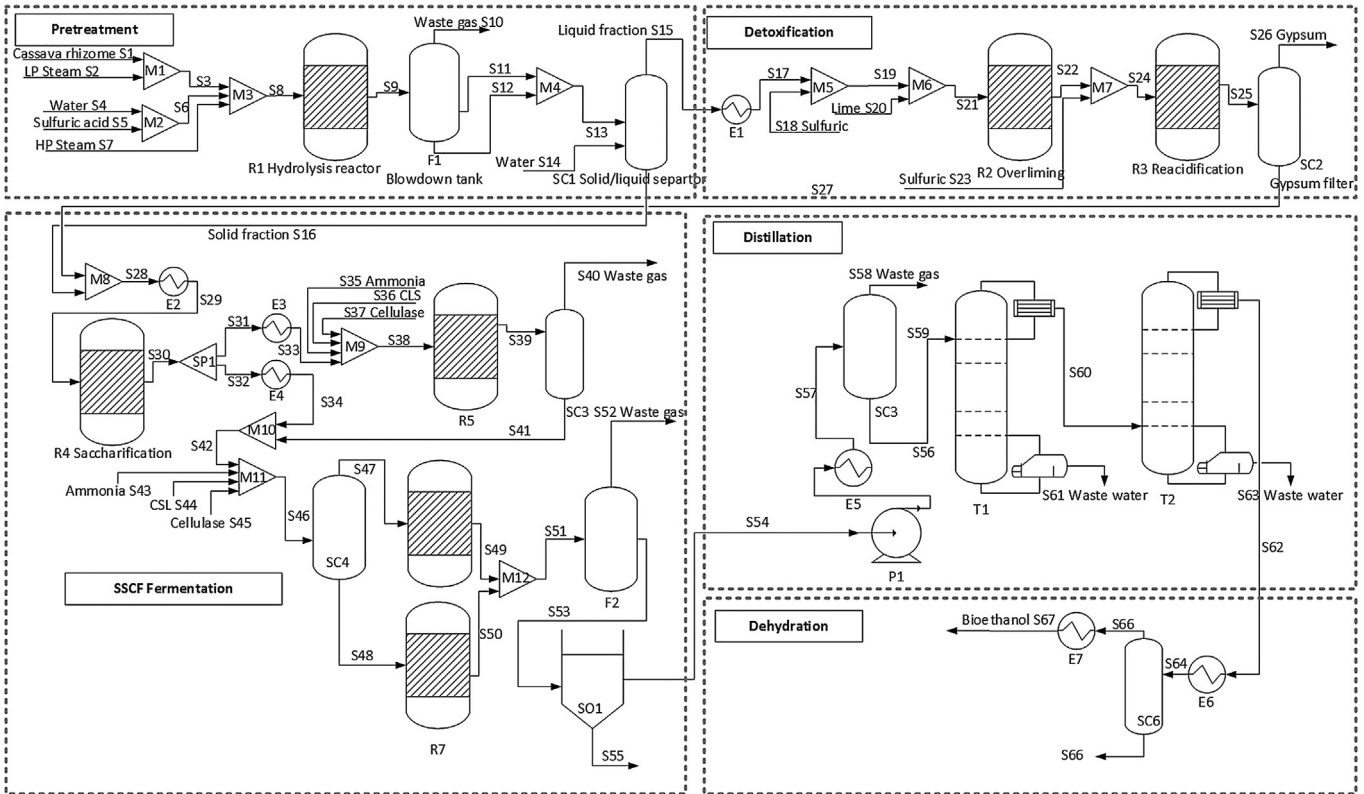


Fig. 5. Flowsheet of the case and LCA boundaries of the case study.

	A	B	C	D	E	F	G	H	I	J	K	L
1	Stream Name		S1	S2	S3	S4	S5	S6	S7	S8	S9	S10
2	Stream Description											
3	Stream Phase		Mixed	Vapor	Mixed	Liquid	Liquid	Liquid	Vapor	Mixed	Mixed	Vapor
4	Temperature	C	30,000	160,000	100,018	25,000	25,000	25,000	268,000	188,002	190,000	103,854
5	Pressure	ATM	1,000	6,000	1,000	1,000	1,000	1,000	13,000	12,100	12,100	1,000
6	Total Molecular Weight		103,896	18,015	84,688	18,015	98,079	18,308	18,015	38,223	40,920	18,725
7	Total Weight Comp. Rates	kg/hr										
8	Cellulose		4680,592	0,000	4680,592	0,000	0,000	0,000	0,000	4680,592	4320,186	0,000
9	Hemicellulose		6674,090	0,000	6674,090	0,000	0,000	0,000	0,000	6674,090	333,705	0,000
10	Lignin		3653,449	0,000	3653,449	0,000	0,000	0,000	0,000	3653,449	3653,449	0,000
11	Glucose		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	364,047	0,000
12	Xylose		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	6825,731	0,000
13	Cellobiose		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	34,584	0,000
14	Ethanol		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
15	Water		129,522	785,091	914,613	4972,114	0,000	4972,114	3153,382	9040,110	8273,831	2371,593
16	Sulfuric Acid		0,000	0,000	0,000	0,000	99,441	99,441	0,000	99,441	99,441	0,000
17	Furfural		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	242,695	115,985
18	Ammonia		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
19	Oxygen		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
20	Carbon Dioxide		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
21	Glycerol		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
22	Succinic Acid		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
23	Lactic Acid		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
24	HMF		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
25	Xylitol		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
26	Acetic Acid		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
27	CornSteep Liquor		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
28	ZM		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
29	Cellulase		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
30	Lime		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
31	CASO4		0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000	0,000
32	Ash		578,255	0,000	578,255	0,000	0,000	0,000	0,000	578,255	578,255	0,000

Fig. 6. Stream table.

Unit	Type of unit	Duty/Work	Unit		Activity	Energy source
			Energy	time		
P1	Pump	5.6979 kW		hr	Electric usage	Electricity, natural gas, at power plant
R2	Reactor	-399.6 MJ		hr	Cooling	Chilled water, engine-driven chiller using natural gas
R3	Reactor	-97.7 MJ		hr	Cooling	Chilled water, engine-driven chiller using natural gas
R4	Reactor	1613.2 MJ		hr	Heating	Natural gas, combusted in industrial equipment
R5	Reactor	-843.3 MJ		hr	Cooling	Chilled water, engine-driven chiller using natural gas
R6	Reactor	-8214.4 MJ		hr	Cooling	Chilled water, engine-driven chiller using natural gas
R7	Reactor	-322.9 MJ		hr	Cooling	Chilled water, engine-driven chiller using natural gas
E1	Heat Exchanger	859.3 MJ		hr	Heating	Wood waste, unspecified, combusted in industrial boiler
E2	Heat Exchanger	1113 MJ		hr	Heating	Wood waste, unspecified, combusted in industrial boiler
E3	Heat Exchanger	235.2 MJ		hr	Heating	Wood waste, unspecified, combusted in industrial boiler
E4	Heat Exchanger	2180 MJ		hr	Heating	Wood waste, unspecified, combusted in industrial boiler
E5	Heat Exchanger	5678.5 MJ		hr	Heating	Wood waste, unspecified, combusted in industrial boiler
E6	Heat Exchanger	4804 MJ		hr	Heating	Wood waste, unspecified, combusted in industrial boiler
E7	Heat Exchanger	4840.4 MJ		hr	Heating	Wood waste, unspecified, combusted in industrial boiler
T1condenser	Column-Condenser	-18089.2 MJ		hr	Cooling	Chilled water, engine-driven chiller using natural gas
T1reboiler	Column-Reboiler	24889.6 MJ		hr	Heating	Wood waste, unspecified, combusted in industrial boiler
T2condenser	Column-Condenser	-19971.2 MJ		hr	Cooling	Chilled water, engine-driven chiller using natural gas
T2reboiler	Column-Reboiler	14371.4 MJ		hr	Heating	Wood waste, unspecified, combusted in industrial boiler

Fig. 7. Equipment table.

sulfuric acid, ammonia, water, ethanol, ammonia, acetic acid, corn steep liquor, cellulose, and calcium sulfate. On the other hand, process data for the production of cassava is not available, although the necessary data can be found in the open literature (Papong and Malakul, 2009). Therefore, new data has to be added to the LCI KB. With this tool, the data from literature is entered into the software and managed with the ontology model, making the work of data addition, maintenance and retrieval easy, fast and reliable.

### 3.2. Step-2 retrieve LCI data

Tool-1 is used to retrieve LCI and LCA-related data for the upstream process (production of raw material) of the system. According to the base-case design, since a small amount of ethanol is emitted from the process, the environmental impacts, such as human toxicity-carcinogenics (HTC), are calculated from the mass of emitted ethanol, the compartment (see Table 2) and the characterization factor of ethanol related to HTC. They are found to be negligible. Note that these calculations are repeated for all other chemicals (such as glucose, sulfuric acid, furfural, ammonia, and carbon dioxide) that are also released.

### 3.3. Step 3 calculate energy consumption

Energy consumption is divided into renewable and non-renewable energy consumption types, depending on the type of resources used in each section. The energy consumption is calculated from heating value of resources. In Table 4, total energy consumption for the case study is given as 12.91 MJ/kg of ethanol

**Table 4**  
Energy consumption calculation results.

Section	Renewable energy consumption (MJ/kg product)	Non-renewable energy consumption (MJ/kg product)	Total energy consumption	% Renewable
(1) Pretreatment	0.00	0.24	0.24	0.00
(2) Detoxification	0.17	0.27	0.44	39.20
(3) SSCF	0.71	0.51	1.22	58.39
(4) Distillation	9.06	0.02	9.07	99.81
(5) Dehydration	1.94	0.00	1.94	100.00
Total	11.88	1.03	12.91	92.03

and percent renewable is 92.03% because the majority of the selected utility comes from heating and wood waste (renewable resource). From this information, section-4 (distillation) consumes the highest energy – this is identified as a future design item to be improved (see Sections 3.7.1 and 3.7.2).

### 3.4. Step 4 calculate carbon footprint

This step is developed for identification of the hot-spots of the process where all equipment in the process flowsheet consumes utilities and/or emits greenhouse gases to the environment. The results are highlighted in Fig. 8, where it is shown that the emissions from utility consumptions mainly come from the reboilers of distillation columns T1 and T2. Therefore, the design of this section should be improved (see Sections 3.7.1 and 3.7.2).

### 3.5. Step 5 assess impacts

Environmental impacts caused by each section are calculated and represented by each impact in the bar chart in LCSoft, as shown in Fig. 9. The distillation section has high contribution in every impact category. In addition, the SSCF section also has high contribution in AP (acidification) impact. Therefore, the design of these sections should be improved (see Sections 3.7.1 and 3.7.2).

### 3.6. Comparison of LCSoft with SimaPro 7.1

In order to test the consistency of the results given by the LCSoft, the environmental impacts for the same case study and system boundaries calculated through LCSoft are compared below with SimaPro 7.1.

In LCSoft, the scope of the case study includes manufacturing phase of raw material, which is the cassava cultivation and production of sulfuric acid, ammonia, corn steep liquor (CSL), and cellulase enzyme. With respect to chemicals included in the simulation results, the following exist in the LCI database: sulfuric acid, ammonia, corn steep liquor (CSL), and cellulase enzyme. Therefore the impacts associated with them are included in the environmental impact assessment. As the cassava cultivation is included, cellulose, hemicelluloses, and lignin that are included in the input streams of the process simulation results are modeled as the sum of the mass of cassava rhizome (lignocellulosic matter).



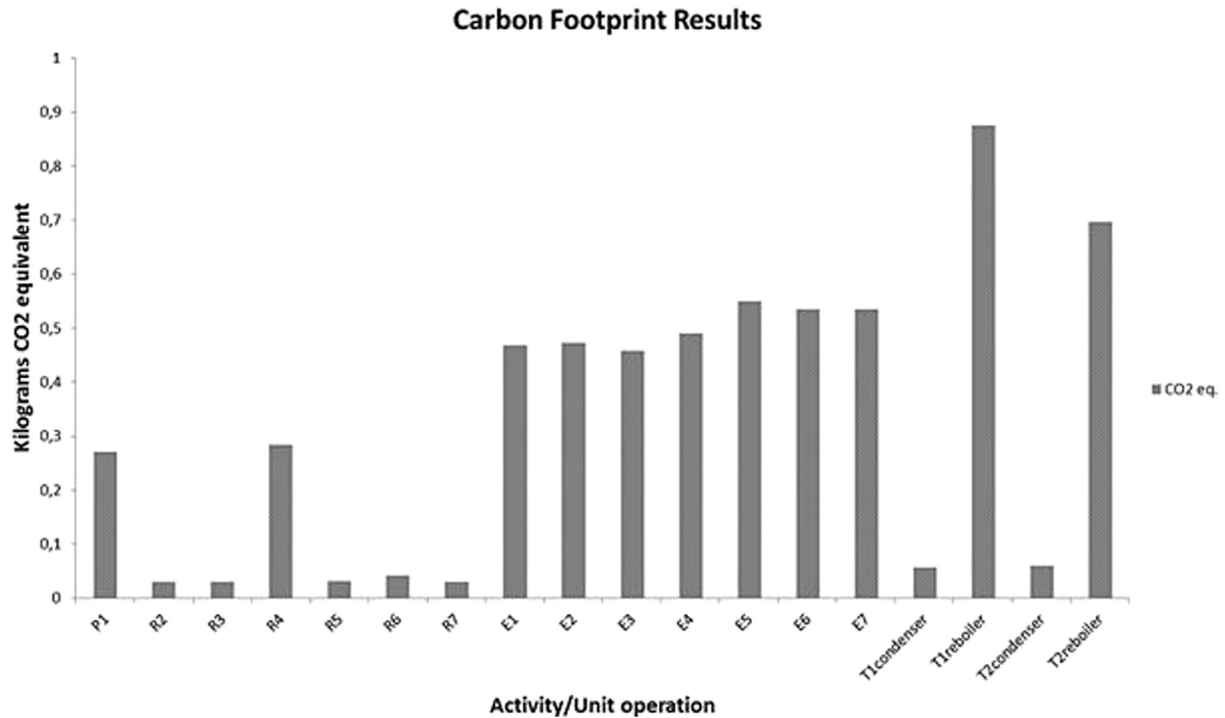


Fig. 8. Carbon footprint results.

Based on the calculations of the environmental impacts in LCSoft, the following chemicals, glucose, xylose, cellobiose, furfural, hydroxymethyl furfural (HMF), lactic acid, succinic acid, and glycerol, are found to have negligible influence. In order to analyze the environmental impacts from using utilities in the bioethanol production process, the unit processes are: electricity using natural gas, natural gas, combusted in industrial boiler and chilled water, and engine-driven chiller using natural gas.

In SimaPro 7.1, raw materials such as sulfuric acid and ammonia exist in their LCI database. On the other hand, CSL and cellulase enzyme were not found in SimaPro 7.1. The cassava cultivation is modeled by the sum of cellulose, hemicelluloses, and lignin and using LCI data from the literature since LCI data for cassava cultivation does not exist in the LCI database of SimaPro 7.1. For utilities, electricity from natural gas, natural gas, combusted in industrial boiler, and cooling water are considered. The method that is used in the case study is TRACI (Tool for the Reduction and Assessment of Chemical and other environmental Impacts) method. This method is midpoint oriented LCIA methodology of US Environmental Protection Agency (EPA) that supports consistency in environmental decision making. TRACI allows the examination of the potential for impacts associated with the raw material consumption and chemical releases resulting from the processes involved in

producing a product. It allows the user to examine the potential for impacts for a single life cycle stage, or the whole life cycle, and to compare the results between products or processes. The purpose of TRACI is to allow a determination or a preliminary comparison of two or more options on the basis of the following environmental impact categories: ozone depletion (ODP), global warming (GWP), acidification (AP), eutrophication (EP), respiratory effects (RE), photochemical oxidation (PCOP), human toxicity-carcinogenics (HTC), human toxicity-non-carcinogenics (HTNC), and ecotoxicity (ET).

Life cycle assessment of the bioethanol process using cassava rhizome is conducted using the TRACI method in SimaPro 7.1. The comparison of the environmental impacts from the two systems is given in Table 5. The insignificant difference between SSE and percent differences of GWP and PCOP values from each software

Table 5  
Comparative results of bioethanol process between SimaPro and LCSoft.

Environmental impacts	Unit	SimaPro	LCSoft	Sum squares error (SSE)	Percent difference (%)
Global Warming (GWP)	kg CO <sub>2</sub> eq.	7.29E-01	7.30E-01	2.04E-06	-0.19
Acidification (AP)	H <sup>+</sup> moles eq.	6.46E-01	1.07E-01	0.29070047	83.5
Carcinogenics (HTC)	kg benzene eq.	8.65E-06	2.89E-07	6.99E-11	96.65
Non carcinogenics (HTNC)	kg toluene eq.	1.44E+00	2.83E+00	1.90745627	-95.63
Ozone depletion (ODP)	kg CFC-11 eq.	4.09E-10	1.14E-10	8.69E-20	72.06
Ecotoxicity (ET)	kg 2,4-D eq.	1.24E-03	6.20E-03	2.45E-05	-397.99
Photochemical oxidation (PCOP)	kg NO <sub>x</sub> eq.	2.40E-02	2.61E-02	4.42E-06	-8.75

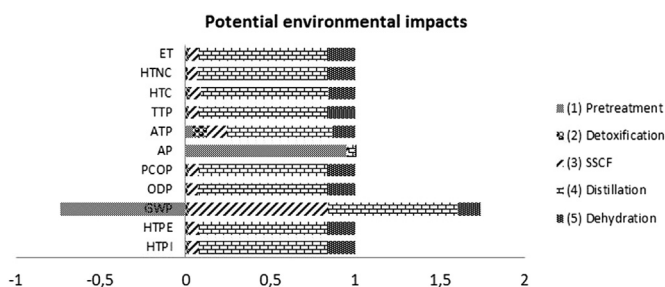


Fig. 9. Impact assessment results.



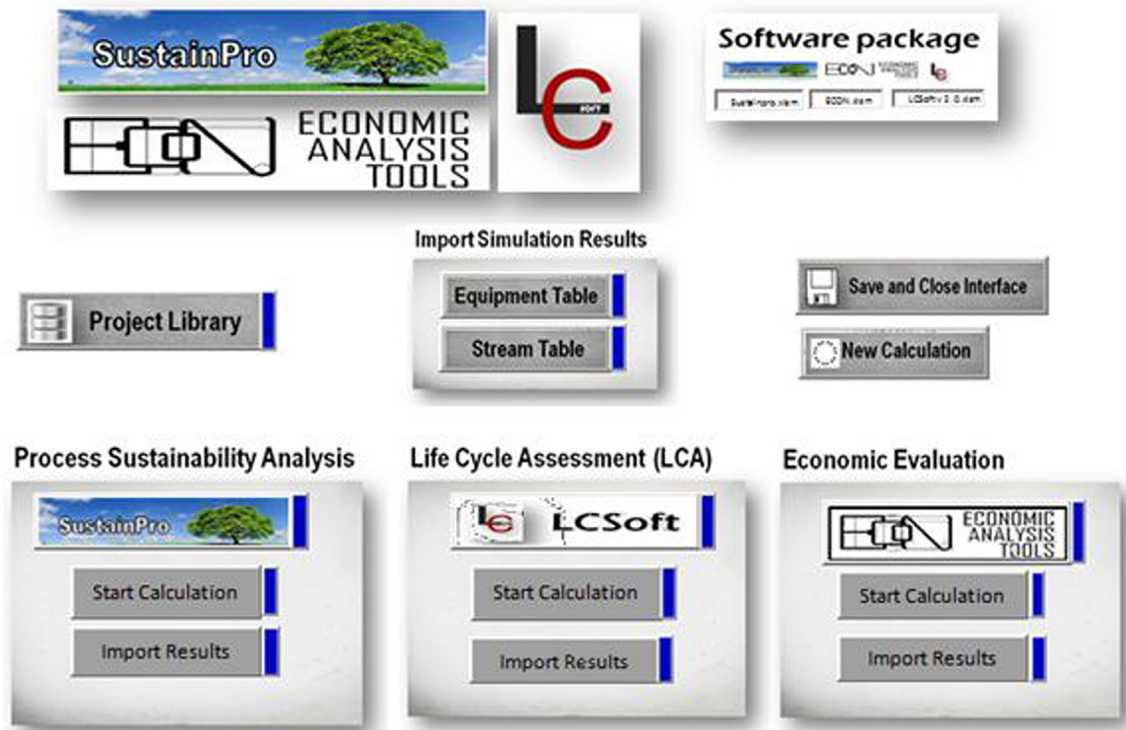


Fig. 10. Main user interface of tools integration.

indicate that the boundary definitions, assumptions in inventories, material flows, and energy flows are the same. The major differences are in the values of AP and HTNC. AP values from SimaPro 7.1 is greater than those from LCSof because the Franklin database model yields larger sets of emission factors associated with the combustion fuels compared with those in LCSof model (De Benedetto and Klemes, 2009). HTNC and ET values from LCSof are greater than the one from SimaPro because LCSof has HTNC characterization factor of isoprene (estimated from Tool-2) which does not exist in SimaPro 7.1. The differences of HTC, ODP, and ET values from either software are considered to be insignificant since these values are in the acceptable ranges.

### 3.7. Multi-objective analysis through tool-4 (Integration of LCSof, ECON, and SustainPro)

The main interface helps the user to reduce steps for data entry. The advantage of this interface is that it allows efficient multi-criteria evaluation of the design process through efficient data-flow consistent with the associated work-flow. Finally, results from all software are sent to the main interface (see Fig. 10).

#### 3.7.1. SustainPro results

This sustainability analysis tool provides targets for improvement in order to make the process more profitable, safer, and more sustainable. SustainPro calculates indicators for each OP and CP and orders them in terms of higher to lower potential for improvement. After entering all necessary data into the software throughout the interface, the paths that have the highest potential for improvement for each indicator are determined as listed in Table 6. The second line of each path states the component and OP it refers to. In cases where the component enters the process through reaction it is written "P" followed by the name of the unit where the reactions take place. For example, Corn Steep Liquor-44-61 means corn steep liquor flows in streams S44 to S61 or Ethanol-P R6-67 means ethanol enters the process through a reaction in the reactor (R6) to stream S67. SustainPro did not calculate indicators for CP (close-path) since there is no recycle path in the case study.

It is necessary to use a good engineering judgment to evaluate which of the targets should actually be improved? The results from SustainPro are given in Table 6. It can be noted that OP 67, OP 43, and OP 50 must reduce their duties since high values of

**Table 6**  
Indicator results of the case study after ordering in SustainPro.

Path	MVA	Probability	Path	EWC	Probability	Path	TVA	Probability
OP 322	-553	High	OP 67	795.49	Medium	OP 322	-1349	High
Corn Steep Liquor-44-61			Ethanol-P R6-67			Corn Steep Liquor-44-61		
OP 206	-506	High	OP 43	270.95	Low	OP 206	-777	High
Water-14-52			Xylose -P R1-61			Water-14-52		
OP 15	-441	High	OP 50	145.35	Low	OP 15	-586	High
Lignin-1-55			Xylose-P R1-61			Lignin-1-55		
OP 318	-376	High	OP 35	102.81	Low	OP 318	-479	High
Corn Steep Liquor-36-61			Glucose-P R4-61			Corn Steep Liquor-36-61		
OP 326	-300	High	OP 62	74.92	High	OP 326	-375	High
Cellulase-45-55			Ethanol-P R5-67			Cellulase-45-55		

Note: text in italic indicates the corresponding path that has the potential for improvement.

Manufacturing Fixed-capital Investment (Direct Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result
Purchased Equipment Delivered	1.1 \$	10,611,227.00
Purchased Equipment Installation	0.47 \$	4,987,276.69
Instrumentation and Controls (installed)	0.36 \$	3,820,041.72
Piping (Installed)	0.68 \$	7,215,634.36
Electrical Systems (Installed)	0.11 \$	1,167,234.36
Buildings (Including Services)	0.18 \$	1,910,020.86
Yard Improvement	0.1 \$	1,061,122.70
Service Facilities (Installed)	0.7 \$	7,427,858.90
<b>Total Direct Cost</b>	<b>\$</b>	<b>38,200,417.20</b>

Nonmanufacturing Fixed-capital Investment (Indirect Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result
Engineering and Supervision	0.33 \$	3,501,704.91
Construction Expenses	0.41 \$	4,350,603.07
Legal Expenses	0.04 \$	424,449.08
Contractor's Fees	0.22 \$	2,334,469.94
Contingency	0.44 \$	4,668,939.88
<b>Total indirect cost</b>	<b>\$</b>	<b>15,280,166.88</b>

Fixed-capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result
Fixed-capital Investment (FCI)		<b>\$ 53,480,584.08</b>

Working Capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result
Working Capital Investment (WC)	0.89	<b>\$ 212,224.54</b>

<b>Total Capital Investment (TCI)</b>	<b>\$</b>	<b>53,692,808.62</b>
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Fig. 11. Total capital investment calculation details.

EWC means that the given path carries important units of energy that could be used for heat integration. These paths all start from the SSCF section and go to the distillation section. Note that LCSOFT also indicated that the distillation section should be improved. This confirms that LCSOFT and SustainPro indicate the same improvements. Another result from SustainPro is that OP 322, OP 15, and OP 326 indicate that corn steep liquor (CSL), lignin, and cellulase (enzyme) lose their value they exit the process since they have high negative values of MVA and TVA. Therefore the excess flow of CSL should be reduced and cellulase should be recovered and recycled, if possible. However, cellulase is difficult to recover and therefore, recycle. Hence, other options, such as, use of the lignin or waste and recycle of water needs to be investigated.

### 3.7.2. ECON results

Economic feasibility of process design alternatives is necessary to ensure economical sustainability of the process. After entering dimensions of all process equipment, the prices of product and raw materials, the data are transferred into ECON through the generic interface. Total capital investment cost, operating cost, and other economic evaluation parameters are calculated and imported from ECON to the interface.

After application of ECON, the net present value (NPV) of this process is found to be \$ 95,125,049.00 with 15% expected internal rate of return (IRR). Therefore, this process has high potential for economic feasibility. In order to find improvement options based on the cost, capital investment, operating cost, and equipment cost

are calculated. Total capital investment is \$ 53,692,808 (see Fig. 11 for additional details). Total operating cost is \$ 20,792,726 (see Fig. 12 for additional details). From these results, the largest fractions of the operating costs are found to involve the raw materials and utilities. 70% of the utility costs are reboiler steam from the distillation column T1 (44%) and T2 (26%), and therefore, distillation units need to be improved. Note that ECON, SustainPro, and LCSOFT are identifying the same deficiencies in the process design, thereby validating each other results. This means that for the process under study, what is more sustainable is also economically more profitable.

## 4. Conclusion

A LCA tool, LCSOFT that can help to evaluate the environmental impacts of a chemical and/or biochemical process has been presented together with a case study highlighting its application. It is based on the developed framework allows a fast, reliable, and systematic calculation of inventories and emissions, and its integration with other important tools for economic and sustainability analysis allows a robust, flexible, and systematic evaluation of sustainable design alternatives. A new database employing a specially developed ontology for knowledge representation has been created and new predictive models for estimation of the environmental impacts have been developed. The LCA of bioethanol production from cassava rhizome has been analyzed. Current and future work is improving and extending the framework with respect to integration with more external tools and the

Items of Operating Cost		Basis	Cost, \$/year
<b>Raw Material</b>			<b>\$ 7,600,517.00</b>
Utilities			\$ 3,459,217.00
Maintenance and Repairs	Fixed Capital Investment		\$ 3,208,835.04
Operating Supplies	Maintenance and Supplies		\$ 481,325.25
Royalties	Total Product Cost		\$ 207,927.26
			<b>Variable Cost \$ 14,957,821.55</b>
Property Taxes	Fixed Capital Investment		\$ 1,069,611.68
Insurance	Fixed Capital Investment		\$ 534,805.84
			<b>Fixed Charges \$ 1,604,417.52</b>
Plant Overhead	Labor + Supervision + Maintenance		\$ 1,925,301.00
			<b>Manufacturing Cost \$ 16,562,239.07</b>
Administration	Labor + Supervision + Maintenance		\$ 641,767.00
Distribution & selling	Total Product Cost		\$ 831,709.04
Research & Development	Total Product Cost		\$ 831,709.04
			<b>General Expense \$ 2,305,185.08</b>
			<b>Total Product without Depreciation \$ 20,792,726.00</b>

Fig. 12. Operating cost calculation details.

addition of sensitivity and uncertainty analysis related to the predicted environmental impacts.

### Nomenclature

$i$	Input from technosphere
$m$	Mass of input from technosphere
$n_r$	Non-renewable resource used to produce input $i$
$x_{r,i}$	Mass of renewable resource $r$ used to produce 1 kg of input $i$ (kg)
$x_{nr,i}$	Mass of non-renewable resource $nr$ used to produce 1 kg of input $i$ (kg)
$HV_r$	Heating value of renewable resource $r$ (MJ/kg <sub>r</sub> )
$HV_{nr}$	Heating value of non-renewable resource $nr$ (MJ/kg <sub>nr</sub> )
$R_{total}$	Total energy from resource consumption per 1 kg of product (MJ/kg <sub>product</sub> )
$R_{renew}$	Total energy from renewable resource consumption per 1 kg of product (MJ/kg <sub>product</sub> )
$R_{non-re}$	Total energy from non-renewable resource consumption per 1 kg of product (MJ/kg <sub>product</sub> )
GHG	Greenhouse gas emitted to air from process
$m_{GHG,air}^{PRO}$	Mass flow rate of GHG emitted to air from the process
$CF_{GHG,air}^{GWP}$	Characterization factor for global warming of GHG
$CO_{2eq}$	Carbon dioxide equivalent per functional unit.
$c$	compartment
$t$	chemical emitted to compartment
$k$	impact category
$CF_{t,c}^k$	The characterization factor of chemical $t$ emitted to compartment $c$ for impact category $k$
$EM_{t,c}$	Mass of chemical $t$ emitted to compartment $c$ per 1 kg of product
$I^k$	The potential environmental impact of chemical $t$ for a specific impact category of concern $k$
sc	Stream component
$o$	Open-path flow
rm	Raw material
$m_o^{sc}$	Flow rate of component sc in the open-path flow $o$
$PP_o^{sc}$	Purchase price

$CA_o^{sc}$	Cost allocation factor calculated by purchase price of the component sc divided by the total purchase price of product
$v_o^{sc}$	Stoichiometry
$M_o^{sc}$	Molecular weight
$PR_o^{(rm)}$	Raw material price
$k$	Path of flow
$u$	Sub-unit operation $u$
$uk$	Sub-unit operation $u$ in path of flow $k$
$PE_u$	Energy price of sub-unit operation $u$
$Q_u$	Sub-unit operation duty
$m_k^{sc}$	Mass flow rate along the path flow $k$ of the component sc
$A_{u,k}^{sc}$	Specific heat capacity

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