CHAPTER III
METHODOLOGY

3.1 Materials and Equipment

3.1.1 Equipment

- Laptop, Intel® Core™ 2 Duo CPU P7550 2.66 GHz, 4 GB of RAM

3.1.2 Software

- LCSoft
- SimaPro7.1
- Visual Basic for Applications

3.2 Experiment

3.2.1 Development of LCI Calculation Function

3.2.1.1 Model Construction

Matrix inversion (Heijungs and Suh, 2002) was used to develop this function. Equations 2.1-2.2 describe the relationship between commodities flow, environmental Intervention flow, and designed product.

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

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

"A" (Technology matrix) is referred to matrix that contains flows of commodities (economic flows), e.g., amount of electricity, amount of fuel, of unit processes. "B" (Intervention matrix) represents matrix that contains flows of environmental Intervention (i.e. emissions or natural resources). "f" represents "Final demand vector", which is the given amount of designed product produced by system. "s" is referred to "Scaling factor", that scale up the economic flows contained in

Technology matrix to meet with target amount defined by Final demand vector. "g" represents "Total intervention vector" that contains set of all environmental Intervention flows given by Intervention matrix and Scaling factor. The principle of LCI calculation function is retrieving inventory data contained in LCSoft database. The commodities flows were filled in Technology matrix and environmental Intervention flows were filled in Intervention matrix. Amount of designed product was filled in Final demand vector. Scaling factor was determined by multiplying of inverted Technology matrix and Final demand vector. The Technology matrix was inverted by using LU decomposition with pivoting method (Ford, 2015). Total intervention vector was multiplying of Intervention matrix and Scaling factor.

3.2.1.2 Validation of LCI Calculation Function

Acetic acid 98 % in H_2O, at plant – RER (Althaus *et al.*, 2007) was used as a case study for validation of new LCI calculation function. LCI results from LCSoft were compared with SimaPro7.1 in order to check accuracy. The model would be modified if LCI results were not meet with accuracy. The development framework is shown in Figure 3.1.

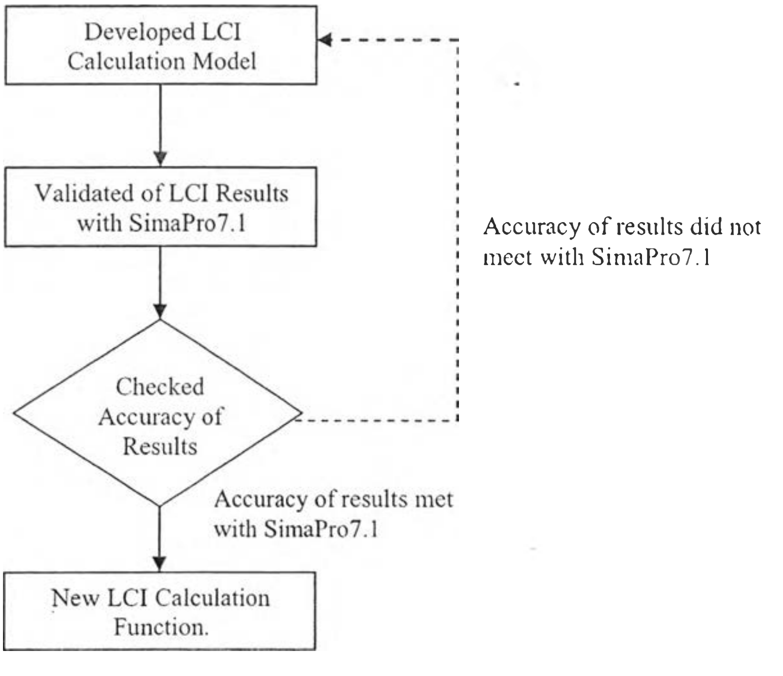

Figure 3.1 Development framework of LCI calculation function.

3.2.2 Extension of Inventory Database

LCI inventory database were mainly collected from U.S. LCI database (NREL, 2015) and the rest from open literatures. LCI database structure of LCSoft was organized to two levels that are LCI KB's first level and LCI KB's second level. LCI KB's first level referred to information of data categories that consist of Material, Transportation, and Utility. LCI KB's second level represents information of input and output flows contained in unit processes.

3.2.3 Improvement of Impact Categories in LCIA Calculation

In order to extend the boundary of LCIA calculation, three impact categories; including deposited wastes, mineral extraction, and water resource consumption; and one renovated impact category, energy consumption, were developed. Equation 2.3 was used to assess potential environmental impacts.

$$I^k = \sum_{t,c} EM_{t,c}\, x\; CF^k_{t,c} \qquad (2.3)$$

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

3.2.3.1 Deposited Wastes

Deposited waste was divided into 3 sub-categories that are Above-ground landfill wastes, Hazardous wastes in underground disposal sites, and radioactive wastes. Characterization factors were collected from Ecological Scarcity 2013 (Frischknecht and Büsser-Knöpfel, 2013), expressed in unit of UBP. Acetic acid, 98 % in H_2O, at plant – RER production (Althaus *et al.*, 2007) was used as a case study for validation of deposited wastes.

3.2.3.2 *Energy Consumption*

In order to simplify and decreasing time of defining heating values of materials in LCI database, Cumulative Energy Demand (CED) was used to determine the energy consumption. The characterization factors in CED method are determined from the amount of energy withdraw from nature and expressed in MJ equivalent. Acetic acid, 98 % in H_2O, at plant – RER production (Althaus *et al.*, 2007) was used as a case study for validation of energy consumption.

3.2.3.3 Mineral Extraction

The CML method, representing the current recommendation in the ILCD framework (EC-JRC, 2011) was used in this part. Characterization factors of element extraction, as a part in Abiotic Depletion Potential (ADP), were collected to calculate mineral extraction, expressed in unit of antimony equivalent. Acetic acid, 98 % in H_2O, at plant – RER production (Althaus *et al.*, 2007) was used as a case study for validation of mineral extraction.

3.2.3.4 Water Consumption

Ecological scarcity (water) is recommended method for assessment of water resource use and consumption (EC-JRC, 2011). In order to assess the impact of water consumption, Characterization factors from Ecological Scarcity 2013 (Frischknecht and Büsser-Knöpfel, 2013), expressed in unit of UBP, were used to assess the impact of water consumption. For validation of water consumption, Acetic acid, 98% in H_2O, at plant – RER production (Althaus *et al.*, 2007) was used as a case study.

3.2.4 Development of Contribution Analysis

Contribution analysis, which is processes contribution, LCI results contribution, and LCIA results contribution, provides information for investigating how results from performing LCA contribute to production stage that would be a useful function for further process development.

3.2.4.1 Process Contribution

Amount of unit processes, which were used to produce certain amount of designed product, used in production system were analyzed and displayed in the results of contribution of processes in each production stage. The results would be shown in exact values and percentage contained in table. Furthermore, results were displayed in graphical format.

3.2.4.2 LCI Contribution

Amount of elementary flow of all unit processes, calculated by LCI calculation function, in production system were analyzed and displayed in contribution of LCI in each production stage.

3.2.4.3 LCIA Contribution

Results of LCIA calculation from production system were shown in contribution of LCIA results in each production stage. Contribution results of specific impact categories could be investigated. Moreover, Contribution of LCIA results in specific impact categories and specific production stage could be shown.

3.2.4.4 Validation of Contribution Analysis Function

In order to validate new contribution analysis, bioethanol process using cassava rhizome as a feed stock was used as a case study. The mass and energy flows were taken from simulation results developed by Mangnimit (2013). The production process was divided into 5 production stages, which are Pretreatment, Detoxification, SSCF Fermentation, Distillation, and Dehydration, as shown in Figure 3.2.

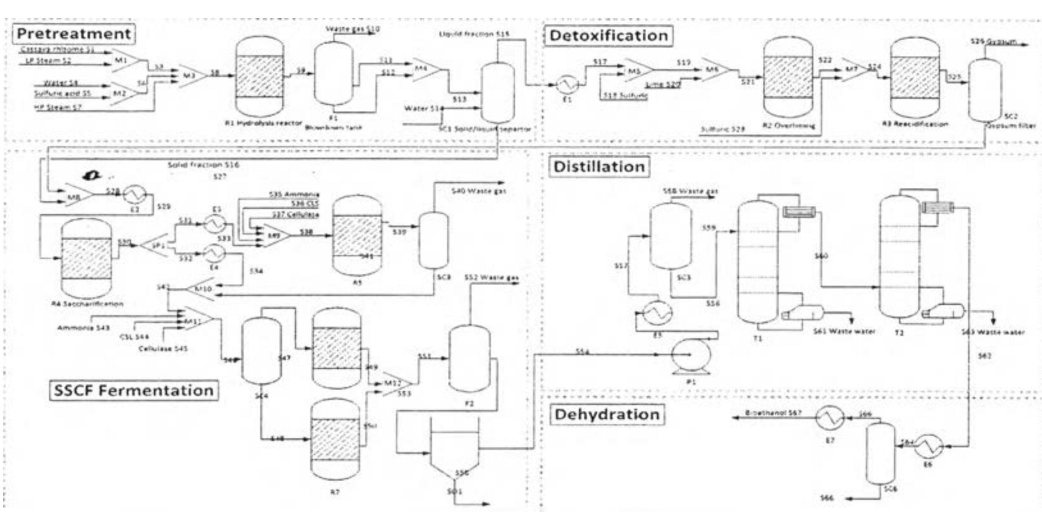

Figure 3.2 Bioethanol production process using cassava rhizome as a feed stock (Kalakul, 2013).

Table 3.1 Unit processes and data sources used in bioethanol production case study

No	Process	Data source
1	Cassava root	Khongsiri, S. (2009)
2	Corn steep liquor	U.S. LCI (NREL, 2015)
3	Enzyme, cellulase	U.S. LCI (NREL, 2015)
4	Ammonia, steam reforming, liquid, at plant	ecoinvent v2
5	Sulphuric acid, at plant	
6	Cooling energy, natural gas, at cogen unit with absorption chiller 100 kW	
7	Electricity, natural gas, at power plant, US	
8	Natural gas, burned in industrial furnace 100kW	

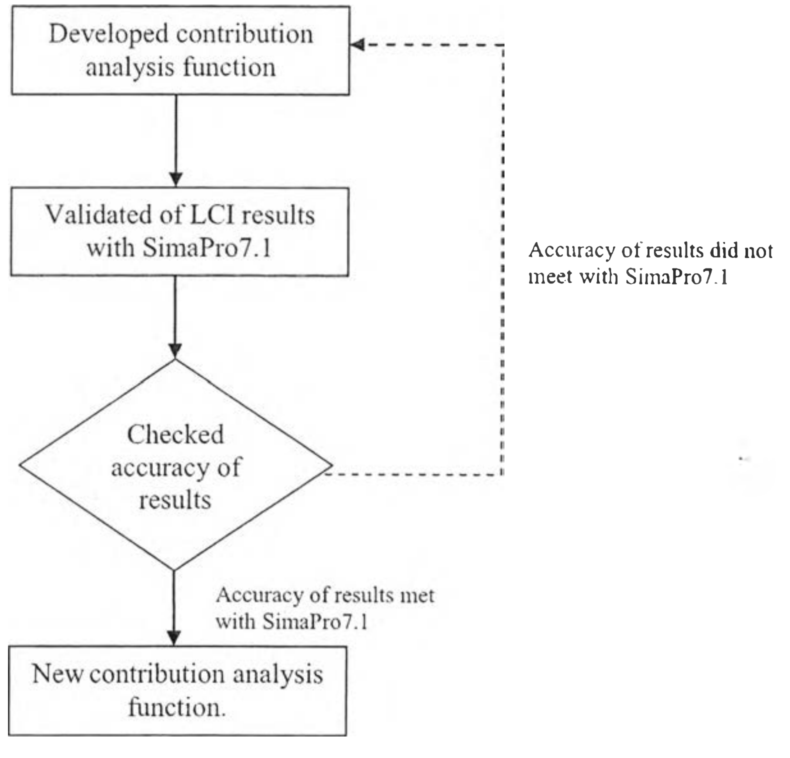

Figure 3.3 Development framework of contribution analysis function.

Amount of related input and output streams are given in Table C1. Detail of used equipment and necessary equipment information are given in Table C2. Development framework of contribution analysis function is shown in Figure 3.3.