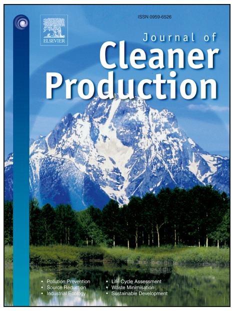

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# Process simulation based life cycle assessment for bioethanol production from cassava, cane molasses, and rice straw

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## Abstract

The process simulation technique is integrated into life cycle assessment (LCA) in this study to reduce biased parameters in process data collection and perform a fair comparison among different processes. Bioethanol production processes from cassava, cane molasses, and rice straw are studied as an example, to show the usability of process simulation. The simulation results are compared with actual bioethanol plant data to validate the reliability of the technique. The study is a comprehensive LCA comparison, based on unbiased process data from simulations, and minimum variations in other settings, i.e., process fuel type, waste recovery options, etc. The results show that cleaner process designs, using simulations with renewable process energy and sustainable waste recovery, improve the energy efficiency, renewability, and environmentally-benign aspects of the three bioethanol feedstocks. Bioethanol from cassava shows the best values of net energy ratio (1.34), renewability (5.16), and reduced greenhouse gas emissions (410 kg $CO_2$ eq/1,000 L). The unbiased LCA results from net energy analysis, and environmental impact assessment, including emissions/hotspot identification and sensitivity analysis, are comprehensively discussed. The simulation technique in this study is also adaptable for future LCA of new/modified processes.

**Keywords:** Process simulation, Unbiased LCA comparison, Bioethanol production, Cassava, Cane molasses, Rice straw

## 1. Introduction

Life cycle assessment (LCA) is a systematic technique to analyze environmental impacts and sustainability improvement approaches for production processes (Zidoniene and Kruopiene, 2015). Recent developments in methodologies have provided standard guidelines to effectively conduct LCA (Owsianiak et al., 2014). However, conventional inventory data collection methods for actual production process plants are time consuming and require large amounts of data through questionnaires, surveys, databases, etc. (Kalakul et al., 2014). These inventory data undergo variations in different production process plants due to biased parameters: plant design, age of individual plants, efficiency degradation based on various locations/technologies used, production scales, labor skills, waste recovery practices applied, etc. (Silalertruksa and Gheewala, 2009). A fair evaluation of LCA among different production processes needs to minimize these biased measurements. Chemical process simulation provides unbiased material/energy data of production processes with reduced time and resource utilization for inventory data collection (Quintero and Cardona, 2011). Simulations have the flexibility of effective process data predictions based on proper thermodynamic properties, design parameters, and actual plant conditions for individual plant designs. In addition, pre-production/modified process plants can be easily predicted using simulations to integrate/modify different alternative scenarios (Kiwjaroun et al., 2009). For example, additions of new materials, technologies, and recycling options into different processes can be easily performed, to evaluate their benefits and decision planning for the industry (Spengler et al., 1998). Therefore, this study focuses on using the process simulation technique to conduct a fair evaluation of LCA for bioethanol production from three agricultural feedstocks, i.e., cassava, cane molasses, and rice straw. The reported data on actual bioethanol plants in the literature are further utilized to validate the reliability of the simulation technique.

Cassava, cane molasses, and rice straw are favorable bioethanol feedstocks due to less competition for availability, food security, and cultivation land occupation, compared to other crops (Gadde et al., 2009; Prapaspongsa and Gheewala, 2016; Silalertruksa and Gheewala, 2010). Bioethanol production from cassava, cane molasses, and rice straw comprises four main product stages: 1) feedstock cultivation, 2) transportation of feedstocks from farm to factory, 3) feedstock preparation, and 4) bioethanol conversion from prepared feedstock to the final product at factory gate. The cultivation stages of these three feedstocks involve agrochemicals production/application and energy consumption by diesel-operated farming machinery (Papong and Malakul, 2010; Silalertruksa and Gheewala, 2013; Silalertruksa et al., 2015). The transportation stages share materials distribution using diesel trucks (Delivand et al., 2011; Nguyen and Gheewala, 2008; Nguyen et al., 2007a). The feedstock preparation stages contain uncomplicated mechanical operations: milling, chopping, drying, etc. These product stages consume relatively low amounts of energy compared to the bioethanol conversion stages (Nguyen et al., 2007b; Nguyen et al., 2008; Silalertruksa and Gheewala, 2013). The unbiased material and energy data of these three product stages can be easily determined using widely available inventory data sources. However, the bioethanol conversion stages of the three feedstocks include distinct process operations. The available inventory data from individual bioethanol plants hold many biased measurements (Silalertruksa and Gheewala, 2009). The bioethanol conversion stage is the most decisive for LCA because, it contributes the majority (60-80%) of the total net energy inputs and environmental impacts (Saga et al., 2010; Silalertruksa and Gheewala, 2009). Therefore, the goal of this study is to evaluate LCA with unbiased process data of bioethanol conversion stages using the process simulation technique. Thus, process simulation can facilitate unbiased analysis of net energy balance, life cycle environmental impacts, and sensitivity parameters.

Recent studies have conducted individual environmental assessments on bioethanol production from cassava, cane molasses, and rice straw (Papong and Malakul, 2010; Silalertruksa and Gheewala, 2013; Silalertruksa et al., 2017). Few studies in the literature compared bioethanol production from cassava and cane molasses (Silalertruksa and Gheewala, 2009). The existing assessments are based on individual plant designs, unequal unit bases, and different impact assessment methods as well as distinctive scenarios on different feedstocks. For example, bioethanol conversion processes from cane molasses and rice straw are fueled by renewable biowaste/biogas recovery within the same process (Silalertruksa and Gheewala, 2013; Silalertruksa et al., 2017). In contrast, bioethanol conversion from cassava has utilized non-renewable fuels (Papong and Malakul, 2010). The variations in process fuel type, waste recovery practices, and biased process data can lead to an unfair LCA comparison among different feedstock processes. No study has been reported on the unbiased LCA comparison of bioethanol production from cassava, cane molasses, and rice straw using the process simulation technique. Therefore, this paper introduces the usability of the process simulation technique for LCA. In this study, the unbiased process data from chemical process simulations with an equal unit basis, unvarying impact assessment method, and minimum variations in fuel type/waste recovery provide a method to conduct a fair comparison among the three bioethanol processes. In addition, this study shows how the simulation technique can be introduced to design cleaner production processes/scenarios for pre-production/modified process plants in different case studies. Thus, process simulation based LCA in this study can also be applied for a fair comparison of other production processes.

## 2. Materials and methods

### 2.1 Goal and scope definition

This study adopts the ISO 14040/44 framework as the LCA methodology (Guinee, 2002). Figure 1 shows the defined cradle-to-gate system boundary for bioethanol production from cassava, cane molasses, and rice straw. The functional unit (FU) is 1,000 L bioethanol at 99.7 vol% purity for all inventory calculations. The cultivation yields (kg/ha), feedstock inputs (kg/1,000 L), and inventory data for cultivation, transportation, and feedstock preparation stages of the three bioethanol feedstocks are selected from referenced data sources (years 2007-2017) related to Thailand, as shown in Table S1 in the supplementary material. Inventory calculations consider real proportions of the feedstock used for bioethanol production in each product stage. The cultivation yield of cassava is entirely utilized for bioethanol production. However, cane molasses is a co-product of sugar manufacturing using sugarcane harvest. Hence, an allocation factor of 0.23 is used to calculate the inventory data for cultivation, transportation, and feedstock preparation stages of bioethanol from cane molasses (Silalertruksa and Gheewala, 2009). Rice straw is also a by-product from paddy rice cultivation stage, where an allocation factor of 0.13 is applied for inventory data calculations (Silalertruksa and Gheewala, 2013).

Figure 1 (P26)

The data of bioethanol conversion stages are evaluated using chemical process simulations. All inventory results are converted into the FU basis and exported to the SimaPro 8.2 LCA software in order to perform LCA analysis. The ReCiPe midpoint (H) V1.12 method is used for environmental impact assessment (Goedkoop et al., 2008). Environmental impacts are compared among the three bioethanol feedstocks using case-specific normalization, i.e., percentage of division-by-maximum (Norris, 2001). The airborne pollutants ($CO_2$, $SO_2$, $NO_x$, particulates, etc.), waterborne pollutants (nitrates, phosphorous, etc.), and soil pollutants (herbicides/pesticides, heavy metals, etc.) are considered as major life cycle environmental emissions. Unbiased calculations/simulations in this study utilize the following literature based assumptions.

1. The carbon neutral rule is applied for biogenic $CO_2$ emissions (Neamhom et al., 2016).
2. In herbicides/pesticides application, 100% of active ingredients are considered as emissions into agricultural soil, and their toxicity impacts are evaluated using the specified characterization factors in the ReCiPe midpoint (H) V1.12 method (Rosenbaum et al., 2015).
3. Agricultural residues and process wastes from each bioethanol process are reused as much as possible, to manure the same cultivation lands and supply energy for the same process (Numjuncharoen et al., 2015; Silalertruksa and Gheewala, 2011).
4. Human labor and socio-economic influences on the system boundary are excluded, as the study is focused on the environmental perspective (Papong and Malakul, 2010).
5. In the scale of study, negligible effects are considered from the infrastructure processes (Silalertruksa and Gheewala, 2009).
6. Fermentation efficiency at 90% and dehydration efficiency at 99% are maintained for the same degree of bioethanol separation among the three feedstock processes (Sriroth et al., 2010; Yoswathana et al., 2010).
7. Wastewater from all bioethanol processes are treated by upflow anaerobic sludge blanket (UASB) reactors. The $CH_4$ amounts in recovered biogas from each process are calculated using Equation 1 (Moriizumi et al., 2012).

   $$CH_4\ amount = Wastewater\ volume \times COD \times 0.3 \times 0.8 \qquad \text{Equation 1}$$

   Zero wastewater release to the environment is considered, as the treated water is reused for onsite cooling water (Silalertruksa et al., 2017).

8. Recovered biogas from anaerobic treatments are used to cogenerate heat and electricity for the same bioethanol conversion processes. The remainder of the process energy requirements are fulfilled by in-plant energy cogeneration using renewable fuels, such as waste wood chips/rice husks, surplus bagasse/cane trash, and lignin/solid residues, for bioethanol from cassava, cane molasses, and rice straw, respectively (Delivand et al., 2012; Nguyen et al., 2010; Numjuncharoen et al., 2015). Biogas and solid fuels are burned in separate boilers.
9. Surplus electricity after individual plant consumption is credited to Thai grid-mix electricity (Gheewala et al., 2011; Krittayakasem et al., 2011).
10. The environmental credit for avoiding open field burning is cancelled out by the opportunity loss of using for manure, because of applying rice straw for bioethanol production (Silalertruksa and Gheewala, 2013).

## 2.2 Literature based energy and emission calculations

This study assumes that all farming machinery in feedstock cultivation, trucks in road transportation, and post-harvest preparation machines consume diesel as the fuel, according to previous studies in Thailand (Silalertruksa and Gheewala, 2009). The energy of diesel consumption ($E_{Diesel}$) is calculated using Equation 2 (Thailand Environment Institute (TEI), 2001). The diesel volumes for cultivation and post-harvest preparation machines are in the data sources shown in Table S1 in the supplementary material. The diesel volumes for road transportation are calculated using Equation 3.

$$E_{Diesel} = 44.5\ (\mathrm{MJ/L}) \times Diesel\ volume\ (L) \qquad \text{Equation 2}$$

$$Diesel\ volume\ (L) = \frac{Distance\ (km) \times Material\ amount\ (tonne)}{Truck\ fuel\ economy\ \left(\frac{km}{L}\right) \times Truck\ capacity\ (tonne)} \qquad \text{Equation 3}$$

Many agrochemicals for feedstock cultivation and enzymes/chemicals for bioethanol conversion are imported materials to Thailand (Silalertruksa and Gheewala, 2009). Energy consumption for their production are retrieved from foreign databases, as listed in Table S2 in the supplementary material. Average energy consumption for nautical transportation ($E_{Nautical}$) from foreign countries to Thailand is calculated using Equation 4 (Papong and Malakul, 2010).

$E_{Nautical}$ = 6,000 (km) × 0.08 (MJ/tonne-km) × *Material amount (tonne)* Equation 4

Emissions to air, water, and soil from agrochemicals application in the cultivation stages are calculated, based on the methodology shown in Tables S3 and S4 in the supplementary material (Agri-footprint, 2015). Table S5 in the supplementary material lists the factors to calculate emissions from combustion of transportation fuels.

## 2.3 Process simulation based data

### 2.3.1 Process simulations of bioethanol conversion stages

Bioethanol conversion processes from prepared feedstocks to the final product are separately modeled in the Aspen Plus V 9.0 (2016) process simulation software. All simulations of the bioethanol conversion processes from cassava, cane molasses, and rice straw utilize the RadFrac rigorous distillation column model for distillation processes, the R-Stoic reactor model for simultaneous saccharification and fermentation (SSF) operations, including other utility equipment models. The NRTL (non-random-two-liquid) thermodynamic property method is applied for all simulations at standard operating conditions of actual bioethanol plants. Table S6 in the supplementary material indicates the feedstock compositions, operating conditions, and the chemical reactions applied in simulations. After fermentation operations, extractive distillation with ethylene glycol is selected for bioethanol dehydration to purify bioethanol to 99.7 vol% (Kumar et al., 2010). The simulation results, including ethylene glycol make-up flow (as the net input), and process energy are used in LCA evaluation.

### 2.3.2 Process energy calculations

The simulated process energy requirements are supplied using combined heat and power (CHP) cogeneration, which is an efficient and cleaner energy production technique (Nielsen et al., 2010). The amounts of process energy generation are calculated based on efficiencies of the cogeneration units and average heating values of the selected fuels, indicated in Table S7 in the supplementary material. The emissions from cogeneration are calculated using the factors listed in Table S8 in the supplementary material.

## 2.4 Scenario description

### (a) Base case

The defined system boundary in Section 2.1 is considered as the base case of bioethanol production for the three feedstocks in this study. The key feature of the base case is, the entire process energy supply using biofuels. Biogas from wastewater treatment can supply a portion of the required process energy for all three bioethanol conversion stages. The remaining process energy requirements can be fulfilled using surplus bagasse with cane trash for bioethanol from cane molasses (Silalertruksa et al., 2017), and using lignin with solid residues for bioethanol from rice straw (Delivand et al., 2012). However, bioethanol conversion from cassava requires an external biofuel like waste wood chips/rice husks in order to satisfy the full mode of renewable process energy in the base case. Thus, wood chips/rice husks transportation to the factory consumes an additional amount of diesel. In addition to the base case, two other scenarios (Scenarios 1 and 2) are considered by making a total of 9 different scenarios to conduct comprehensive LCA. Unbiased alterations are applied to the base cases of the three feedstock processes to obtain Scenarios 1 and 2 for a fair comparison.

### (b) Scenario 1 for non-renewable process energy supply

Many existing bioethanol production plants still rely on coal as the primary fuel for process energy (Nguyen et al., 2008; Papong and Malakul, 2010; Silalertruksa and Gheewala, 2009). Hence, Scenario 1 replaces the solid biofuels with lignite coal to supply process energy for bioethanol conversion stages of the three feedstocks. Process energy from biogas and other inventory in the base case are remained unchanged. In this study, Scenario 1 of cassava, and base cases of cane molasses and rice straw represent the fuel type used in existing bioethanol plants.

### (c) Scenario 2 for waste recovery and toxicity evaluation

Agricultural residues and process wastes, such as cassava stems/leaves, 50% cane trash, vinasse, filter cake, and gypsum from the three bioethanol processes are reused as organic manure in the base case. The calculations show that they can replace an average of 10% of chemical fertilizers for individual feedstock cultivations (Silalertruksa et al., 2017; Trivelin et al., 2013). In many LCA studies, the herbicides/pesticides emissions into agricultural soil are excluded from the emissions inventory due to the absence of a consistent life cycle toxicity evaluation model (Rosenbaum et al., 2015). Therefore, Scenario 2 is considered with 10% of the chemical fertilizers replaced by organic wastes, and zero herbicides/pesticides emissions in all three feedstock processes. Scenario 2 can also be considered as a sustainability improvement option for the cultivation stages of all feedstocks.

## 3. Results and discussion

### 3.1 Process simulation results

Figure 2 illustrates the detailed material flow diagrams of bioethanol production from (a) cassava, (b) cane molasses, and (c) rice straw. The diagrams show the results for material/resource inventory flows related to all product stages (basis: 1,000 L at 99.7 vol%). The major material/resource inventory flows are summarized in Table S9 in the supplementary material. The material/resource utilization by the three feedstock processes are compared. The comparison shows that in the cultivation stages, cassava conserves herbicides/pesticides and diesel for farming machinery, and rice straw saves agricultural land, crop water, and fertilizers. However, cane molasses consumes relatively large amounts of materials/resources in the cultivation, transportation, and feedstock preparation stages. The inventory results of cane molasses feedstock preparation includes the allocated share of process energy consumption to generate sugar rich syrup (pH adjusted and purified) after the final centrifuge operation in the sugar refinery process. The dash lines in Figure 2 demark the boundaries of bioethanol conversion stages that are evaluated using process simulations.

Figure 2(a), Figure 2(b), Figure 2(c) (P27-P29)

The detailed process simulation flowsheets for bioethanol conversion stages from (a) cassava, (b) cane molasses, and (c) rice straw are shown in Figure S1 in the supplementary material. The simulation results for energy consumption by individual process operations are also classified in Tables S10 to S12 in the supplementary material. The simulation based total process energy consumption is, 12,986 MJ for cassava, 18,868 MJ for cane molasses, and 23,170 MJ for rice straw, to produce 1,000 L bioethanol at 99.7 vol%. The results are compared with referenced LCA studies related to different locations and bioethanol feedstocks (years 2007-2017) as shown in Table S13 in the supplementary material. The simulated process energy results in this study approximate the actual plant data reported for bioethanol from: cassava (Liu et al., 2013; Silalertruksa and Gheewala, 2009), cane molasses (Nguyen et al., 2008; Silalertruksa and Gheewala, 2009), and rice straw (Saga et al., 2010). The use of energy efficient bioethanol separation technologies, such as SSF, extractive distillation, pretreatment at low temperatures, in simulations of this study have resulted in slightly decreased process energy consumption, compared to some case studies (Khatiwada et al., 2016; Papong and Malakul, 2010; Silalertruksa and Gheewala, 2013). Nonetheless, the simulated process energy results in this study are within the process energy data ranges reported in the literature, i.e., 10,000-20,000 MJ for cassava, 15,000-27,000 MJ for cane molasses, and 10,000-30,000 MJ for rice straw, irrespective of location/yield parameter variations (Khatiwada and Silveira, 2009; Le et al., 2013; Soam et al., 2016). Therefore, the reliability of the process simulation technique in this study is validated to obtain unbiased process data for a fair LCA evaluation.

The unbiased material/energy results from process simulations, along with other inventory results, are analyzed for energy efficiency, renewability, and environmental impacts. The comprehensive LCA covers the results and discussion: 3.2 net energy analysis, 3.3 environmental impact assessment, 3.4 environmental emissions and hotspot analysis, and 3.5 sensitivity analysis.

### 3.2 Net energy analysis

Table 1 indicates the net energy balance for the base cases of bioethanol production from the three feedstocks. The total net energy inputs are, 17,716 MJ for cassava, 29,260 MJ for cane molasses, and 29,797 MJ for rice straw (basis: 1,000 L at 99.7 vol%). The results exhibit that cassava only consumes around 60% of the total net energy inputs with respect to cane molasses and rice straw. The results also show that the total process energy consumption is 73.3%, 64.5%, and 77.8% of the total net energy input for bioethanol from cassava, cane molasses, and rice straw, respectively. Bioethanol conversion from rice straw is more energy intensive than other feedstocks due to the energy consumption in pretreatment operations. The energy performance indicators, such as net energy value (NEV), net energy ratio (NER), net renewable energy value (NRnEV), and renewability (Rn) are calculated for all scenarios in Table 1, to study the energy performance of the three feedstock processes.

Table 1 (P31)

The results in Table 1 show that the base cases of bioethanol from cassava and cane molasses have net energy gains, with positive values of NEV (5,733 MJ and 2,774 MJ) and NER > 1 (1.32 and 1.09). In contrast, bioethanol from rice straw indicates a net energy loss, implied by NER < 1 (0.85). However, all three feedstocks display renewability gains in the base case, denoted by positive NRnEV and Rn > 1. The 100% use of renewable process energy is the key reason for the renewability gains. Despite the additional diesel consumption for wood chips/rice husks transportation, bioethanol from cassava demonstrates an enhanced renewability of 4.96, which is above 1.5 times greater than that of other two feedstock processes. The non-renewable energy shares relative to the total net energy inputs in the base cases, are 26.7%, 35.5%, and 22.2% for bioethanol from cassava, cane molasses, and rice straw, respectively. Even though the non-renewable energy share is high for bioethanol from cane molasses, there is a greater NRnEV in the base case due to the surplus energy from bagasse and cane trash.

In Scenario 1, all energy indicators drop off as a result of the lignite coal usage for process energy. The results show that cassava can still hold a net energy gain (NER>1) while cane molasses and rice straw undergo net energy losses. Cassava shows a renewability gain of Rn = 1.21) in Scenario 1, where cane molasses obtains almost complete renewability (Rn ≈ 1. In Scenario 2, the energy indicator results of all feedstocks exhibit increased values compared to the base case. Bioethanol from cassava in Scenario 2 obtains the best values of 1.34 for NER and 5.16 for Rn.

Energy indicator results of all scenarios in this study show improved NER and Rn for cassava compared to related studies in the literature. The NER and Rn for Scenario 1 of cassava approximate the values of actual bioethanol plants reported in (Papong and Malakul, 2010) and (Silalertruksa and Gheewala, 2009), respectively. However, the NER and Rn for the base case and Scenario 2 of cassava are greater than the values reported in the literature. In addition, bioethanol production from cassava in this study demonstrates an enhanced renewability, relative to LCA studies of many other first generation bioethanol feedstocks, such as cane molasses, maize, sugar beet, and sweet potato (Foteinis et al., 2011; Persson et al., 2009; Silalertruksa and Gheewala, 2009; Wang et al., 2013). Assessments in the literature reported that cane molasses and rice straw are more energy efficient and renewable bioethanol feedstocks than cassava (Silalertruksa and Gheewala, 2009; Silalertruksa and Gheewala, 2013). Comparison among individual studies on different bioethanol feedstocks is unfair due to availability of many biased parameters. Hence, the process simulation based energy analysis in this study provides useful findings for decision making, i.e., the effect of biased parameters on different processes, unbiased feedstock selection, cleaner process designs, etc.

### 3.3 Environmental impact assessment

Table 2 indicates the scenario-based environmental impact results of ten major impact categories for bioethanol production from cassava, cane molasses, and rice straw (basis: 1,000 L at 99.7 vol%). The results show that cassava in the base case with renewable process energy contributes low environmental impacts, compared to cane molasses and rice straw. Starting with the base case of cassava, the climate change, acidification, and fossil depletion impacts are 425.1 kg $CO_2$ eq, 7.0 kg $SO_2$ eq, and 93.7 kg oil eq, respectively. The results of Scenario 1 in Table 3 show that non-renewable fuels for process energy increase many environmental impacts. For example, the climate change, acidification, and fossil depletion impacts in Scenario 1 of bioethanol from cassava are increased to 1,703.6 kg $CO_2$ eq, 24.9 kg $SO_2$ eq, and 437.6 kg oil eq, respectively. Unlike in the base case, cane molasses shows a lesser climate change impact of 1,637.1 kg $CO_2$ eq in Scenario 1, compared to that of cassava. One of the reasons for this lesser climate change impact is the relatively low amount of lignite coal utilization in Scenario 1 by cane molasses. Eutrophication and ecotoxicity are the only impact categories that show insignificant changes in Scenario 1 compared to the base case.

Table 2 (P32)

Results in Table 2 show that the extent of agrochemicals application in the feedstock cultivation stages is also a key factor for toxicity impacts. The toxicity impacts of all feedstock processes drastically decrease in Scenario 2 due to zero herbicides/pesticides emissions, compared to the base case. For the case of bioethanol from rice straw, the toxicity impacts are diminished in Scenario 2, i.e., human toxicity from 81.2 to 31.3 kg 1,4-DB eq, terrestrial ecotoxicity from 371.8 to 0.4 kg 1,4-DB eq, and freshwater ecotoxicity from 60.1 to 1.2 kg 1,4-DB eq. Hence, this study suggests a way to evaluate the net toxicity potentials of herbicides/pesticides emissions in LCA rather than the conventional method of excluding them from the emissions inventory. In addition, Scenario 2 shows a considerable decrease in eutrophication impacts due to the chemical fertilizer being replaced by organic wastes. For bioethanol from cane molasses in Scenario 2, the freshwater eutrophication decreases from 1.0 to 0.9 kg P eq, and marine eutrophication decreases from 10.5 to 9.5 kg N eq.

This study has identified the environmental benign potentials of bioethanol production from cassava, cane molasses, and rice straw with unbiased scenarios of fuel type and waste recovery, compared to the literature. The climate change impact (410 kg $CO_2$ eq/1,000 L) for bioethanol from cassava in Scenario 2 is the most environmental benign, relative to many LCA studies on different bioethanol feedstocks (Foteinis et al., 2011; Garcia et al., 2011; Le et al., 2013; Macedo et al., 2008; Persson et al., 2009; Wang et al., 2013). The climate change impacts in Scenario 1 of cassava and cane molasses are also less severe compared to the results from similar studies that used coal as a process fuel (Nguyen et al., 2008; Papong and Malakul, 2010). The impact results for bioethanol from cane molasses in this study are close to those reported in (Silalertruksa et al., 2017) with the ReCiPe impact assessment method. However, most of the individual assessments in the literature have followed different impact assessment methods (CML, IMPACT 2002+, etc.), and the impact results are not comparable among cassava, cane molasses, and rice straw. Hence, this study offers an unbiased comparison of environmental assessments among the three production processes with cleaner bioethanol plant designs using the process simulation technique.

Figure 3 shows the relative environmental impacts for the base case of bioethanol production from cassava, cane molasses, and rice straw. The relative impacts were obtained by computing the percentage of division-by-maximum for the impact results in Table 3. The results indicate that all the relative impacts for the base case of bioethanol from cassava are less than 80%. Bioethanol from cane molasses has the highest severities (100%) of freshwater eutrophication, human toxicity, photochemical oxidant formation, and fossil depletion. Meanwhile, bioethanol from rice straw shows the most severe climate change, acidification, and terrestrial ecotoxicity impacts in the base case. The severities of climate change impacts in the base cases of cassava and cane molasses are 28% and 37%, relative to rice straw, respectively. The environmental impact variations among the three feedstocks can be correlated to the inventory results, using the environmental emissions and hotspot analysis.

Figure 3 (P30)

### 3.4 Environmental emissions and hotspot analysis

Table 3 presents the total inventory results of major environmental emissions from the three scenarios of bioethanol production from cassava, cane molasses, and rice straw on the basis of 1,000 L at 99.7 vol%. Bioethanol from cassava in the base case shows comparatively lower emission levels than other two feedstocks. The relatively low greenhouse gas emission levels, ($CO_2$ of 230.7 kg, $CH_4$ of 1.2 kg, $N_2O$ of 0.6 kg, and $NH_3$ of 2.1 kg) have low climate change impacts in the base case of cassava. In contrast, bioethanol from rice straw in the base case generates excessive greenhouse gas emissions, i.e., $CH_4$ of 46.1 kg, $N_2O$ of 0.9 kg, and $NH_3$ of 7.7 kg, corresponding to a high climate change impact. In rice straw cultivation, $CH_4$ is formed under anaerobic conditions of flooded paddy rice fields, and $N_2O$ and $NH_3$ are released due to nitrification processes after fertilizers application. The majority of $CO_2$, $NO_x$, and $SO_2$ emissions in the base cases originate from diesel burning in farming and transportation operations. The relatively lowest emissions of $NO_x$ (2.8 kg) and $SO_2$ (0.3 kg) in the base case of bioethanol from cassava are the reasons for the low terrestrial acidification impact.

Table 3 (P33)

The results exhibit unfavourable $CO_2$, $NO_x$, and $SO_2$ emissions in Scenario 1 of bioethanol from all three feedstocks. For example, the $CO_2$, $NO_x$, and $SO_2$ emissions of bioethanol from cassava increase to 1,445.3 kg, 9.4 kg, and 14.5 kg, respectively. The amount of lignite coal burned for process energy is the hotspot for increasing the $CO_2$, $NO_x$, and $SO_2$ emissions. In comparison, cane molasses shows a lower $CO_2$ emission of 1343.3 kg in Scenario 1 that causes a lower climate change impact than cassava. The particulates and NMVOC levels are lower in Scenario 1 than those due to biomass combustion for process energy in the base case. However, the increased levels of $NO_x$ and $SO_2$ emissions in Scenario 1 cause increased photochemical oxidant formation and particulate matter formation for all feedstocks. The results also show that the nitrates and phosphorus emission levels in Scenario 2 of all feedstock processes decrease, compared to the base case. Hence, the nitrates and phosphorus emissions from chemical fertilizers application have major contributions to the eutrophication impacts. The herbicides/pesticides application, as well as heavy metals leaching from chemical fertilizers, are the major environmental hotspots for toxicity impacts.

The scenario-based impact assessment and emissions/hotspot analysis clearly investigated the effect of biased settings with fuel type and waste recovery practices for a fair LCA comparison of different bioethanol processes. The uncertainty parameters also lead to divergences in energy efficiency, renewability, and environmental impacts. Thus, life cycle consequences due to variations in uncertainty parameters are discussed using sensitivity analysis.

### 3.5 Sensitivity analysis

The process simulation based LCA can facilitate the unbiased sensitivity analysis even for multiple scenarios of different processes. In this study, sensitivity analysis is performed for the base case by varying three major uncertainty parameters, i.e., cultivation yield (tonne/ha), bioethanol yield (L/tonne), and process energy consumption (MJ/1,000 L). The uncertainty parameters and their ranges for sensitivity analysis are determined, based on the actual data reported in the literature (Table S13 in the supplementary material). These parameter ranges and their integrated emissions in each bioethanol process are defined in SimaPro 8.2 LCA software and decreased/increased accordingly for sensitivity analysis.

Table 4 indicates the sensitivity results of environmental impacts, NER, and renewability for parameter variations in the base case. The cultivation yield holds the highest uncertainty, and the corresponding variation shows wide impact ranges for all three bioethanol processes. For example, bioethanol from cassava in the base case shows a climate change impact range of 360-569 kg $CO_2$ eq/1,000 L for cultivation yield variation. However, the corresponding sensitivity range is 394-506 kg $CO_2$ eq/1,000 L for bioethanol yield variation and 418-427 kg $CO_2$ eq/1,000 L for process energy variation. Thus, high sensitivity to cultivation yield implies that the majority of environmental impacts of the base case in this study originate from the feedstock cultivation stages.

Table 4 (P34)

Sensitivity analysis in this study also evaluates the effect of biased settings (process data, fuel type, waste recovery) in uncertainty parameters on environmental impacts, NER and renewability. The results show that the bioethanol yield variation leads to the second highest sensitivity, and the variations in process energy consumption show narrow environmental impact ranges in the base case. Hence, utilization of 100% renewable process energy has decreased the sensitivity of process energy parameter towards the environmental impacts. Nevertheless, the results exhibit high fluctuations in NER when process energy consumption is varied. A process energy decrease from 20,000 to 10,000 MJ/1,000 L for bioethanol from cassava improves the NER from 0.86 to 1.79. In addition, all parameter variations in the base cases of the three feedstocks obtain similar sensitivity ranges for the renewability. Collaborative improvements in both yield and process energy efficiencies are recommended, to further promote the renewability. Thus, the process simulation based LCA in this study contributes effective decision making (cleaner process designs, feedstock selection, etc.) for sustainable bioethanol production, in terms of energy and environmental perspectives.

## Conclusion

This study shows that the process simulation technique effectively provides an unbiased LCA comparison of different processes. The simulation results, compared with actual data in referenced studies, validate the reliability of the technique. The unbiased LCA analysis reveals useful findings for cleaner bioethanol production from cassava, cane molasses, and rice straw. From the unbiased comparison, cassava is the most energy efficient, renewable, and environmentally benign bioethanol feedstock, followed by cane molasses, and finally, rice straw. The relatively low levels of materials utilization, energy consumption, and environmental emissions in the inventory with reduced biased parameters cause cassava to be a superior bioethanol feedstock. Renewable process energy, enhanced waste recovery, and green manuring with low herbicides/pesticides inputs are recommended to promote renewability and mitigate the environmental impacts of bioethanol production from all three feedstocks. This study contributes decision making for the sustainability of future bioethanol industry with cleaner production designs, i.e., feedstock selection from unbiased energy and environmental perspectives, renewable fuels for process energy cogeneration, options for maximum waste recovery, energy efficient ethanol conversion technologies, etc. The process simulation technique developed in this study can also be applied to other case studies on different processes/feedstocks, in order to obtain new/modified plant designs and unbiased inventory data for LCA analysis.

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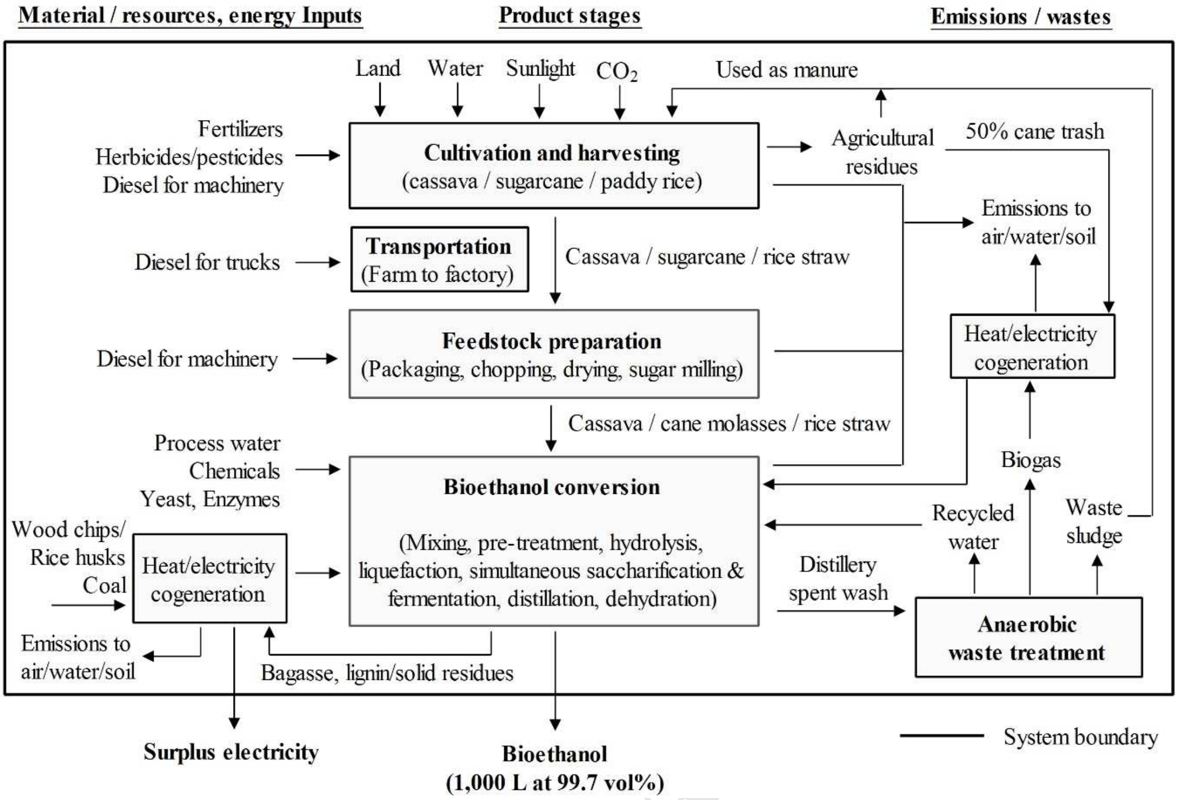


Figure 1: Cradle-to-gate system boundary for bioethanol production

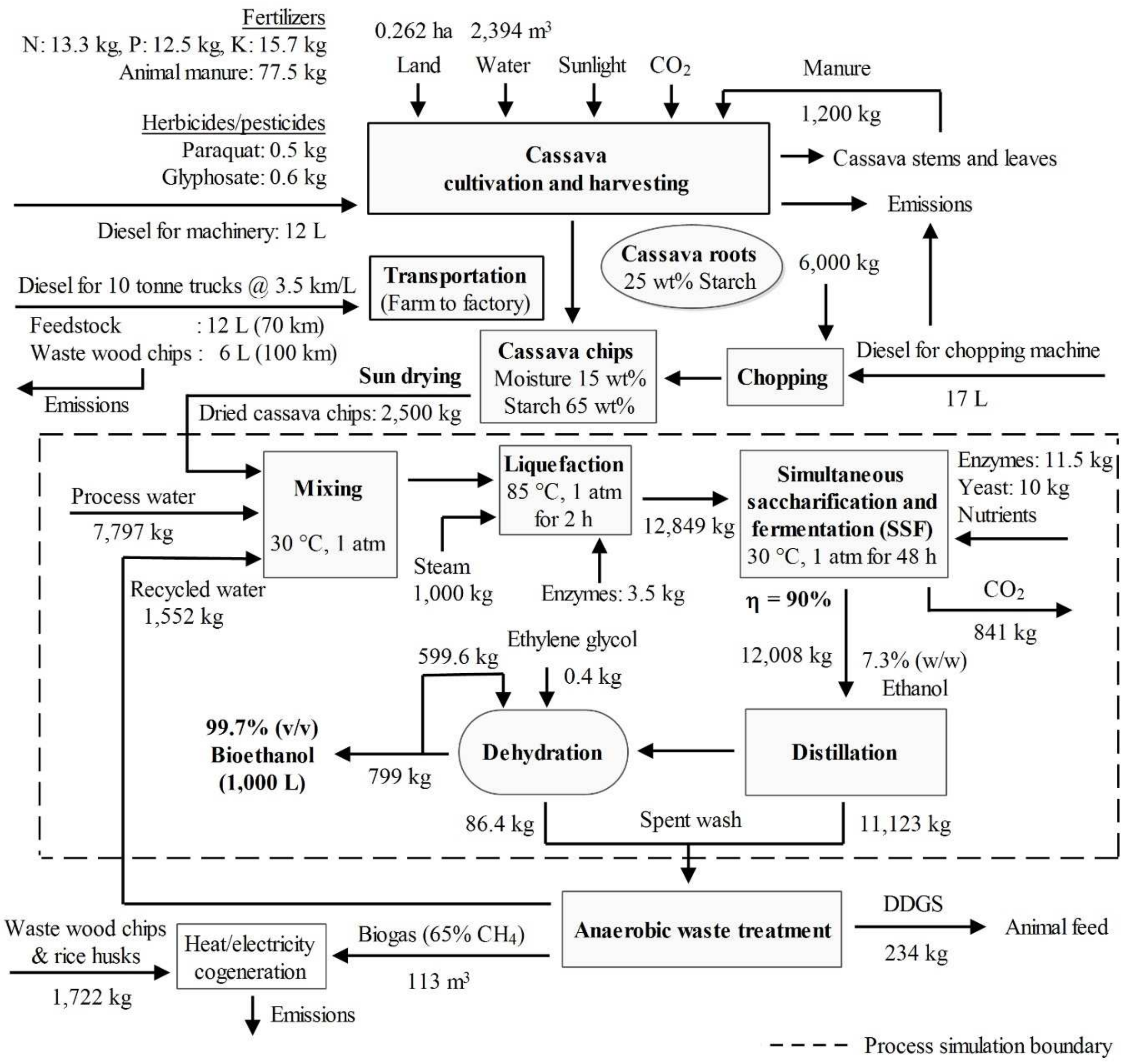
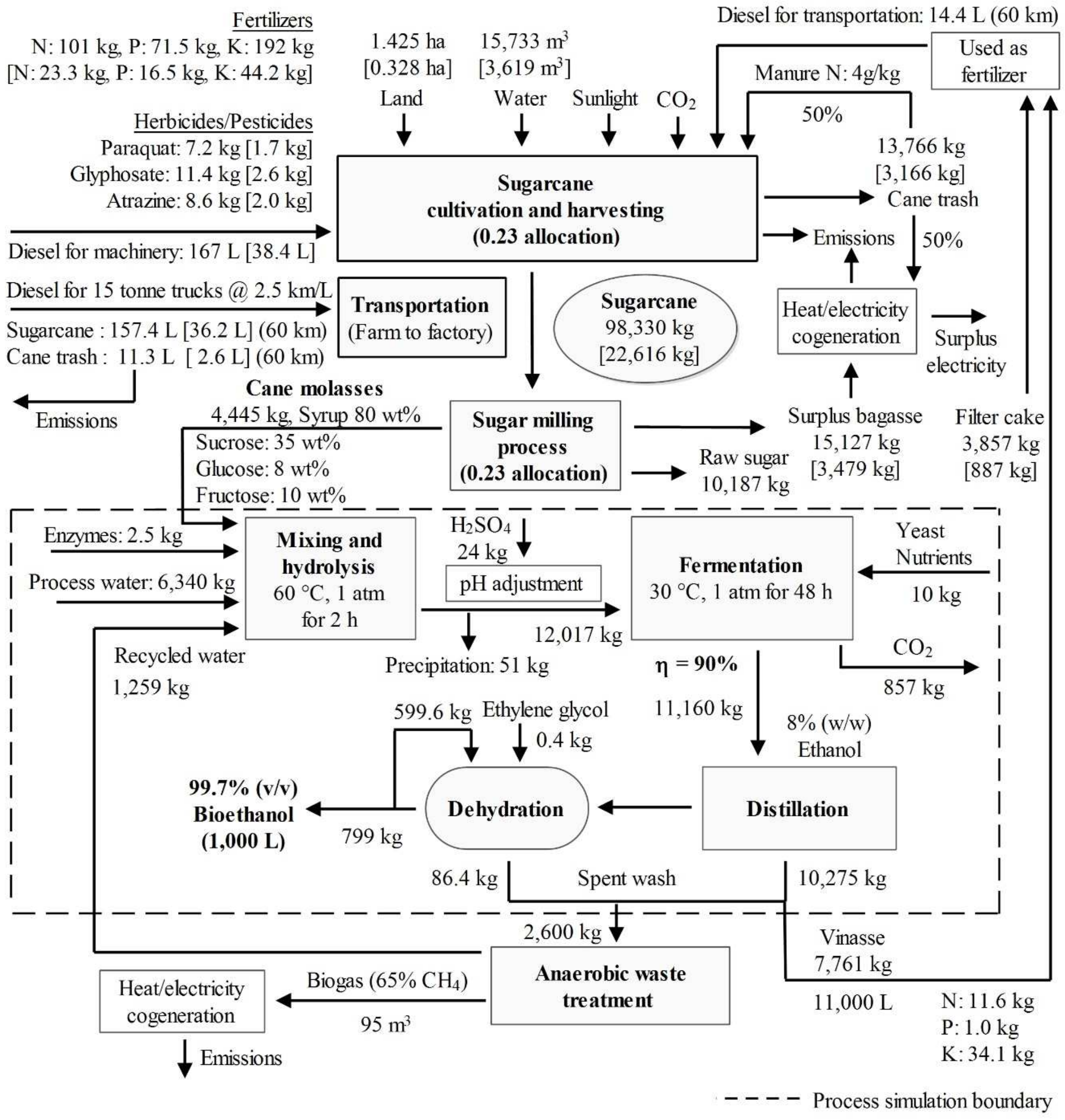


Figure 2(a): Material flow diagram for base case of bioethanol from cassava

(Basis: 1,000 L at 99.7 vol%)



Note: [ ] Values in brackets are the data with 0.23 allocation for cane molasses

Figure 2(b): Material flow diagram for base case of bioethanol from cane molasses

(Basis: 1,000 L at 99.7 vol%)

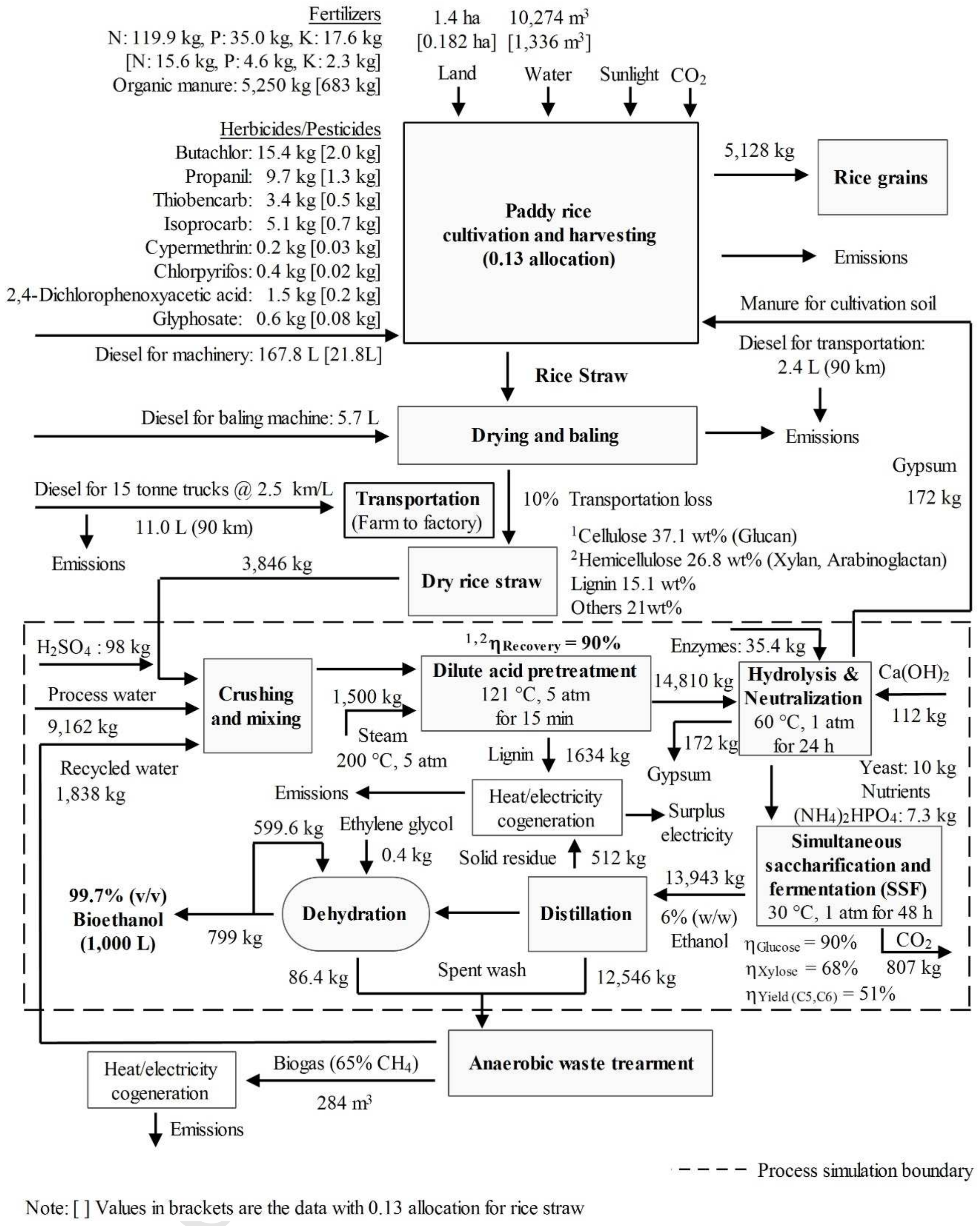


Figure 2(c): Material flow diagram for base case of bioethanol from rice straw

(Basis: 1,000 L at 99.7 vol%)

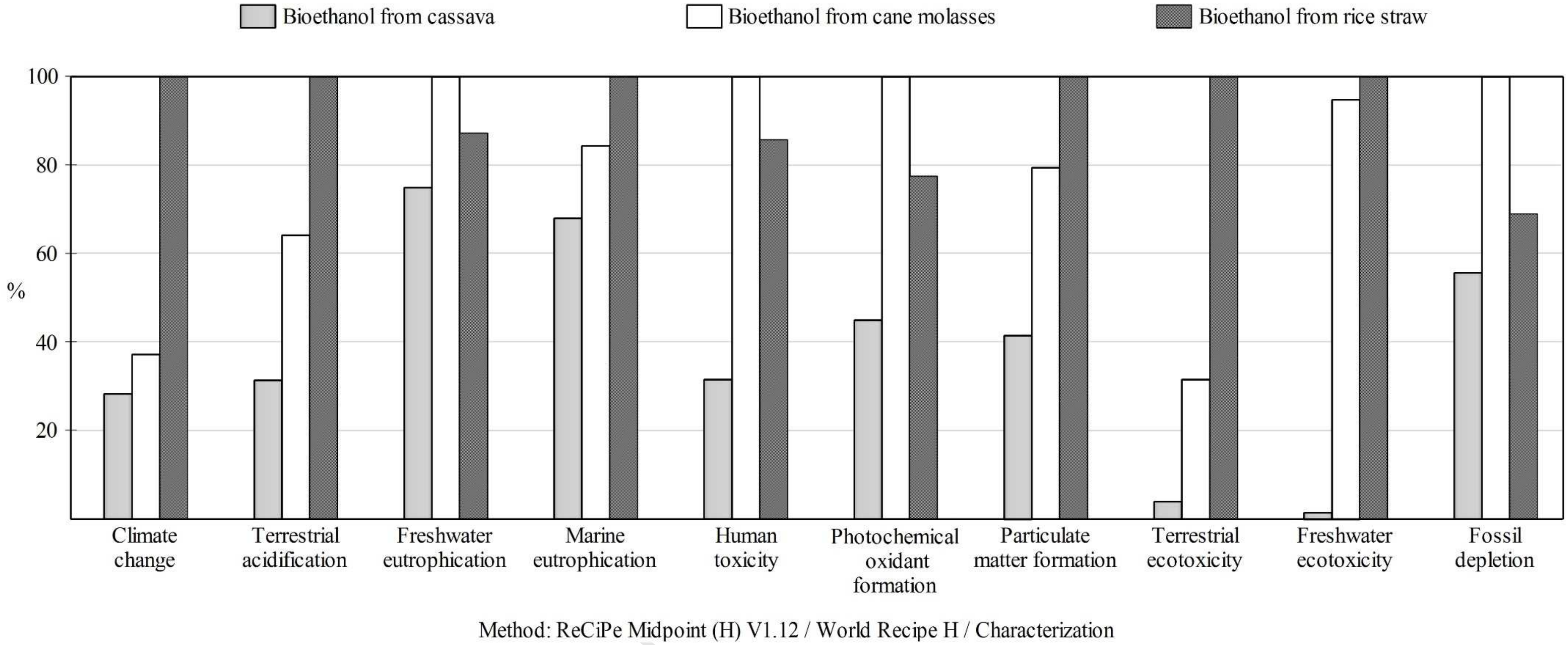


Figure 3: Relative environmental impacts for base case of bioethanol from cassava, cane molasses, and rice straw

Table 1: Energy analysis for base case and scenarios (basis: 1,000 L bioethanol at 99.7 vol%)

| Energy input/output | Cassava | | Cane molasses | | Rice straw | |
|---|---|---|---|---|---|---|
| (All units are in MJ) | Total | Non-renewable | Total | Non-renewable | Total | Non-renewable |
| <u>Cultivation stage</u> | | | | | | |
| Fertilizers (NPK, manure) | 1,881 | 1,881 | 3,893 | 3,893 | 1,785 | 1,785 |
| Herbicides/pesticides | 501 | 501 | 2,343 | 2,343 | 1,806 | 1,806 |
| Farm machinery | 534 | 534 | 1,709 | 1,709 | 970 | 970 |
| <u>Transportation stage</u> | | | | | | |
| Feedstock transportation | 534 | 534 | 1,849 | 1,611 | 489 | 489 |
| Process fuel/waste transportation | 267 | 267 | 757 | 757 | 107 | 107 |
| <u>Feedstock preparation stage</u> | | | | | | |
| Preparation operations | 757 | 757 | 9,277[a] | | 254 | 254 |
| <u>Bioethanol conversion stage</u> | | | | | | |
| Chemicals | 256 | 256 | 81 | 81 | 1,216 | 1,216 |
| Energy production | | | | | | |
| Steam | 11,929 | | 23,764 | | 21,014 | |
| Electricity | 3,306 | | 5,936 | | 6,244 | |
| Energy consumption[a] | | | | | | |
| Steam[a] | 9,680[a] | | 6,514[a] | | 17,467[a] | |
| Electricity[a] | 3,306[a] | | 2,837[a] | | 5,703[a] | |
| Surplus energy | | | | | | |
| Steam | 2,249 | | 7,973 | | 3,547 | |
| Electricity | | | 2,861 | | 541 | |
| Total net energy inputs | 17,716 | 4,730 | 29,260 | 10,394 | 29,797 | 6,627 |
| Total net energy outputs[b] | 23,449 | | 32,034 | | 25,288 | |
| Total net bioenergy outputs[c] | 23,449 | | 32,034 | | 25,288 | |

| Indicator | Cassava | | | Cane molasses | | | Rice straw | | |
|---|---|---|---|---|---|---|---|---|---|
| | Base case | Scenario 1 | Scenario 2 | Base case | Scenario 1 | Scenario 2 | Base case | Scenario 1 | Scenario 2 |
| NEV[d] (MJ) | 5,733 | 1788 | 5,921 | 2,774 | (-9,826) | 3,163 | (-4,509) | (-11,490) | -4,331 |
| NRnEV[e] (MJ) | 18,719 | 3,607 | 18,907 | 21,640 | 980 | 22,029 | 18,661 | (-6,918) | 18,840 |
| NER[f] | 1.32 | 1.09 | 1.34 | 1.09 | 0.68 | 1.11 | 0.85 | 0.65 | 0.85 |
| Rn[g] | 4.96 | 1.21 | 5.16 | 3.08 | 1.05 | 3.20 | 3.82 | 0.75 | 3.92 |

Energy content of bioethanol = 21,200 MJ/1,000 L bioethanol (Silalertruksa and Gheewala, 2009).

[a] Process simulation based energy results.

[b] Total net energy outputs = 21,200 MJ + surplus energy

[c] Total net bioenergy outputs = 21,200 MJ + surplus bioenergy

[d] NEV = total net energy outputs – total net energy inputs.

[e] NRnEV = total net bioenergy outputs – total net fossil energy inputs.

[f] NER = net energy outputs/net energy inputs.

[g] Rn = total net bioenergy outputs/total net fossil energy inputs.

Table 2: Scenario-based environmental impacts (basis: 1,000 L bioethanol at 99.7 vol%)

| Impact category | Units | Base case | | | Scenario 1 | | | Scenario 2 | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | Cassava | Cane molasses | Rice straw | Cassava | Cane molasses | Rice straw | Cassava | Cane molasses | Rice straw |
| Climate change | kg $CO_2$ eq | 425.1 | 558.1 | 1,501.9 | 1,703.6 | 1,637.1 | 3,660.7 | 410.2 | 505.7 | 1,488.7 |
| Terrestrial acidification | kg $SO_2$ eq | 7.0 | 14.3 | 22.2 | 24.9 | 25.6 | 51.9 | 6.6 | 13.4 | 21.8 |
| Freshwater eutrophication | kg P eq | 0.7 | 1.0 | 0.8 | 0.7 | 1.0 | 0.8 | 0.7 | 0.9 | 0.8 |
| Marine eutrophication | kg N eq | 8.5 | 10.5 | 12.4 | 8.7 | 10.6 | 12.9 | 8.0 | 9.5 | 11.3 |
| Human toxicity | kg 1,4-DB eq | 30.0 | 94.7 | 81.2 | 38.1 | 100.6 | 94.8 | 24.2 | 72.1 | 31.3 |
| Photochemical oxidant formation | kg NMVOC | 3.1 | 6.9 | 5.3 | 10.8 | 11.0 | 17.9 | 3.1 | 6.6 | 5.3 |
| Particulate matter formation | kg PM10 eq | 2.1 | 4.1 | 5.2 | 5.8 | 6.1 | 10.9 | 2.1 | 3.9 | 5.1 |
| Terrestrial ecotoxicity | kg 1,4-DB eq | 15.0 | 117.3 | 371.8 | 15.0 | 117.3 | 371.8 | 0.2 | 0.3 | 0.4 |
| Freshwater ecotoxicity | kg 1,4-DB eq | 0.9 | 57.0 | 60.1 | 0.9 | 57.0 | 60.1 | 0.3 | 0.6 | 1.2 |
| Fossil depletion | kg oil eq | 93.7 | 168.1 | 116.0 | 437.6 | 437.2 | 692.8 | 90.0 | 152.9 | 113.4 |

Table 3: Major environmental emissions (basis: 1,000 L bioethanol at 99.7 vol%)

| Emissions | Base case | | | Scenario 1 | | | Scenario 2 | | |
|---|---|---|---|---|---|---|---|---|---|
| (All units are in kg) | Cassava | Cane molasses | Rice straw | Cassava | Cane molasses | Rice straw | Cassava | Cane molasses | Rice straw |
| $CO_2$ | 230.7 | 307.8 | 217.5 | 1,445.3 | 1,343.3 | 2,270.8 | 224.6 | 272.1 | 214.4 |
| CO | 2.1 | 3.6 | 4.0 | 1.9 | 2.9 | 3.4 | 2.1 | 3.5 | 4.0 |
| $CH_4$ | 1.2 | 1.5 | 46.1 | 1.3 | 1.5 | 46.2 | 1.2 | 1.4 | 46.1 |
| $NO_x$ | 2.8 | 6.3 | 4.3 | 9.4 | 9.7 | 15.0 | 2.8 | 6.1 | 4.3 |
| $N_2O$ | 0.6 | 0.7 | 0.9 | 0.6 | 0.7 | 0.9 | 0.5 | 0.7 | 0.8 |
| $NH_3$ | 2.1 | 3.6 | 7.7 | 2.1 | 3.6 | 7.7 | 1.9 | 3.4 | 7.5 |
| $SO_2$ | 0.3 | 1.8 | 1.0 | 14.5 | 11.3 | 24.6 | 0.3 | 1.8 | 1.0 |
| NMVOC[a] ($\times 10^{-3}$) | 171.3 | 190.3 | 285.2 | 123.3 | 180.4 | 183.9 | 170.1 | 168.6 | 284.5 |
| Particulates ($\times 10^{-3}$) | 818.7 | 1,230.4 | 1,590.3 | 303.3 | 724.6 | 478.4 | 816.1 | 1,216.5 | 1,589.1 |
| Heavy metals ($\times 10^{-3}$) | 41.8 | 104.5 | 43.5 | 43.6 | 105.8 | 46.5 | 37.9 | 94.8 | 39.6 |
| Herbicides/Pesticides | 1.1 | 6.2 | 4.8 | 1.1 | 6.2 | 4.8 | - | - | - |
| Nitrate | 35.5 | 43.1 | 50.2 | 35.5 | 43.1 | 50.2 | 33.7 | 38.8 | 45.3 |
| Phosphorous | 5.9 | 8.9 | 4.1 | 5.9 | 8.9 | 4.1 | 5.4 | 8.2 | 3.9 |

[a] Non-methane volatile organic compounds

Table 4: Sensitivity analysis for base case (basis: 1,000 L bioethanol at 99.7 vol%)

| Description | Units | Varied by cultivation yield (tonne/ha) | | | Varied by bioethanol yield (L/tonne) | | | Varied by process energy (MJ/1,000 L) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | Cassava | Cane molasses | Rice straw | Cassava | Cane molasses | Rice straw | Cassava | Cane molasses | Rice straw |
| Parameter values in this study | | 22.9 | 69.0 | 3.66 | 166.7 | 225.0 | 260.0 | 12,986 | 18,868 | 23,170 |
| Decreased/increased range | | 15-30 | 40-90 | 3.0-8.0 | 140-180 | 200-280 | 240-350 | 10,000-20,000 | 15,000-27,000 | 10,000-30,000 |
| Climate change | kg $CO_2$ eq | 360-569 | 436-757 | 768-1800 | 394-506 | 449-628 | 1,116-1,627 | 418-427 | 514-633 | 1,283-1,533 |
| Terrestrial acidification | kg $SO_2$ eq | 5.8-9.7 | 12.0-18.0 | 12.0-26.4 | 6.5-8.3 | 11.5-16.1 | 16.5-24.1 | 6.7-7.3 | 14.0-14.4 | 20.8-22.4 |
| Freshwater eutrophication | kg P eq | 0.6-1.1 | 0.7-1.3 | 0.4-1.0 | 0.7-0.9 | 0.8-1.1 | 0.6-0.9 | 0.7-0.7 | 1.0-1.0 | 0.8-0.8 |
| Marine eutrophication | kg N eq | 6.5-12.8 | 8.1-14.4 | 5.9-15.1 | 7.8-10.1 | 8.4-11.8 | 9.2-13.5 | 8.4-8.5 | 10.5-10.5 | 12.3-12.5 |
| Human toxicity | kg 1,4-DB eq | 23-45 | 73-129 | 40-98 | 28-36 | 76-107 | 60-88 | 30-30 | 94-95 | 80-81 |
| Photochemical oxidant formation | kg NMVOC | 3.0-3.4 | 6.5-7.6 | 4.6-5.6 | 2.9-3.7 | 5.5-7.7 | 4.0-5.8 | 2.8-3.8 | 6.6-7.0 | 4.3-5.7 |
| Particulate matter formation | kg PM10 eq | 1.9-2.6 | 3.7-4.7 | 3.7-5.8 | 2.0-2.5 | 3.3-4.6 | 3.8-5.6 | 1.9-2.7 | 4.0-4.1 | 4.8-5.4 |
| Terrestrial ecotoxicity | kg 1,4-DB eq | 12-23 | 90-162 | 170-453 | 14-18 | 94-132 | 276-403 | 15-15 | 117-117 | 372-372 |
| Freshwater ecotoxicity | kg 1,4-DB eq | 0.7-1.4 | 43.7-78.6 | 27.6-73.3 | 0.9-1.1 | 45.8-64.1 | 44.7-65.1 | 0.9-0.9 | 57.0-57.0 | 60.0-60.1 |
| Fossil depletion | kg oil eq | 81-121 | 137-219 | 83-129 | 87-112 | 135-189 | 86-126 | 93-94 | 163-178 | 90-120 |
| Net Energy Ratio (NER) | | 1.22-1.38 | 0.91-1.17 | 0.82-0.93 | 1.13-1.42 | 1.01-1.27 | 0.79-1.09 | 0.86-1.79 | 0.64-1.41 | 0.58-2.31 |
| Renewability (Rn) | | 3.74-5.80 | 1.98-3.75 | 3.34-6.18 | 4.24-5.32 | 2.86-3.58 | 3.57-4.92 | 4.48-5.59 | 2.30-3.45 | 3.20-5.80 |

**Highlights of the manuscript:**

- Integration of process simulation technique into LCA for unbiased comparison.
- Case of bioethanol production from cassava, cane molasses, and rice straw.
- Results were compared, and reliability of the simulation is validated.
- Cassava shows the best net energy gain (1.34) and renewability (5.16).
- All relative environmental impacts from cassava are less than 80%.