Life Cycle Assessment of Biomass-Derived Resin for Sustainable Chemical Industry

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Life cycle assessment (LCA) is a strong tool for quantifying the environmental impact associated with a product life cycle. To implement LCA into process design of biomass-derived resin, the lack of inventory data should be addressed by computer-aided process engineering (CAPE) tools. This study proposes the procedure of life cycle system design of biomass-derived resin. In this procedure, missing inventory data can be estimated by process simulation with design information extracted from literatures and design heuristics. At this time, the sensitivity of design settings to LCA results is analyzed and considered in process analysis. The categories of environmental impacts are specified on the scenarios definition originating from the decision by other stakeholders in the life cycle. This study demonstrates the proposed procedure by a case study of biomass-derived polyethylene (PE) and polypropylene (PP). At the case of synthesizing PP through synthesis gas from biomass, resin production phase has the largest contribution to the total GHG emission. In the case study, it is demonstrated that the detailed design of unit operation can lead to the increase of environmental impact by substituting biomass for fossil resources as raw materials.

1. Introduction

Biomass-derived resin has been expected to substitute for fossil-derived resin, because of its renewability. However, the much amount of biomass is required as raw materials for such substitution and new environmental impacts may arise due to the increase of the land use for cultivation such as water use, land use, nutrient enrichment and acidification. The changes of raw materials may result in the increase of the emission of the green house gas (GHG). To avoid such negative effects by the utilization of biomass, it is necessary to design a life cycle system of biomass-derived resin based on an appropriate environmental assessment. Although Life cycle assessment (LCA) has been applied for environmentally-conscious process design (Azapagic and Clift, 1999; Sugiyama et al., 2006), the lack of inventory data of producing biomass-derived resin in planning phase might be a hard obstacle to perform LCA. CAPE tools have great potentials to tackle this difficulty by process simulation for the estimation of process inventories. To enable us to perform LCA at the planning phase where available design
information is limited, standardized procedure of process simulation as inventory estimation is strongly needed. This paper demonstrates a collaboration of LCA and CAPE tools for environmentally-conscious process design of biomass-derived resin. A procedure of life-cycle system design of biomass-derived resin is proposed. As CAPE tools, process simulators are applied into the estimation of process inventories required for LCA. Life cycle system design is demonstrated on a case study of biomass-derived polyethylene (PE) and polypropylene (PP).

2. Life Cycle System Design of Biomass-derived Resin

Figure 1 shows the proposed procedure of life cycle system design of biomass-derived resin. The design starts from “Life cycle modeling”, where the candidates of target resin, the amount of production, synthesis routes and procurement routes are proposed. To perform LCA, inventory data of all life cycle stages are needed. Especially for the inventory data of production stages, the data can be obtained by “Inventory estimation by process simulation”.

In the life cycle system of biomass-derived resin, there are various stakeholders including farmer, resin producer and trader. Environmental impacts are occurred according to their decision making. For example, the amount of nitrogen fertilizer used at the cultivation stage makes a large difference in the total GHG emission. It means that scenario-based LCA must be performed and the inventory data and reference information about other life cycle stages have to be collected for individual possible scenarios. At the phase of “Scenario investigation of environmental impacts” in Figure 1, the relationship between such scenario and environmental impacts is investigated. Based on the collected and estimated inventory data, “Life cycle assessment” is performed. At last, “Process analysis” is performed based on the results of LCA and collected reference information. If the sensitivity of production phase becomes a critical

Figure 1 Procedure of Life cycle system design
factors changing decision, the design parameters regarded as the sensitive factors must be determined carefully based on the analysis results.

3. Case Study

3.1 Life cycle modeling
Life cycle modeling begins from the settings of target resin and production amount. The candidates of synthesis routes of the target resin are examined based on literatures, patents, and past cases. In this case study, the synthesis of PE and PP through bio-ethanol and bio-syngas are selected as production routes as shown in Figure 2. To determine the candidates of procurement route, the total amount of biomass consumption needs to be considered and is estimated based on block flow diagram (BFD) of each production route. BFD is drawn by using design information on reaction and separation, the conditions of which are extracted from available literatures. In this case study, biomass procurement routes were determined on the availability of biomass in possible exporting countries.

3.2 Inventory estimation by process simulation
Process inventory data of double lined processes in Figure 2 were estimated by process simulation by Aspen Plus™ and Aspen HYSYS™. As an example of process simulation, process flow diagram (PFD) of dimerization process in the ethanol route is shown in Figure 3. This process includes the reactor for the dimerization and the separator network composed of three distillation columns for separating products and by-products. In the separation parts within dimerization process, butene and by-products are separated and unreacted ethylene is recycled to the reactor. Design parameters including reaction temperature, pressure and conversion ratio are obtained from literatures. Regarding heat exchanging, power, and separation systems, unit operations are designed based on available design heuristics. For example, designing heat exchanging system, we followed pinch technology and set the minimum approach temperature between hot
fluid and cool fluid ($\Delta T_{\text{min}}$) as 50 °C. Designing power system, the maximum compression ratio of each compressor was set at 2.5 and the maximum decompression ratio of each gas turbine at 0.4 (Lorenz T. Biegler et al., 1997). Designing separation system, reflux ratios were designed as one and a half times of the minimum reflux ratios. Based on this process simulation, process data including the amount of raw materials and products, energy consumption and recovery, and emissions to the environment could be obtained for LCA. In this case study, there are by-products outputted at high purity. The environmental loads were allocated to all outputs based on the weight. Although the inventory data estimated through the process design based on heuristics can be regarded as a representative data, the change of the estimation by the modification of design parameters should be taken into account. Table 1 organizes the examples of such sensitivity analysis for the design parameters, which have been regarded as highly sensitive ones to process inventories. Considering theoretical and practical limitations, the analysis ranges for each target were specified.

**Table 1 Examples of sensitivity analysis**

<table>
<thead>
<tr>
<th>Analysis target</th>
<th>Design parameter requiring sensitivity analysis</th>
<th>Analysis range (min ~ representative ~ max)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat exchanging system</td>
<td>Minimum approach temperature between hot fluid and cool fluid ($\Delta T_{\text{min}}$).</td>
<td>0 degree C ~ 50 degree C ~ 100 degree C</td>
</tr>
<tr>
<td>Power system</td>
<td>Compression ratio of each compressor.</td>
<td>Isentropic ~ 2.5 ~ 10</td>
</tr>
<tr>
<td></td>
<td>Decompression ratio of each gas turbin.</td>
<td>0.1 ~ 0.4 ~ Isentropic</td>
</tr>
<tr>
<td>Separation system</td>
<td>Reflux ratio of distillation</td>
<td>minimum reflux ratio $\times$1.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\sim$ minimum reflux ratio $\times$1.5 ~</td>
</tr>
<tr>
<td></td>
<td></td>
<td>minimum reflux ratio $\times$3.0</td>
</tr>
<tr>
<td>Recycling process</td>
<td>Recycling feed ratio</td>
<td>0.90 ~ 0.95 ~ 0.99</td>
</tr>
</tbody>
</table>
3.3 Scenario investigation of environmental impacts
This phase begins from dividing a product life cycle to sub-processes. In this case, the sub-processes were defined as raw material production, resin production, transportation, resin use, and waste management. Based on the sub-processes, the environmental impacts were investigated, and the relationships between the decision making by stakeholders and environmental impacts were characterized. The way of land preparation for cultivation is an example of considerable scenario related with environmental impact. If farmer transforms land use style to prepare crop land, the amount of fixed carbon in ground will vary over the year. At the case of transformation of land from forest to agricultural land for sugarcane, the fixed carbon in the ground decreases from 95.8 Mg/ha to 72.8 Mg/ha in fifty years (Rhoades C. C. et al., 2000). Because decreased carbon in the ground is emitted to the air as CO₂, such transformation of land use results in the increase of global warming impacts.

3.4 Life cycle assessment and process analysis
Based on the sensitivity of design parameters and scenarios on the decision by other stakeholders to environmental impacts, LCA was performed for the production of biomass-derived PE and PP. The procedure of process analysis based on the results of LCA and collected reference information was demonstrated on a case of synthesizing PP through synthesis gas derived from waste wood (waste wood-syngas-PP route). The LCA result on GHG emission is shown in Figure 4. The total GHG emission originating from “Raw material production” and “Transportation” of waste wood-syngas-PP route are much less than that of “resin production”. This is because the energy consumption in the raw material production, that is, cultivation, is small. Additionally, the short distance between production sites might be a reason of small impact originating from "transportation". From Figure 4, syngas to methanol process can be regarded as a critical process among the life cycle stages. When ΔT_{min}, a highly-sensitive design parameter for this process data, was set at 100 °C, the total GHG

![Figure 4 Sensitivity analysis of ΔT_{min} about methanol production process](image)
emission of waste wood-syngas-PP route gets closer to that of fossil resource–PP route. This result can demonstrate that $\Delta T_{\text{min}}$ needs to be managed carefully at detailed design phase for construction of the production process of waste wood–syngas-PP route.

4. Conclusion

A procedure of life cycle system design of biomass-derived resin is proposed. LCA has an important role of quantifying the environmental impacts due to the utilization of biomass as the raw materials for chemical productions. At that time, CAPE tools have great potential to address the lack of data at the production of biomass-derived resin. Process simulators with available design information extracted from literatures and design heuristics can estimate the missing inventory data. In this time, the sensitivity of the design parameters to environmental impacts must be carefully analyzed, because the results can be significantly changed and the decision may become different. The environmental impacts originating from the life cycle of biomass-derived resin have strong relationship with the decision by other stakeholders within the life cycle. The categories of environmental impacts should be considered based on the scenarios on such decision cases.

The proposed procedure was demonstrated on an actual case study of designing production process of biomass-derived PE and PP. LCA results based on estimated and collected inventory data was used to analyze each sub-process. At the case of waste wood-syngas-PP route, resin production has the largest contribution to the total GHG emission. According to the value of minimum approach temperature at heat exchanging system, merit of biomass-derived PP against fossil resource-derived PP can be lost. Based on the process analysis, the constraints on detailed design before construction or information for process improvement can be extracted.

References