Design and Assessment of Bio-Ethanol Based Chemical Process for Sustainability

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1. Introduction

Originated from renewable resource, bio-ethanol has been used as a substitute for fossil-based fuel. Moreover, it is also expected to be used as a key chemical for future organic chemical industry. However, utilization of bioethanol cannot guarantee actual sustainability unless bioethanol based processes are examined from the viewpoints of not only renewability but also other sustainability indicators. In this study, we investigate the bio-ethanol based production processes of ethyl acetate, one of the most essential solvents of chemical industry. The sustainability of these processes is examined by considering both monetary and non-monetary issues such as environmental impacts and safety hazards.

2. Sustainability evaluation

In this study, the sustainability of the production processes is evaluated by three indicators: production cost, environmental impacts and inherent safety hazards.

Production cost indicator

The production cost, including costs of raw materials and utilities used in the processes, is calculated.

Environmental impact indicator

With the increasing concern on global warming, CO_2 emission can be considered as an important sustainable indicator. Cumulative Energy Demand (CED) [1] is used to quantify CO_2 emission caused by manufacturing processes of fossil-based raw materials and utilities supplied to the production processes of ethyl acetate. For bio-ethanol based processes, the life cycle of bio-ethanol feedstock derived from sugarcane [2] is considered to calculate the amount of CO_2 emitted from its production. In addition, CO_2 emitted from the waste treatment is also counted

Inherent safety hazard indicator

The inherent safety index (ISI) method [3] is applied to evaluate the inherent safety hazards of the alternative processes. Requiring only data available at early design phase, it considers the inherent safety hazards of both chemical (I_{CI}) and process (I_{PI}). I_{CI} accounts for heat of main reaction, heat of potential side reaction, flammability, explosiveness, toxicity, corrosiveness and incompatibility of chemicals. I_{PI} involves inventory of chemicals, process temperature, and pressure, type of equipment and structure of process. The sum of I_{CI} and I_{PI} gives the total inherent safety index of the whole process. The high total index results in high hazard potential process.

3. Case study on Ethyl acetate production process

Ethyl acetate can be produced by different synthesis routes. The esterification of ethanol and acetic acid with the aid of acid catalysts is the main technology to produce ethyl acetate. Therefore, it is selected as the base case, in which the raw materials ethanol and acetic acid are produced by the catalytic hydration of fossil derived ethylene and carbonylation of fossil derived methanol, respectively. Besides this route, the potential alternative routes considered in this study are:

- One step ethanol route (route alternative 1)
- Dehydrogenation of ethanol by using copper-based catalyst (route alternative 2)
- Addition of acetic acid to ethylene, by using clay or heteropoly acid as a catalyst (route alternative 3)

Except the base case, the other alternative routes, named bio-ethanol based routes, use bio-ethanol derived from sugarcane as the initial raw material.

These processes are designed to produce ethyl acetate with purity 99.95 wt% and productivity 100,000 tons/year. The waste liquid streams output from the process can be incinerated to generate steam or electricity to supply for the production process, depending on the amount of waste water included. **4. Results**



CO2 emission [kg/kg product]
□ Inherent safety index/10 [-]

Fig. 1: Evaluation results

Figure 1 shows that the bio-ethanol based alternative processes 1 and 2 have high potential toward the sustainable chemical industry. They give both better cost saving and lower CO_2 emission than fossil-based process.

Among the alternative routes, the bio-based alternative process 1 can be considered as the most promising to produce ethyl acetate. Since it has high ISI value, more attention should be paid during operation and control.

Although more case studies on bio-ethanol based chemicals and more rigorous evaluations especially on the sustainability must be needed, this study provides good visions for further research and development in bioethanol based chemical industry.

References

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