論 文 の 内 容 の 要 旨

論文題目　Structured Framework Supporting Design of Bio-based Chemical Process toward Sustainability
（和訳：　持続性に向けたバイオマス原料による化学プロセス設計支援の構造化フレームワーク）

氏　　名　　ゲェン　ティ　ホン　テュイ　　Nguyen Thi Hong Thuy

1. Introduction

Security supply of energy and raw materials together with economically healthy and environmentally friendly production processes are decisive factors for sustainable development of future chemical industry. Substitution of bio-based feedstocks for the fossil-based is a potential paradigm for sustainable chemical production. In addition, designing sustainable bio-based chemical production processes can positively contribute to sustainable development.

The sustainability of the chemical process is determined by three integrated elements: input raw material, synthesis process and output product. To be sustainable, the input feedstock needs to be renewable and available. The sustainability of synthesis process and output product needs to be assessed considering not only production cost but also environmental problems and health and safety hazards. The sustainability of chemical process cannot be guaranteed, unless the sustainability of these elements is evaluated. Nevertheless, such integrated assessment has not been addressed in almost all guidelines of process design and evaluation, e.g., [1-3].

Biomass has been considered as sustainable resource. The concept of utilizing biomass for chemical production has received many attentions. The economic and environmental assessment has been performed to provide some forecasts about the potential of bio-based chemicals [4, 5]. However, to solve complicated issues related to utilizing bio-based feedstock for chemical production such as resource availability and production process feasibility, a more comprehensive approach is needed.

In this study, I developed a structural framework to support design and assessment of bio-based chemical process for sustainability. It addresses the important issues of bio-based chemical production: designing sustainable production process, evaluating and selecting sustainable input bio-based feedstock and output products.

2. Structural framework supporting design and evaluation of bio-based chemical process

Figure 1 shows the schematic framework supporting design and assessment of bio-based chemical process. It consists of six main stages. At the first stage, the environmental problems caused by running processes are defined. Market demand, company and local conditions are checked to define desired function of output chemical and available bio-based raw materials as well. At the second stage, alternative chemicals are generated and synthesis routes are investigated based on literature, patent and available information. At the third stage, alternative processes producing alternative chemicals are designed with the aid of computer-aided process engineering tools. The running fossil-based process is examined if it can be modified to switch to using bio-based feedstock in replacement of fossil-based. At the fourth stage, evaluation of bio-based chemical alternatives is performed by assuming a representative bio-based feedstock. At this stage, production cost, CO_2 emission and fossil energy consumption are evaluated, since they are the main criteria determining the success of bio-based chemicals versus the fossil-based in the

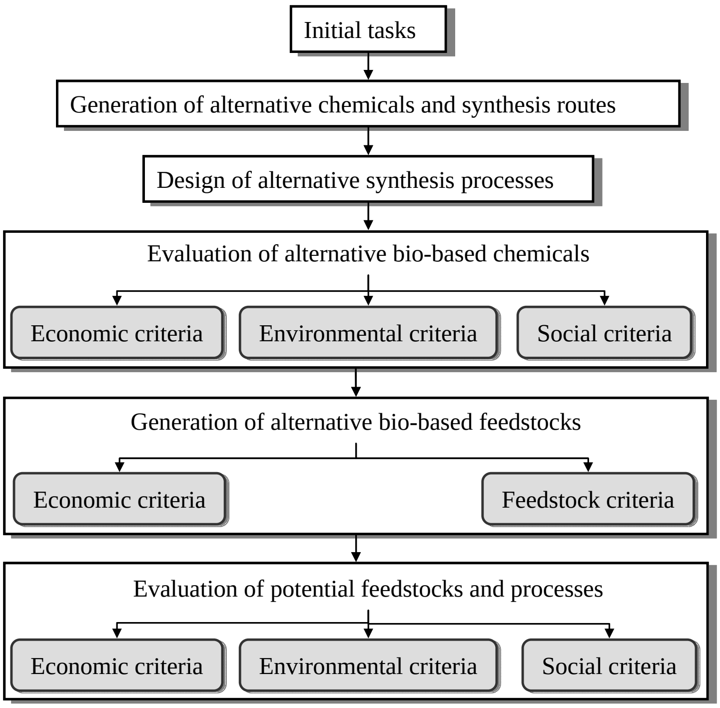

Fig.1 Framework of design of bio-based chemical process

commercial market. The social criteria such as health and safety hazards can also be assessed to find potentially safer processes. At the fifth stage, the potential feedstock alternatives are generated considering feedstock criteria including renewability, availability and collectability and economic criteria represented by investment and transportation costs. At the last stage, the investigated potential bio-based feedstocks together with the process alternatives are further evaluated. Since the plantation of bio-based feedstocks caused many environmental problems, different environmental criteria are assessed at this stage such as CO_2 emission, fossil energy consumption, eutrophication, acidification and ozone depletion. While the evaluation boundary of the fourth stage consists of only the process converting bio-based feedstock to the target chemical, the last stage includes not only the conversion but also the plantation and collection stages of bio-based feedstock. The processes that cannot satisfy desired environmental performance are eliminated. Among the satisfying processes, the most sustainable is selected if it gives good performances toward economic and social criteria. Pareto optimum curve is applied when the processes have trade-off results of economic and social criteria.

3. Case study on design of bio-based chemical process

The applicability of developed framework is demonstrated through a case study on design of bioethanol based chemical process. Before the complete case study, I focus on the design of separation system, which has strong influence on the sustainability of the whole process, performing a separate case study on MAA purification.

3.1. Case study on MAA purification

The case study on extraction of MAA (Methyl Methacrylic acid) from water and acetic acid in the production process of MMA (Methyl Methacrylate) is considered.

To extract MAA, three feasible alternative solvents are selected based on patents: heptane, xylene and mixture of MMA and xylene. Due to the differences of split fractions, boiling points and the possibilities of forming azeotropic mixtures between solvents and process substances, feasible extraction processes are designed and modeled individually.

The alternative processes are designed and evaluated considering three indicators: production cost represented by Net Present Value (NPV), CO_2 emission calculated based on CED (Cumulative Energy demand) [6] and safety hazards evaluated by applying EHS method [7]. The evaluation result shows that Heptane and (MMA + Xylene) processes are rather comparative to each other for all evaluation indicators. Xylene process has the worst performances toward these evaluation objectives. Applying weighting method (multiplying weighting factors 0.5, 0.3, 0.2 to production cost, safety hazard and CO_2 emission indicators, respectively), the most suitable process is selected. Among the process alternatives, Heptane process is the best process for purification of MAA.

With the case study on MAA purification, method of designing separation process included in the developed framework was clearly illustrated.

3.2. Case study on bio-chemical production

Three kinds of high volume chemicals are accounted in this case study: ethyl acetate, acetic acid and ethylene.

Generation of synthesis routes and design of alternative synthesis processes

Possible synthesis routes of the chemicals considered are investigated based on literatures. Based on these synthesis routes, bio-based alternative processes are designed and examined for the potential of substituting for the fossil-based processes.

Evaluation of alternative bio-based chemicals

Sugarcane is selected as the representative bio-based feedstock to produce bioethanol and bioethanol derivatives supplied to the process alternatives. To succeed in the commercial market, the bio-based chemicals must not only bring more environmental benefits but also be more economic attractive than the fossil-based. Thus, three kinds of indicators are considered to select the most appropriate chemical: production cost, CO_2 emission and fossil energy consumption.

The evaluation results show that all process alternatives producing the chemicals considered help reduce marked amount of CO_2 emission. Among the chemicals considered, bio-based ethyl acetate is the most attractive as it helps reduce marked amount of fossil energy consumption and save lot of production cost.

Generation of alternative bio-based feedstocks

To generate the alternative bio-based feedstocks, it is necessary to consider economic and feedstock criteria. The economic criteria are represented by investment cost of process alternatives and transportation cost of bio-based feedstocks. The feedstock criteria are represented by renewability, availability and collectability. The local conditions have strong influence on the performance evaluated at this stage. This fact is illustrated by the case study which is described in detail in the next chapter.

Evaluation of potential feedstocks and processes

In addition to production cost, different categories of environmental impacts such as fossil energy consumption, eutrophication, global warming, ozone depletion, acidification and photooxidant formation are considered, because the plantation of biomass has caused many environmental problems. The evaluation results of these categories are normalized before being summed up to give the total environmental index. The inherent safety index is considered to assess the potential hazards of the process alternatives by applying ISI method [8]. The higher the indexes are, the worse the performances of the process alternatives are.

Based on the evaluation results, the most sustainable process together with input bio-based feedstock which possesses desired environmental performance and the lowest inherent safety index and production cost is selected for producing the selected chemical.

4. Case study on impacts of local conditions on bio-based chemical process design

The local conditions strongly influence the criteria that need to be considered in the stage of generation of bio-based feedstock alternatives. In this chapter, the availability, distribution and transportation of biomass are considered in the local conditions of Vietnam.

Different kinds of bio-based feedstocks (sugarcane, corn, cassava, corn stove, rice straw and rice husk) and different scales of production are accounted to highlight the impact of local conditions on the design of bio-based chemical process. Two scenarios of producing target bio-based chemical are developed: 1) Centralized plant: bio-based feedstock is collected to the centralized gathering plant, and all amount of target chemical is produced at that plant, 2) Distributed plant: bio-based resource is collected to the multiple plants distributed close to the available resource. The production scale of distributed plant is divided by the determined productivity of target chemical to the number of distributed plants.

The evaluation result clearly shows that within the centralized plant scenario, the collection cost is markedly high with the increase of production scale when bio-based feedstock is widely distributed. In distributed plant scenario, the collection cost dramatically decreases while the investment cost increases. The distribution, available amount and the transportation distance of bio-based feedstock are the main factors determining the collection cost of raw material. Thus, they strongly influence the economic performance of bio-based chemical process, especially the processes utilizing large amount of input raw material. Directly, the local conditions have strong impact on the selection of bio-based feedstock, production scale, synthesis process and its plant set-up.

5. Developed framework under IDEF0 representation

From the performance of the case studies above, the developed framework is improved and modified by adding more necessary information to clarify input and output, supporting resources and the constraints that need to be considered during the performance of each stage.

Under IDEF0 (Integration DEFinition language 0), the framework supporting design of bio-based chemical process is described in more detail as shown in **Fig.2**. There are 6 main activities included in the main level activity. The activities A2 to A5 are

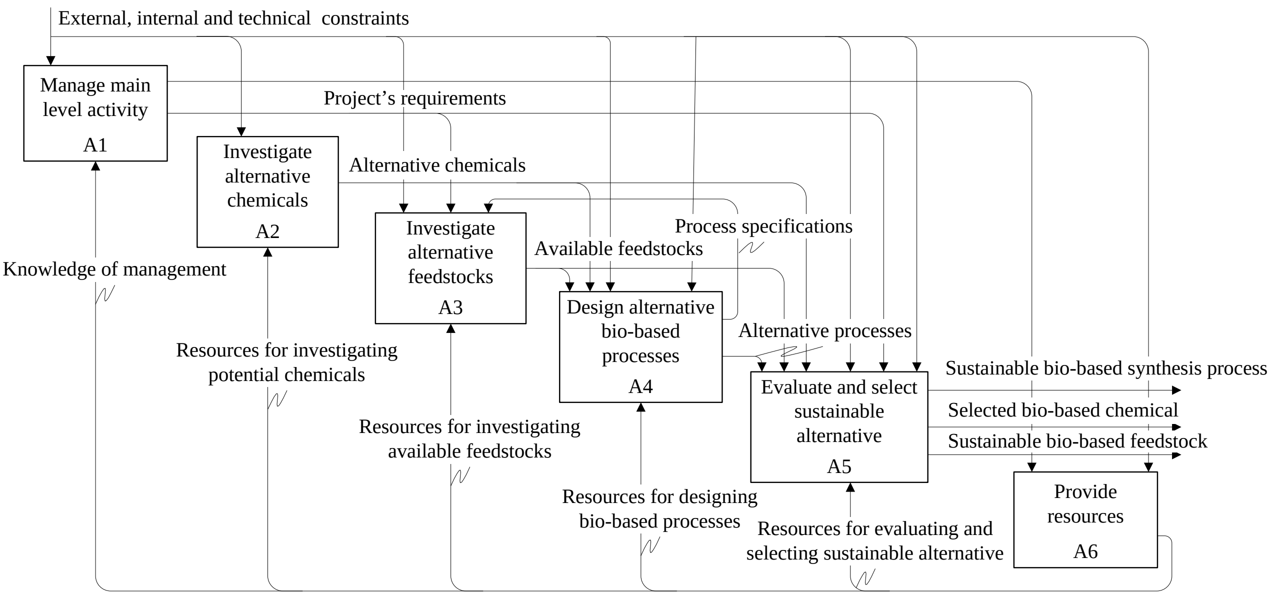

Fig.2 Illustration of developed framework by IDEF0 model

performed under the management of activity A1 and with the support resources provided by activity A6. Each activity is described in detail by being decomposed into some sub-layer activities. The top side arrows show the constraints controlling the performance of the activities such as external (e.g., market demand and governmental laws), internal (e.g., company policies and capacity) and technical constraints (e.g., conditions and performances of running processes). The left and right side arrows are the input and output of each activity, respectively. The bottom side arrows are the mechanisms, necessary tool and information supporting the performance of each activity.

Output from activity A2 are the chemical alternatives that meet the market demand and satisfy the conditions of company's situation. Within activity A3, all possible feedstocks are investigated and checked for feasibility respect to local conditions. The process alternatives producing target chemicals are designed by performing activity A4. Besides investigating new synthesis routes, the fossil-based process is also examined if it can be modified to use bio-based resource for producing target chemical. The alternative processes are evaluated within activity A5. Suitable evaluation models which include considered indicators and evaluation methods are developed. As the final targets, sustainable synthesis process, output chemical and input bio-based feedstock are produced after the activity A5.

6. Conclusion and outlook

6.1 Conclusion

- A novel framework supporting design of bio-based chemical process was developed. It addressed the important issues related to utilization of bio-based feedstock for chemical production.
- Using the flowchart diagram, the necessary stages included in the framework are clearly displayed, supporting designers to fulfill the tasks of design and assessment of bio-based chemical process for sustainability. The framework is modeled by IDEF0 in more detail, facilitating more effective communication and discussion among designers.
- With the performance of the concrete case studies, the applicability of the developed framework was verified. The framework provides practical business model for further research and development of bio-based and thus sustainable chemical industry.

6.2 Outlook

The following points should be considered in the future research:

- Process integration and multi-product integration
- Assessment of land use impact and water use impact
- Rigorous assessment of social issues: job creation, change of local status, etc.

References

[1] Sugiyama *et al*., *AIChE J.*, 54, 1037-1053 (2008).

[2] Chen and Shonnard, *Ind. Eng. Chem. Res.*, 43, 535-552 (2004).

[3] Tugnoli *et al*., *Environ. Sci. Technol*., 42, 4555-4562 (2008).

[4] Hermann *et al*., *Environ. Sci. Technol.*, 41, 7915-7921 (2007)

[5] Hermann and Patel, *Appl. Biochem. Biotech.*, 136, 361-388 (2007).

[6] Huijbregts *et al*., *Environ. Sci. Technol.*, 40, 641-648 (2006).

[7] Koller *et al*., *Ind. Eng. Chem. Res.*, 39, 960-972 (2000).

[8] Heikkilä *et al*., *Comput. Chem. Eng.*, 20, S115-S120 (2000)