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Hierarchical Decomposition Approach for Process Synthesis of Integrated Biorefinery

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Process synthesis is one of the most important activities in chemical process design. In the past decades, development in process synthesis has been dominantly targeted for petrochemical or petroleum-based industries. However, in recent years, the industries have been searching for alternative sustainable resources to replace fossil fuels. Biomass has been identified as one of the most promising alternatives. Biomass can be used to produce fuel, energy and chemicals in an integrated biorefinery. In order to synthesise and design an integrated biorefinery, many researchers have extended and modified current available process synthesis approaches, in which they have been mainly developed based on petrochemical industries. Although these reported approaches are useful in designing the integrated biorefinery; however, they are mainly mathematical optimisation approaches which require either high computational efforts or intensive modelling of the system. Based on the literature, there are limited works on developing hierarchical approach that can provide guidance for designer to synthesise an integrated biorefinery systemically. Due to the diversification in compositions and characteristics of biomass feedstock, as well as limited physical and chemical properties of biomass, additional considerations are required to modify the current available hierarchical approaches for integrated biorefinery synthesis. In this work, a well-established hierarchical decomposition approach is extended for synthesis of integrated biorefinery. The revised hierarchical approach now includes a new level, which is known as "characterisation and standardisation of biomass". Besides, appropriate modifications are also made on the other levels (i.e. level 2- 6) to accommodate the requirements of synthesis of integrated biorefinery.

1. Introduction

Since industrialisation, society has been dependent on finite fossil resources (i.e., petroleum) for power generation, and as the sources of various transportation fuels. Besides, fossil resources are converted into various petrochemicals for different applications. According to Cherubini (2010), almost 4 % of the petroleum resources in worldwide are used for chemical and polymer productions. For example, majority of chemical products can be obtained from petroleum refinery. Consequently, the development and establishment of chemical engineering have been dominated by the petroleum or petrochemical industries. In particular, chemical process synthesis has been established with the underlying chemical and physical science, as well as operational knowledge in petrochemical industries.
In the recent year, due to the decreasing in fossil resource reserves and increasing environmental concerns (i.e. global warming), the industries are motivated to seek for sustainable renewable resources to replace fossil resources as raw materials for chemical processes. Among all the available renewable sources (e.g. solar, wind, hydro, etc.), biomass has been identified as one of the most promising renewable sources. Biomass is defined as any organic matter that is available on a renewable or recurring basis, including dedicated energy crops and tress, agricultural residues, algae and aquatic plants, wood and wood residues, animal wastes, and other waste materials usable for the production of energy, fuels, chemicals, and materials (Kamm et al., 2005). In order to convert biomass into value-added products such as fuels, materials and chemicals, the biomass can be processed in a processing facility known as integrated biorefinery. To maximise the energy and material recovery within the integrated biorefinery,

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systemic synthesis and design of such processing facility is needed. In addition, due to the complexity of the chemical structure and variation in composition of biomass, it is challenging to synthesise integrated biorefinery based on the current established process synthesis approaches. Therefore, additional considerations need to be taken into consideration for synthesis of integrated biorefinery. In this work, a well-established hierarchical decomposition approach that is firstly proposed by Douglas (1985) is extended for the synthesis of integrated biorefinery.

2. Process synthesis in chemical process design

Process synthesis is one of the most important activities in chemical process design. According to Nishida et al. (1981), process synthesis can be defined as an activity of determining the optimal interconnection of processing or operation units, as well as the optimal type of the design of the units within a processing system. To date, various systematic approaches for process synthesis have been presented, such as hierarchical approaches, graph theoretic approach (i.e. P-graphs), mathematical optimisation approaches, etc. By using these process synthesis approaches, one can eliminate poor projects and process alternatives at a minimum cost of effort (Douglas, 1988). Moreover, the previous works have shown that systematic process synthesis can reduce energy requirements by 50 % (Siirola, 1996) and costs by 35 % for chemical industries (Dimian and Bildea, 2008).

Since the pioneering work of Rudd et al. (1973), there have been significant developments and contributions in the area of process synthesis over the past decades. Consequently, several subtopics of process synthesis have been maturely established, such as flowsheet synthesis (e.g. Douglas, 1988), reaction pathways, reactor network and separation network syntheses (e.g. Seider et al., 2004), mass exchanger network synthesis (e.g. El-Halwagi, 2006), heat exchanger network synthesis (e.g. Kemp, 2007) and resource conservation network synthesis (e.g. Foo, 2012). These subtopics can be collectively viewed as important elements that form a systematic framework for process synthesis in designing a most optimal chemical process flowsheet. It is noted that, based on the literature studies, according to their publication years, one of the earliest researches in process synthesis had been focusing on developing and proposing systematic approaches that can guide designer to synthesise a process (i.e. flowsheet synthesis). For example, Grossmann (1985) proposed mixed-integer programming approach; while Douglas (1985) proposed a hierarchical decision procedure for flowsheet synthesis. The hierarchical decomposition approach is one of the most well-known approaches. Such approach provides guided procedures to address process flowsheeting activity through a hierarchy of decision levels, where more fine structure is added to the process flowsheet at each decision level. In this approach, essential decisions for developing a flowsheet at each level are identified, and if these decisions are altered, then process alternatives can be generated. Designers are often included in the synthesis activity since the decisions are normally made by the designers. Note that, the essence of this approach is a sequential design procedure, and each decision level normally terminates with an economic analysis. By using this approach, the whole chemical process flowsheet can be synthesised systematically. Besides, the approach is also able to generate a base-case design that can be used for the successive detailed engineering analysis in the later design stage.

3. Synthesis and design of integrated biorefinery

Biorefinery is a processing facility that converts biomass into value-added products, such as fuel, energy, and chemicals. It is proposed based on the similar concept of petroleum refinery (Kamm et al., 1998). In order to enhance the overall process and economic performances, the concept of integrated biorefinery which maximises the energy and material recovery within the biomass processing system is proposed by Fernando et al. (2006). Note that an integrated biorefinery integrates multiple biomass conversion technologies (e.g. biomass feedstock handling, biomass pre-treatment, biomass conversion, etc.) as a whole integrated processing system (Ng, 2010). In terms of process synthesis, the problem statement for integrated biorefinery synthesis can be stated as followed: Given a set of biomass feedstock and a set of desired bio-based final products with specifications, it is desired to determine the optimal interconnection of processing or operation units, as well as the optimal type of the design of these units within a processing system for converting biomass into the desired products.

Over the past few years, research works have seen intensive on developing systematic approaches for integrated biorefinery synthesis and design. Consequently, different aspects have been taken into considerations. For instances, approaches to synthesise integrated biorefinery with optimal processing configuration and processing pathway have been proposed via two-stage approach (Pham and El-Halwagi, 2012), disjunctive programming formulation (Ponce-Ortega et al., 2012), transhipment models with superstructure (Zondervan et al., 2011), etc. On the other hand, Voll and Marquardt (2012) proposed an optimisation-based reaction network flux analysis to identify and analyse large number of reaction pathways in the synthesis of integrated biorefinery. Besides, other aspects such as environmental concern and social impact are also taken into consideration together with process synthesis. For examples, simultaneous considerations of economic and social aspects (El-Halwagi et al., 2013), simultaneous considerations of economic, social and environmental aspects (Santibañez-Aguilar et al., 2014) are reported in optimal planning and site selection of biorefineries. On the other hand, business and other system engineering aspects have also been taken into account; for instance, supply chain (e.g. Lam et al., 2013), supply network (e.g. Čuček et al., 2014) and enterprise-wise optimisation (e.g. Quaglia et al., 2013). On the other hand, there are some works working on the different feedstock, such as microalgae (Garcia Prieto et al., 2014).

However, most of these reported works are mainly relied on mathematical optimisation approaches which require either high computational effort or intensive modelling of the system. There are limited works reported on hierarchical approach which can provide a framework to guide designer in synthesising an integrated biorefinery. In this work, the well-established hierarchical decomposition approach (Douglas, 1985) is adapted. Note that the proposed approach provides systematic guidance to process flowsheet construction for the integrated biorefinery.

4. Hierarchical decomposition approach for synthesis of integrated biorefinery

Hierarchical decomposition approach has been proven to be very successful in industrial applications (Martín and Grossmann, 2013). It is firstly proposed by Douglas (1985) to design conventional chemical process. Conventional chemical process (i.e. petrochemical process) usually processes petroleum-based or petroleum-derived raw materials that can readily be utilised for chemical production. For example, in a benzene production process, petroleum-based raw materials (i.e. toluene and hydrogen gases) can directly participate in a hydrodealkylation reaction to produce benzene. However, in integrated biorefinery, biomass raw materials typically vary in both compositions and properties. As a result, biomass cannot be directly utilised into conversion process in an integrated biorefinery. For instance, rice straw (biomass) cannot be directly used in fermentation process (i.e. conversion process) to produce bioethanol. Thus, rice straw is required to be pre-treated into more appropriate and useful forms. In such regards, the biomass has to be particularly standardised into bio-precursor, which is defined as a compound that can be readily utilised in first biomass conversion unit of the integrated biorefinery process to produce useful intermediates or products. Before the biomass can be pre-treated into bio-precursor, it is necessary to understand the compositions and properties of the biomass, such as moisture contents, lignocellulose contents, etc. This step can be defined as characterisation of biomass. The characterised biomass then can be pretreated into bio-precursors corresponding to the first biomass conversion unit. This step can be defined as standardisation of biomass, in which biomass raw material inputs are standardised to an appropriate form that can be readily utilised in the conversion process. Various biomass pretreatment technologies (e.g. drying, delignification, etc.) can be applied to standardise the biomass. It is important to note that biomass standardisation procedure is usually subjected to the first biomass conversion system. For instance, in order to produce bioethanol from rice straw, there are two possible pathways, namely thermochemical and biological pathways. Thermochemical pathway uses thermal decomposition methods while biological pathway uses micro-organisms to break down the biomass. In the case where the biomass is processed into bioethanol via thermochemical pathway, gasification is identified as the first biomass conversion system. In order to prepare the biomass in such that it can be readily used for gasification, it has to be grinded and dried into the form with acceptable size and moisture content. In the event that the biological pathway (fermentation process) is taken into consideration, the biomass needs to be pre-treated to remove lignin in order to expose the celluloses for fermentation. Additionally, the delignified biomass then needs to be hydrolysed into fermentable sugars for fermentation. Note that, regardless of which pathway is selected, the biomass is required to be pretreated. Pretreatment system is essential for an integrated biorefinery. Figure 1 shows the general structure of an integrated biorefinery. As shown, an integrated biorefinery typically has a biomass pretreatment system before its main conversion process. Once the biomass is treated in the pretreatment system, the remaining processing steps of the conversion process in the integrated biorefinery is similar with the conventional chemical process where reactor and separation systems are required to form a total process.

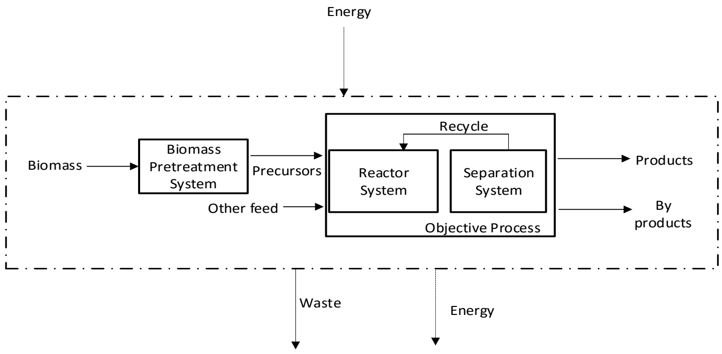

Figure 1: General representation of an Integrated Biorefinery

In this work, the existing hierarchical decomposition approach is adapted and modified to accommodate the above-discussed steps for synthesis of integrated biorefinery, A new level (i.e. Level 2: Characterisation and standardisation of biomass) is added onto the hierarchical decomposition approach. Note that, Levels 3 – 5 in the revised hierarchical approach are similar with Levels 2 – 4 in the previous hierarchical decomposition approach (Douglas, 1985), as shown in the section below. The last level (Level 6) in the revised hierarchical approach is modified to consider both mass and energy integration opportunity instead of only consideration of energy integration. Additionally, it is also modified to consider the possibility to use biomass residues as process fuel for the biorefinery. This is important as part of the design in order to ensure that integrated biorefineries do not depend on fossil resources for power and heat consumptions. Therefore, the flowsheet synthesis problem of integrated biorefinery can now be decomposed into six hierarchical levels as followed:

- Level 1: List of input information and operation mode selection
- Level 2: Characterisation and standardisation of biomass
- Level 3: Input-output structure of the flowsheet
- Level 4: Considerations of the recycle structure of the flowsheet
- Level 5: Considerations of separation
- Level 6: Considerations of resource conservation and biomass residue utilisation

4.1 Level 1: List of input information and operation mode selection

In this level, necessary information which are required to develop a process flowsheet or a base-case design are collected. Table 1 shows some of the important information. Note that, the information listed in Table 1 is only the example information that required. In order to synthesise integrated biorefinery, more information may be required. On the other hand, operation mode (e.g. continuous, semi batch and batch) of the process is also decided in this level.

Table 1: Example of important input information

1. Information of the desired product (e.g. production rate, product specifications, etc.)
2. Information of the objective process (e.g. reactions data and catalyst, if any, etc.)
3. Information of any processing constraints
4. Information of plant and site data
5. Information concerning the safety, toxicity, and environmental impact of all the materials involved

4.2 Level 2: Characterisation and standardisation of biomass

As discussed in the previous sections, due to the complexity of chemical structures, and variation in compositions, biomass has to be characterised and standardised into bioprecursor before it can be readily used in the conversion process. For instance, empty fruit bunches in palm oil industry normally come in the forms with different composition and moisture contents. Even if they are originally sourced from a same palm oil mill at the same time, their properties and compositions may not be uniform. It is thus necessary to standardise the biomass before they can be utilised in a conversion process. However, before standardisation of biomass can be done, their properties and compositions must be determined. This is because information and characteristics of biomass are essential to help in deciding appropriate pretreatment technologies to prepare the biomass into bioprecursors. After characterisation, the biomass is then prepared and standardised into bioprecursor according to the respective first biomass conversion system of the biorefinery process. In other words, decisions are made on how to characterise and standardise the biomass into bioprecursors in this level. Note that, characterisation of biomass can be achieved by using various analysis techniques, such as proximate and ultimate analyses; while standardisation of biomass can be achieved by application of different biomass pretreatment technologies. For example, in order to obtain fermentable sugars for ethanol production via biochemical route, acid hydrolysis can be considered as the biomass pretreatment technology.

4.3 Level 3: Input and output structure of the flowsheet

This level of detail will consider and describe all the streams that are fed to the integrated biorefinery and those leave the integrated biorefinery. In other words, decisions are required to fix the input and output structure of the flowsheet. Attentions are given on what raw materials are fed to the process and what products and by-products are removed. For instance, one should consider and decide if there is any additional raw material other than the bio-precursors is required for the conversion process.

4.4 Level 4: Considerations of the recycle structure of the flowsheet

As shown in the previous level, the input-output structure of the flowsheet can be fixed. In this level, decisions are made to determine the recycle structure of the flowsheet; besides, the number of reactor systems, number of recycle streams, etc. need to be determined. The recycling decisions often depend on the excess reactant at the reactor inlet, the addition of diluent and the need for adding external solvents to the process. By recycling, the requirement of raw materials can be reduced.

4.5 Level 5: Consideration of separation systems

In this level, synthesis of separation system to recover solid, liquid and gaseous components are taken into consideration. The considerations of separation systems can be mainly categorised as general structures, solid recovery system, vapour recovery system and liquid separation system (Douglas, 1985). in this level, decisions are to be considered and made regarding to the selection of separation system. For instance, if one attempts to synthesise a vapour recovery system, two example decisions are normally required: 1) which are the best location of such system in the entire flowsheet, and 2) what type of vapour recovery system (e.g. condensation, absorption, adsorption and etc.).

4.6 Level 6: Consideration of resource conservation and biomass residue utilisation

Final level considers the opportunities of resource conservation (i.e. mass and energy conservations) within the process. For example, from the material conservation aspects, if fresh water is intensively used in the integrated biorefinery, water recovery system can be considered and synthesised to reduce fresh water consumption. From the energy conservation perspective, specifications of utility targets and network design for energy integration via heat exchangers network synthesis are determined in this level. Additionally, in case that there is any biomass residue (i.e. process biomass by-products) which are not utilised in the integrated biorefinery for chemical production, decisions can be made on using them for power and heat generation. Note that, this final level is only sensible after pre-treatment, reactors and separation systems have been fixed based on the abovementioned levels.

5. Conclusions

In this work, the well-established hierarchical decomposition approach, which is originally developed for conventional chemical process (i.e. petrochemical process) synthesis, is adapted for the synthesis of integrated biorefinery. Such biorefinery is a processing facility that integrates multiple biomass processing technologies as a whole to convert biomass into various value-added products. In general, biomass has different characteristics, compositions and properties. Therefore, biomass must be characterised and standardised into bioprecursors in order to be directly utilised in a conversion process. In such regards, a new level is added to the hierarchical decomposition in order to accommodate this consideration. As a result, one can decompose the whole synthesis problem of integrated biorefinery into six hierarchical levels as follows: Level 1: List of input information and operation mode selection; Level 2: Characterisation and standardisation of biomass; Level 3: Input and output structure of the flowsheet; Level 4: Considerations of the recycle structure of the flowsheet; Level 5: Consideration of separation systems; Level 6: Consideration of resource conservation. Note that, the essence of the original hierarchical decomposition is to consider process flowsheeting as a sequential activity. Hence, the revised hierarchical approach also shares the same uniqueness as the original one.

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