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Automated Targeting For the Synthesis of an Integrated Biorefinery with Multiple Products

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In this work, an optimisation-based, automated targeting procedure to determine the maximum revenue level in an integrated biorefinery with multiple products is presented. The proposed approach is based on the concept of pinch analysis and allows targets to be determined prior to detailed design of the biorefinery flowsheet. A hypothetical case study is shown to illustrate the proposed approach.

1. Introduction

The exhaustion of natural resources such as coal, oil and natural gas will soon become the global major crisis. As a result, there is an increased attention on the issues of energy security, environmental protections, and sustainable development. In addition, the increase in global energy demands and the desire to reduce damages to the environment motivate a shift to use more renewable energy sources. Biofuels are recognised as some of the most promising forms of alternative energy in reducing greenhouse emissions. An integrated biorefinery is designed to provide a sustainable supply of biochemicals which includes methanol, syngas, glycerol, ether, etc. with minimum fresh resources consumption and waste generation. Via in-plant material recovery, generation of waste can be minimised. Furthermore, the residual of biomass can be used as fuel to generate steam and electricity to fulfill the processes requirement. Thus, the overall energy consumption of an integrated biorefinery will be lower as compare to the process that operates independently.
Due to the complexity of the chemical structure and variation in composition of biomass, there are many challenges in designing an integrated biorefinery. In addition, the unique features of an integrated biorefinery make the process design more difficult than the conventional chemical processes. Therefore, many existing approaches for the synthesis and design of chemical processes may not be directly applicable for the synthesis of integrated biorefineries.
According to the philosophy of pinch analysis, the overall performance targets can be located prior to the detailed network design, which is essential for gaining insight into process bottlenecks. Therefore, it is important to develop a systematic procedure to find performance targets prior to the detailed design of an integrated biorefineries.

In this work, pinch based automated targeting approach that was originally developed for the synthesis of resource conservation networks (Ng et al., 2009b, 2009c) is extended to determine the maximum revenue target for an integrated biorefinery with multiple products. In addition, based on the resulting target, the detailed allocation of raw material (biomass) and intermediate products (e.g., alcohol, syngas, etc.) for different processes to produce final products can be determined. Note that the revenue target for a given feedstock can be determined prior to the detailed process flowsheet and network design of an integrated biorefinery.

2. Problem Statement

The problem of synthesis of an integrated biorefinery may be formally stated as follows. Given a set of biomass sources, SR_i that may be converted to intermediates *p*, INTER_p or products *p'*, $\mathrm{PD}_{p'}$. Each source has given a flowrate, $F_{\mathrm{SR}i}$ and is characterised by carbon fraction, C_i. A set of sinks, SK_j which are process units that can convert sources *i* into intermediates *p*, and products *p'*, is specified. Each sink is characterised by a predefined minimum carbon fraction requirement (C_j^{min}). In addition, the process conversion factors of sources *i* to intermediates *p* (X_{ijp}) and intermediates *p* to products *p'* ($X_{pjp'}$) via SK_j are also specified. The objective of the methodology is to determine maximum revenue from a mix of multiple products and the network design of the integrated biorefinery that meet the target.

3. Automated Targeting

The automated targeting technique was originally developed for mass exchange network synthesis (El-Halwagi and Manousiothakis, 1990). It was then extended to the synthesis of resource conservation network (Ng et al., 2009b, 2009c) based on cascade analysis (Manan et al., 2004). In this work, automated targeting is further extended to the synthesis of an integrated biorefinery. Apart from setting maximum performance target, the model can also determine the network design of the integrated biorefinery.

Based on these previous works (Ng et al., 2009b, 2009c), the technique involves arranging sources/sinks in descending sequence, with highest quality (lowest impurity concentration) located at the top of the cascades. In this work, the sources, sinks, intermediates and products are arranged in a descending order based on carbon fraction level (C_{k}), from the highest level $k = 1$ to the lowest level $k = n$. This step of procedure is called as the construction of a *biorefinery cascade diagram* (BCD) as shown in Figure 1.

The highest value of carbon fraction is added as the first level, if this does not already exist among the process sinks and sources. In addition, a final fictitious level of zero ($C_n = 0$) is added at the bottom of the cascade to allow the calculation of residue carbon load (ε). Next, material flowrate cascading is performed across all levels. At each level *k*, the difference between the total available material sinks ($\Sigma_j F_{\mathrm{SK}j}$) and sources ($\Sigma_i F_{\mathrm{SR}i}$) is determined. The *net material flow* cascaded from the earlier level $k - 1$ (δ_{k-1}) with the flow balance at level *k* form the net material flowrate of each *k*-th level (δ_k) as below:

$$\delta_k = \delta_{k-1} + (\Sigma_i F_{\mathrm{SR}i} - \Sigma_j F_{\mathrm{SK}j})_k \quad (1)$$

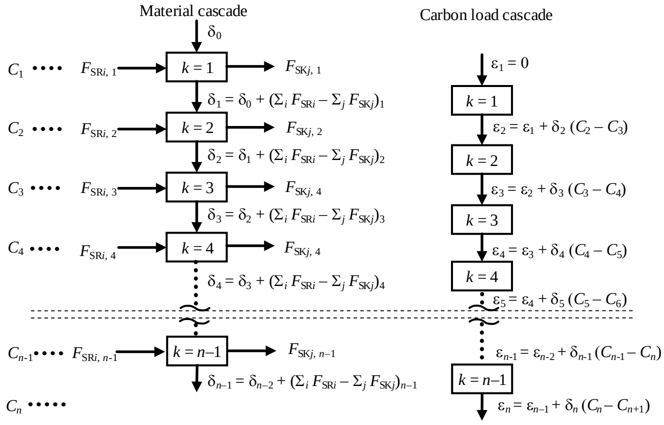

Figure 1: Generic Biorefinery Cascade Diagram (BCD)

To ensure that no additional biomass flow is generated from the final level n, as that level is only used for the calculation of residual carbon load, a new constraint (as shown in Equation 2) is needed.

$$\delta_k = 0 \tag{2}$$

Carbon load cascading is performed next. Within each interval, the carbon load is given by the product of the net material flow from level k and the difference between two adjacent levels. As in the material flow cascade, residual of the carbon load of each level k (ε_k) is cascaded down to the next level. Hence, carbon load balance at the k-th level is determined by Equation 3.

$$\varepsilon_k = \varepsilon_{k-1} + \delta_k\,(C_k - C_{k+1}) \tag{3}$$

where ε_{k-1} is the residue carbon load that is cascaded from level $k - 1$.
Conversely, the residual impurity load, ε must take a positive value, which implies that a feasible carbon load cascade is achieved (Manan et al., 2004; Ng et al., 2009b, 2009c). As such, the maximum allowable carbon load of sink in each level is fulfilled. Equation 4 is included as a constraint in the formulation of the model.

$$\varepsilon_k \geq 0 \tag{4}$$

Note that when the residual carbon load is determined as zero in the model solution at level k ($\varepsilon_k = 0$), a pinch point occurs. In physical terms, the zero carbon load means that, at the optimal solution, the minimum carbon load requirement of all sinks above the pinch point are fulfilled by the sources in order to operate the process sinks (Manan et al., 2004; Ng et al., 2009b, 2009c). Note also that the above formulation is a linear programming (LP) model that can be solved easily to yield global optimal solution if a solution exists.
To determine the maximum revenue solution can be obtained for cases with multiple products which generated from multiple feedstocks, the optimisation objective is set as

Maximise $\Sigma_{p'}$ $(\mathrm{REV}_{p'} \cdot F_{\mathrm{PD}p'})$ (5)

where $\mathrm{REV}_{p'}$ and $F_{\mathrm{PD}p'}$ are the revenue and flowrate of product *p'* respectively. In this work, a hypothetical case study is solved to illustrate the proposed automated targeting for synthesis of integrated biorefinery.

4. Case Study

Tables 1 and 2 show the conversion table and data for a hypothetical case that are used to illustrate the application of the automated targeting approach to the synthesis of an integrated biorefinery. In this work, an idealised biomass (Holtzapple and Grada, 2009) that contains 31.7% lignin ($CH_{1.12}O_{0.377}$) and 68.3% polysaccharides ($C_6H_{10}O_5$) on an ash-free basis is assumed as raw material. The carbon fraction of the biomass is calculated as 0.477. As shown in Table 1, four processes (i.e., digestion, fermentation, gasification and pyrolysis) that convert raw material (biomass) to intermediates are taken into consideration. In addition, four other processes that further convert the intermediates to final products are also included. Theoretical or empirical conversions of raw material to intermediates/products are also included in Table 1.

Since the residuals of biomass from digestion and fermentation processes contain high carbon content and energy potential; hence, further recovery these residues allow the enhancement of the production of biofuel. Thus, both biomass residues are taken as sources in Table 2. The carbon fraction of biomass residues can be estimated based on theoretical or experiment data that reported in the literature. The carbon fractions of digested and fermented biomass residues are given as 0.474 and 0.17 respectively.

On the other hand, four processes (i.e., digestion, fermentation, pyrolysis and gaisification) that accept similar raw materials (i.e., biomass, biomass residue, or mixture of both) to produce various intermediates are taken as sinks (see Table 2). As shown, the minimum requirements of carbon fraction ($C_j^{\min}$) of the sinks to produce intermediates/products are also specified for each sink. It is noted that the processes that further convert intermediates to final products are not taken as process sinks in Table 2 because such processes are not constrained by the carbon fraction of intermediates. In addition, those processes require different raw materials or intermediates to produce final product (biofuel). Examples include Fischer-Tropsch, dehydration and synthetic fuel processes require syngas (carbon monoxide and hydrogen), alcohol and methane/bio-oil, respectively, to produce biofuel.

Table 1: Conversion Table of Biomass to Intermediate and Final Products

Process sink *j*	Raw material	Intermediate *p* / product *p'*	Conversion, X_{ijp} or $X_{pjp'}$ (kg product/kg raw material)
Digestion	biomass	methane (CH_4)	0.147
		biomass residual	0.79
Fermentation	biomass	ethanol	0.27
		biomass residual	0.61
Gasification	biomass	syngas (CO)	0.18
Pyrolysis	biomass	bio-oil	0.54
Dehydration	ethanol	biofuel	0.65
Synthetic fuel	methane	biofuel	0.286
Synthetic fuel	Bio-oil	biofuel	0.1425
Fischer–Tropsch	syngas	biofuel	0.9

Table 2: Data for a Hypothetical Case Study

	Source	Available source (kg)	Carbon fraction (C_i)
SR1	Wood waste	5,000	0.490
SR2	Energy crop	5,000	0.477
SR3	Digested residual biomass	79% inlet biomass to digestion	0.474
SR4	Fermented residual biomass	61% inlet biomass to fermentation	0.170
Sink		**Minimum requirement of carbon fraction (C_j^{min})**	
SK1	Digestion	0.477	
SK2	Fermentation	0.477	
SK3	Pyrolysis	0.250	
SK4	Gasification	0.250	

To locate the performance target, Equations 6 and 7 are included in the automated targeting formulation (Equations 1 – 4).

$$F_{\text{INTER}p} = X_{ijp}\, F_{\text{SR}i} \tag{6}$$

$$F_{\text{PD}p'} = X_{pjp'}\, F_{\text{INTER}p} \tag{7}$$

Based on Equations 6 and 7, the flowrates of intermediates *p* ($F_{\text{INTER}p}$) and final product *p'* ($F_{\text{PD}p'}$) can be determined. Since the biomass residues are taken as SR_i and the flowrates of these sources can only be determined once the model is optimised. Thus, $F_{\text{SR}i}$ of biomass residues are included as variables. To locate the maximum revenue from the product portfolio, the revenue of final products *p'* ($\text{REV}_{p'}$) is specified. In this work, revenue of biofuel, methane, ethanol and bio-oil is given as 0.93 $/kg, 1.02 $/kg, 0.78 $/kg and 0.008 $/kg respectively. Since each intermediate *p* has a market value, it can be considered as final product. To determine the flowrate of multiple products, the mass balances of processes (Equation 8) are included in the model.

$$F_{\text{PD}p'} = F^{\text{I}}_{\text{PD}p'} - F^{\text{I}}_{\text{INTER}p} \tag{8}$$

where $F^{\text{I}}_{\text{PD}p'}$ is the flowrate of product *p'* that produced from first process. Meanwhile, $F^{\text{I}}_{\text{INTER}p}$ denotes the flowrate of product *p'* that require further processing (which also considered as intermediate *p*).

Solving the model with the objective function in Equation 5, subject to Equations 1 – 4 and 6 – 8, yields the results shown in Figure 2. Note that digestion (SK1), fermentation (SK2) and gasification (SK4) processes are involved in this scenario. As shown in Figure 2, 2161.6 kg and 7838.4 kg of biomass are digested into methane and fermented to ethanol, respectively. In this scenario, there are two types of residual biomass (SR2 and SR3) are generated from digestion and fermentation processes. Based on Equation 6, flow of SR2 and SR3 are determined as 1707.7 kg and 4781.4 kg respectively. In addition, the maximum revenue target is found to be $ 2953 when 10,000 kg of biomass is processed. Based on the optimised model, 2116.4 kg of ethanol and 317.8 kg of methane from fermentation and digestion processes, respectively, are taken as final products. Meanwhile, 6489.1 kg of biomass residues from both processes are gasified to

1168 kg of syngas, and then further converted to 1051.2 kg of biofuel via Fischer–Tropsch process. The network design that achieves the target is shown in Figure 3.

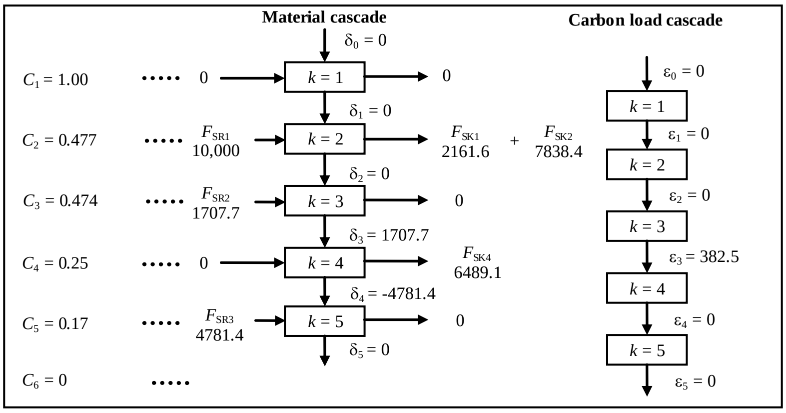

Figure 2: Biorefinery Cascade Diagram for Case Study

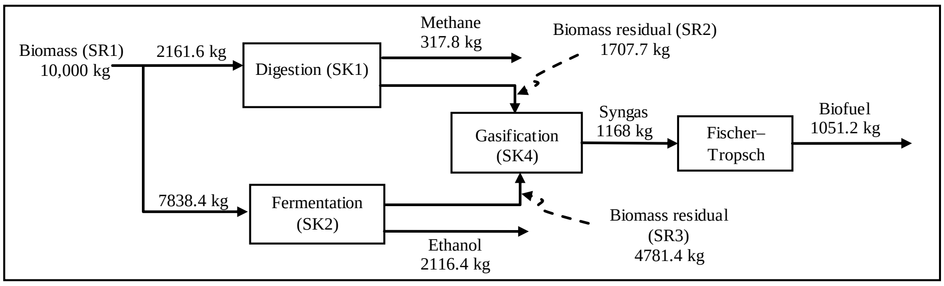

Figure 3: Network design for Case Study

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