Process Synthesis and Optimization of Biorefinery Configurations

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DOI 10.1002/aic.12640

Recently, there has been a growing interest in the development of cost-effective technologies for the production of biofuels. A common approach to biofuel research is to invent or improve a biochemical or thermochemical conversion step. Subsequently, other conversion and separation steps are added to form a complete biorefinery flowsheet. Because this approach is structured around a specific conversion step, it may limit the possibilities of configuring optimal and innovative biorefineries. This article proposes a novel and systematic two-stage approach to the synthesis and optimization of biorefinery configurations, given available feedstocks and desired products. In the synthesis stage, a systems-based approach is developed to create a methodical way for synthesizing integrated biorefineries. This method is referred to as "forward-backward" approach. It involves forward synthesis of biomass to possible intermediates and reverse synthesis starting with the desired products and identifying necessary species and pathways leading to them. In the optimization stage, Bellman's principle of optimality is applied to decompose the optimization problem into subproblems in which an optimal policy of available technologies is determined for every conversion step. An optimization formulation is utilized to determine the optimal configuration based on screening and connecting the optimal policies and generating the biorefinery flowsheet. A case study of alcohol-producing pathways from lignocellulosic biomass is solved to demonstrate the merits of the proposed approach. © 2011 American Institute of Chemical Engineers *AIChE J*, 58: 1212–1221, 2012

Keywords: process synthesis, design

Introduction

With the growing attention to sustainable development, the concept of biorefineries is gaining an increasing attention. A biorefinery is a processing facility that receives biomass feedstocks and produces one or more chemical products and/or biofuels through a system of physical/chemical/biological processes. The resurging interest in biorefineries has been motivated by the dwindling fossil fuel resources and the increasing attention in strategies to reduce greenhouse gas emissions. Several laboratory-scale concepts have been developed for the production of biofuels. However, there are still very few pathways that have been commercialized to meet the technoeconomic criteria for biofuels.

A common approach to the design of biorefinery configurations is to start with a core conversion technology, which is usually in the front end of a biorefinery (e.g., pretreatment, hydrolysis, fermentation, digestion, gasification, and pyrolysis), then add preprocessing and postprocessing units for feedstock preparation and product separation and upgrading. Another common approach is to scale up the same units developed at the laboratory scale and revise the process configuration based on the practical aspects of large-scale production. Although these approaches can lead to process

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configurations that work, their overall performance may not be attractive. Furthermore, they may severely hinder the innovation of new configurations.

This article proposes a novel two-stage approach to the synthesis and optimization for the design of biorefinery configurations. In the synthesis work with specified feedstocks and products, possible pathways are created to include conversion steps that are based on proven reactions or available technologies. A pathway synthesis method referred to as the ''forward-backward'' approach is introduced. It involves forward synthesis of biomass to possible intermediates and reverse synthesis starting with desired products and identifying necessary species and pathways leading to them. In the optimization work to determine an optimal configuration from the synthesized pathways, a preprocessing step of selecting an optimal policy in every conversion step of the pathways is performed. This preprocessing step reduces the size of the subsequent optimization calculations.

Problem Description

The problem can be described as follows: Given a set of biomass feedstocks with known flowrates and characteristics and a desired final product with specifications, it is desired to develop a systematic methodology for the generation of optimal configurations from feedstocks to products. Available for service is a set of conversion technologies with known performance. Various objectives may be considered such as the highest yield, the highest energy efficiency, the shortest route (the least number of processing steps), the minimum-cost route, or the most sustainable route (as characterized by sustainability metrics) Figure 1 shows the inputs and outputs of the problem.

Figure 1. Schematic problem description.

Literature Review

Several important pathways for the production of transportation fuels and chemicals from biomass can be found in literature. Huber et al.[1] provided a review of current and possible future pathways for obtaining transportation fuels. Kamm and Kamm[2] and Fernando et al.[3] reviewed product trees of four biorefinery systems: lignocellulosic feedstock biorefinery, green biorefinery, whole corn biorefinery, and biorefinery with integration of thermochemical and biochemical platforms. Fernando et al.[3] proposed an integration between biorefineries and petroleum refineries to produce 12 potential chemicals in addition to conventional fuels.

Databases of biomass-derived chemicals were developed at National Renewable Energy Laboratory. Werpy and Petersen[4] reported a large collection of chemicals that can be derived from sugar and syngas. Holladay et al.[5] made a similar effort to find the most promising chemicals derived from lignin.

Various techniques have been developed for reaction pathway synthesis. The earlier work in the 1970's was reviewed by Agnihotri and Motard[6] and Nishida et al.[7] Proposed techniques in that period included matrix synthesis approach,[8] symbol triangle approach,[9] retrosynthesis approach,[10,11] minimum Gibbs free energy approach,[12] and geometry synthesis approach.[13] The approach using Gibbs free energy was further developed in the 1980's.[6,14,15] In the 1990's, environmental aspect was incorporated in the synthesis of reaction pathways.[16–18] Recently, optimization-based approaches[19,20] and an evolutionary technique[21] for reaction path synthesis were introduced.

A systematic approach to the synthesis of optimal biorefinery pathways was reported by Bao et al.[22] The approach is based on the development of a superstructure of conversion technologies and resulting intermediate chemicals then using a tree-branching and searching technique to determine candidate pathways.

Several articles have focused on the technoeconomic analysis and optimization of specific production pathways such as ethanol,[23–27] biodiesel,[28,29] mixed alcohols and transportation fuels,[30–32] and energy.[33,34] There is also research to establish processing routes with minimum energy consumption before establishing the optimal products.[3,35–37] Elms and El-Halwagi[38] introduced an optimization routine for feedstock selection and scheduling for biorefineries and included the impact of greenhouse gas policies on the biorefinery design. Pokoo-Aikins et al.[39] included safety metrics along with process and economic metrics to guide the design and screening of biorefineries.

The optimization problem to determine the best pathway from the synthesized ones has been investigated by several researchers. Optimization has been carried out based on yield,[22] entropy analysis,[40] optimization framework,[41] and modular platform.[42] Ng[43] used a pinch analysis for an automated targeting procedure to find the highest production rate and revenue without a detailed design of biorefineries. Alvarado-Morales et al.[35] applied principles of group-contribution for prediction of pure component properties to simultaneously model, design, and synthesize biorefineries.

Proposed Approach

The next two sections discuss the proposed approaches for the synthesis and the optimization tasks. Subsequently, the overall framework with key steps for solving the problem will be described.

The synthesis problem

To avoid the generation of complex (and potentially impractical) configurations, the number of conversion steps in the synthesis problem is limited to five. Each conversion step is a reaction system (a reactor or a set of reactors), followed by separation units necessary to purify the produced chemicals to appropriate levels for the next conversion steps. Pretreatment of lignocellulosic biomass is not counted as one of the conversion steps. The synthesis approach involves forward synthesis of biomass to possible intermediates and reverse synthesis starting with the desired products and identifying the necessary species and pathways leading to them. Once the feedstock-forward and the product-backward pathways are synthesized, two activities are carried out:

"matching" (which corresponds to direct connection of two species if one of the species synthesized in the forward step is also generated by the backward step) and "interception" (which refers to the addition of a conversion steps to convert a forward-generated species to a backward-generated species). The interception task may be detailed by identifying known processes to achieve such conversion or by using reaction pathway synthesis to link the two species.

Figure 2 is an illustrating example of the branching trees. Each node represents an intermediate compound (i.e., a species) and each arc represents a conversion step. In the forward branching problem, the branching starts from the feedstock node. The nodes connecting to the feedstock node are compounds that can be directly produced from the feedstock through one conversion technology. Two forward steps are allowed from the feedstock. For example, a carbohydrate feedstock can be converted into methane (by digestion), sugar (by enzymatic hydrolysis), syngas (which is a mixture of carbon monoxide and hydrogen, by gasification), and so on. The next layer of nodes lists compounds that can be produced from the compounds at the previous nodes. For example, acetylene is produced from methane (by cracking). This is called the "forward problem" because the branching direction is cocurrent with the processing flows.

In the reverse problem, the branching originates from the final product node and is counter-current to the processing flows. Two backward steps are taken from the final product. For example as shown by Figure 2, node bromoethane (C_2H_5Br) connects to node ethanol because bromoethane can be hydrolyzed into ethanol. One of the chemicals that can be used to produce bromoethane (by hydrobromination) is ethylene.

Next, nodes from the forward branching tree and from the backward branching tree are connected in one of two ways: matching or interception. An example of matching is when sugar appears as both forward and backward nodes (see Figure 2). By connecting the two sugar nodes, a pathway is created from biomass to ethanol. An example of interception is the use of hydrogenation step (see Figure 2) to connect nodes acetylene (C_2H_2) and ethylene (C_2H_4), making another complete pathway from the biomass to the ethanol.

As a result of the synthesis problem, one or more complete pathways connecting a feedstock and products are found. Although based on known building blocks, the generated pathways can be novel because of their interconnections. The generated pathways can also be quickly constructed and screened. Figure 3a is an example of a superstructure of synthesized pathways. Lettered nodes represent intermediate compounds. Between each two nodes, there can be more than one pathway (e.g., the pathway from Feedstock to E) or arc (e.g., A-G, D-E, E-H, and F-I). It is useful to identify optimal pathways between nodes. This is described in the next section.

The optimization problem

In this proposed approach, a parameter-optimization step is performed first. In this step, a set of design parameters $\boldsymbol{x}_{ntn'}$ is designated for each conversion technology, t, that produces species n' from species n. The objective is to optimize the objective values $r_{ntn'}$ as follows:

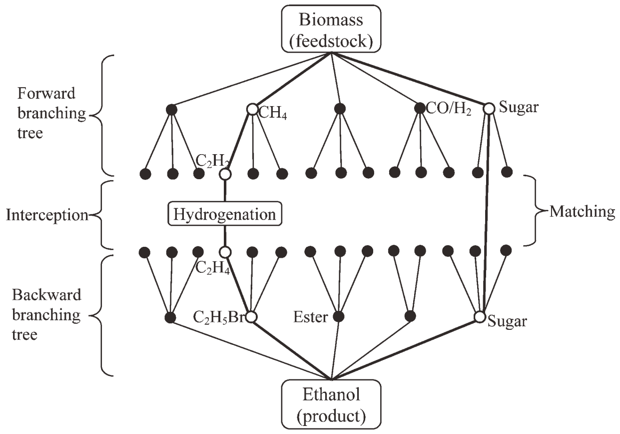

Figure 2. Exemplary forward and backward branching trees.

Problem P_0:

$$r_{ntn'} = \min_{x} Y(x_{ntn'}) \text{ for every } t \tag{1}$$

$$\text{Subject to}: h(x_{ntn'}) \le 0 \tag{2}$$

$$g(x_{ntn'}) = 0 \tag{3}$$

The objective function of this optimization problem may be defined as the conversion step with the highest yield, the highest energy efficiency, the simplest, the minimum cost, the maximum profit, and so om. The constraints of the formulation include:

- Key performances of processing technologies: yield, conversion, and so on.
- Mass balances.
- Energy balances.
- Capital cost.
- Operating cost.

In this step, detailed analysis can be performed using available data and/or appropriate levels of simulation.

It is not uncommon to have multiple routes connecting two adjacent nodes. To reduce the complexity of the design problem, it is useful to determine optimal routes among the nodes. In this context, it is proposed to use Bellman's principle of optimality[44] to decompose the optimization problem into several subproblems. The principle of optimality is stated as follows[44]: "An optimal policy has the property that whatever the initial state and initial decision are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision."

For network problems of the type addressed here in the biorefinery pathway synthesis, the principle of optimality may be stated as follows[45]: "There exists a policy that is optimal for every node."

Hence, an optimal policy is first identified for subproblems. Each subproblem corresponds to identifying the optimal conversion route between a pair of nodes. Specifically, two types of subproblems are considered:

Arcs directly connecting two adjacent nodes (e.g., the three arcs connecting nodes F and I in Figure 3a).

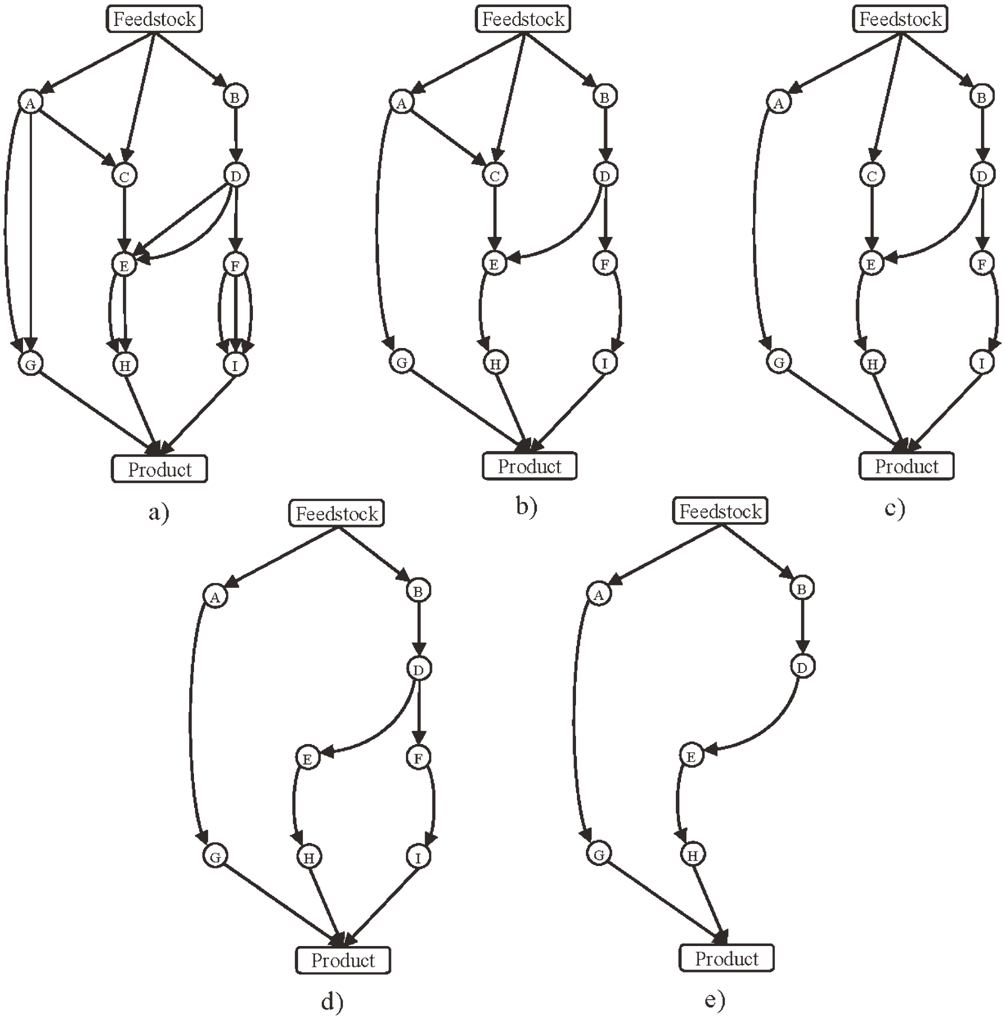

Figure 3. A superstructure of synthesized pathways representing conversion technologies (arcs) and intermediate chemicals (nodes).

(a) With all brainstormed arcs and nodes, and after applying the principle of optimality to pathways connecting: (b) every pair of adjacent nodes, (c) Feedstock—C, (d) Feedstock—E, and (e) D—Product.

Problem P_1:

$$r_{nn'} = \min_{t} r_{ntn'} \tag{4}$$

where $r_{nn'}$ is the objective value of the optimum arc connecting two adjacent nodes, $r_{ntn'}$ is the objective value of the arc using technology t and connecting the two adjacent nodes n and n'.

Routes connecting two nonadjacent nodes through different intermediates (e.g., in Figure 3a, nodes Feedstock and E connected through the route Feedstock-C-E vs. the route Feedstock-B-D-E).

Problem P_2:

$$r_{ij} = \min_{t} f(r_{ntn'}) \tag{5}$$

where r_{ij} is the objective value of the optimum route connecting two nonadjacent nodes i and j, and $r_{ntn'}$ is the objective value of the arc using technology t and connecting the two adjacent nodes n and n'.

As a result of solving Problems P_1 and P_2, optimal policies are determined and the superstructure is simplified to one of the levels as shown in Figure 3b–e. This is done before solving the superstructure-optimization problem.

Next, an optimal configuration from the synthesized and locally optimized pathways (the simplified superstructure) is determined by solving either a linear programming formulation or dynamic programming algorithm. As for the approach of linear programming formulation, the following problem is solved:

Problem P_{3a}:

$$r_{1N} = \min_{i,j} f(r_{ij}) \tag{6}$$

where r_{1N} is the objective value of the optimum pathway connecting nodes feedstock and product, and r_{ij} is the objective value of the optimum route connecting two nonadjacent nodes i and j.

If the objective functions are nonlinear, Problem P_{3a} is difficult to solve globally. In such cases, the following approach of dynamic programming is recommended to obtain the global optimum. The approach of dynamic programming algorithm is based on the functional equation:

Problem P_{3b}:

$$r_{1n'} = \min_{n} f(r_{1n}, r_{nn'}) \tag{7}$$

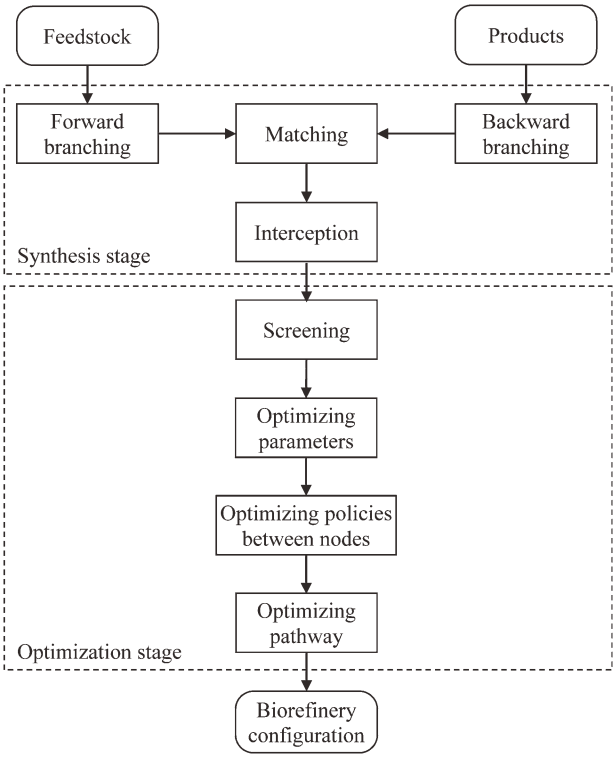

Figure 4. Framework for the synthesis and optimization of biorefinery configurations.

where r_{1n} and $r_{1n'}$ are the objective values of the optimum routes connecting nodes Feedstock – n and Feedstock – n' respectively. n and n' are two adjacent nodes and the path direction is $n \rightarrow n'$.

Using the functional equation, $r_{1n'}$ can be determined once r_{1n} is known for every n and n' such that (n, n') is an arc. The algorithm starts from the first node (feedstock) and ends at the last node (product). This algorithm is called forward optimization in dynamic programming. The reverse algorithm that starts from the last node and is similarly developed is also applicable.

Framework for the synthesis and optimization of biorefinery configurations

The proposed framework for the synthesis and optimization of biorefinery configurations is shown in Figure 3. Starting from the input information on feedstock and products, the following steps are performed in sequence:

1. Forward and backward branchings: These two branching steps enumerate as many intermediate compounds (and associating conversion technologies) as possible. Those compounds can be produced from the feedstock (in forward branching problem) or converted into the final product (in reverse branching problem).
2. Matching: Some of the branches of the two trees are connected to yield complete pathways (from the feedstock to the final product) by identifying the identical intermediate compounds.

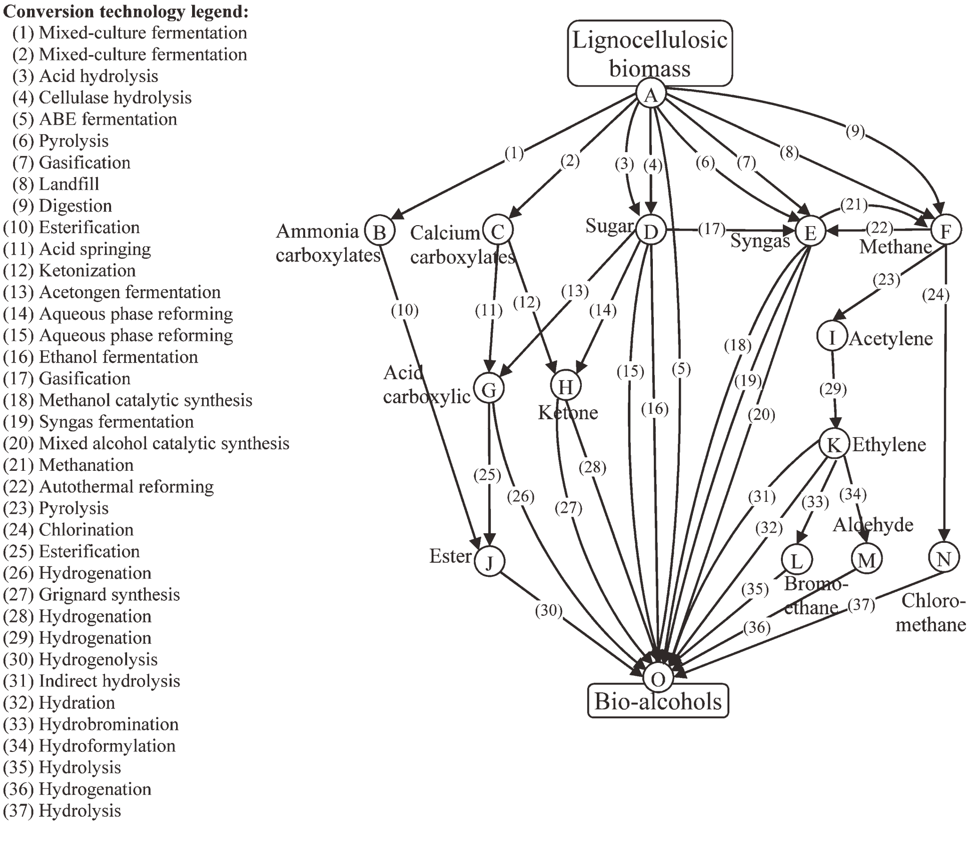

Figure 5. Part of the branching trees for the production of bio-alcohols from lignocellulosic bio-mass.

Table 1. Conversion Steps Eliminated Based on Low Yield

Conversion step	Feed	Product	Yield	Yield base	Reference
(6) Pyrolysis	Biomass	Syngas	Max 29.2%	Biomass weight	Goyal et al.[48]
(14) Aqueous phase reforming	Sugar	Ketones	23.7%	Fed carbon weight	Blommel and Cortright[49]
(15) Aqueous phase reforming	Sugar	Alcohols	8.7%	Fed carbon weight	Blommel and Cortright[49]
(19) Syngas fermentation	Syngas	Alcohols	53.1%	Carbon monoxide weight	Piccolo and Bezzo[50]
(24) Chlorination	Methane	Chloro-methane	Max 12%	Methane weight	Schmittinger[51]

3. Interception: When two compounds on the edging layers of the branching trees are not connected, it is possible to identify known processes or reactions that will link the two compounds. This is referred to as ''interception.''

4. Screening: Based on simple technical and economic analyses, this step eliminates the synthesized pathways that are too complex, thermodynamically infeasible, economically infeasible, or have too low yields. The elimination reduces the work load in the next steps without sacrificing optimal pathways.

5. Optimizing parameters: Before solving the superstructure-optimization problem, the design parameters are optimized for every synthesized pathway in this optimization step. Analyses (include simulation and technoeconomic analysis) can be performed at different levels of details.

6. Optimizing policies between two nodes: Based on the connectivity between the nodes, two types of these subproblems are solved: adjacent and nonadjacent. For the former subproblem, technologies that process the same nodes are compared for the identification of an optimal one. However, there can be cases in which a series of conversion steps are considered at the same time for a global optimum. For these cases, the latter subproblem is solved. Based on the principle of optimality, this step reduces the number of synthesized pathways without affecting the final results of the optimization problem.

7. Optimizing pathways: Either a linear programming formulation or dynamic programming algorithm is used to determine the optimal configuration from the superstructure of synthesized pathways.

These steps are categorized into two stages: a synthesis stage (which includes the first three steps) and an optimization stage (which includes the remaining four steps). The output of the framework is a biorefinery configuration, which is technically feasible and optimum according to the given data. The configuration comprises not only the optimized pathways between feedstock and final products but also some open branches connecting to the pathways which represent byproduct production.

Case Study

It is desired to synthesize pathways that produce fuel-grade alcohols from lignocellulosic biomass and to determine the most cost-effective pathway. The proposed procedure for the solution is applied as described in the ensuing steps.

First, the branching and matching were performed. A tree of forward branching search from the feedstock was constructed. This tree tracks the compounds that can be produced from the lignocellulosic biomass within two conversion steps. Another tree starting from the bio-alcohol node

Table 2. Data for the Pathway Nodes and Prescreening Results

Node	Feed	Product	Route*	Key comment	Reference
A → F	Biomass	Methane	(7) Gasification and (21) Methanation	Production cost: \$8.53/GJ of methane	Gassner and Maréchal[52]
			(8) Landfill	Production cost: \$1.90-\$3.79/GJ of methane	EPA[53]
			(9) Digestion	Production cost: \$0.20-\$0.55/GJ of methane	Gray[54]
A → E	Biomass	Syngas	**(7) Gasification**	Energy efficiency: 82.8%	Hamelinck and Faaij[55]
			(9) Digestion and (22) Autothermal reforming	Energy efficiency: 63%	Calculation
H → O	Ketones	Alcohols	(27) Grignard synthesis	Yield is 82-88%	Carey and Sundberg[56]
			(28) Hydrogenation	Yield is 100%	Chang[57]
K → O	Ethylene	Ethanol	(31) Indirect hydrolysis	Well developed and commercialized in 1960s but phased out due to less economic than hydration.	
			(32) Hydration	Simple, direct, and most costly effective pathway	
			(33) Hydrobromination and (35) Hydrolysis	Involve many more steps than hydration pathway	
			(34) Hydroformylation and (36) Hydrogenation	Involve many more steps than hydration pathway	
G → O	Acid carboxylic	Alcohols	**(25) Esterification and (30) Hydrogenolysis**	Include mild esterification (203 kPa and 50°C) and hydrogenation (160°C and 405 kPa)	Kiff and Schreck[58]
			(26) Hydrogenation	Involve furnace, intense hydrogenation (230-270°C and 4.1-7.1 MPa), and expensive molecular sieve.	Kiff and Schreck[58]
E → O	Syngas	Methanol	**(18) Methanol synthesis**	Production cost (\$2010): \$19.98/GJ methanol†	Hamelinck and Faaij[55]
	Syngas	Alcohols	(20) Mixed alcohol synthesis	Production cost (\$2010): \$19.98/GJ methanol‡	Bechtel[59]

*The numbers in parentheses correspond to the conversion technologies with the numbers listed in Figure 5. Bold routes are optimal ones connecting the two nodes based on pre-screening.
†20% was added to account for additional cost of processing municipal solid waste.
‡A additional cost of \$0.425/gal was added to account for biomass feedstock.[60]

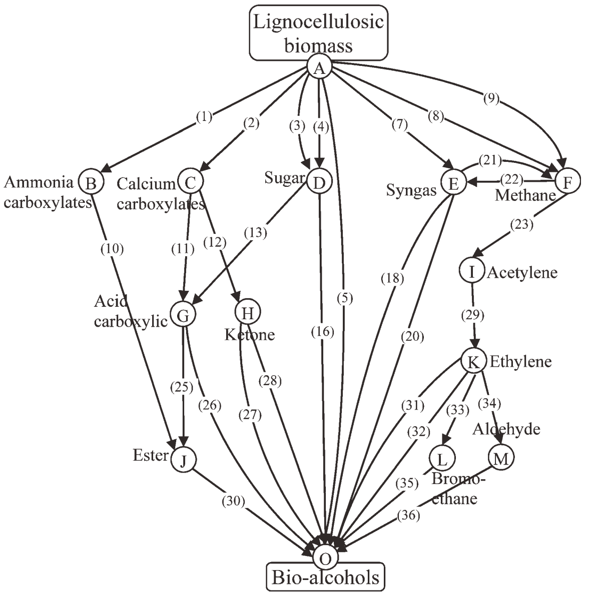

Figure 6. The superstructure of synthesized pathways after the screening step.

was built to enumerate compounds from which the bio-alcohols can be derived. The enumeration in each direction is limited to two conversion steps to avoid an unnecessarily exhausting blind search. After the branching searches were done, the matching and interception steps were performed to identify complete pathways. Figure 4 shows a part of the two branching trees with identified complete pathways. Compounds, associating conversions, and unmatched branches are not presented for a clearer presentation. In the figure, it is not necessary to note to which layer a specific compound belongs. The left-hand side of the figure collects biochemical pathways while the other side collects mostly thermochemical routes. The upper half (which is front-ends of biorefineries) includes biological conversions while the lower half involves chemical conversions.

Next, the screening step was performed. The processing technologies 6, 14, 15, 19, and 24 are eliminated due to their very low yields (Table 1). Arc 37 is disregarded despite its high theoretical yield, because the associating pathway is incomplete after the elimination of the arc 24. In another case, arc 17 is eliminated based on a simple economic analysis (it is not economically feasible to obtain syngas by performing expensive hydrolysis[46] (arcs 3 and 4), then drying the sugar solution and gasifying the produced sugar (arc 17). The direct gasification of the feedstock (arc 7) is obviously more cost-effective to produce the syngas, because it uses less equipment, conversion, and separation steps. Note that although the routes involving arcs 3–17 and 4–17 are eliminated, the arcs 3 and 4 are kept because they are parts of other routes, for instance, through the one involving arcs 3, 14, and 28. Figure 6 shows the superstructure after the screening step. It is possible for an arc to connect the feedstock and the product to form a pathway. For example, the pathway via arc 5 comprises only one conversion step, which is acetone-butane-ethanol (ABE) fermentation (pretreatment as well as other treatment and separation are not considered as conversion steps in this branching-tree presentation).

In this case study, the parameter-optimization step to optimize the process designs (Problem P_0) was not performed, because the overall objective values (production costs) of most of the pathways can be found in the available literature on the technoeconomic analyses (with some extent of optimization).

The next step is to optimize the policy between nodes. The technologies used for adjacent nodes were compared to find the most costly effective ones (Problem P_1). These pairs of technologies were considered: (27 vs. 28) and (18 vs. 20). Then, another type of subproblems (Problems P_2) is solved to determine the optimal routes connecting the nonadjacent nodes: A → E, A → F, K → O, and G → O. The objective function of these subproblems is the minimization of the production costs which has to be identical to that of the overall optimization problem. This work uses information of the production costs of these conversion steps from published data (with adjustments for the time value of money, location, and production capacity). In some cases where such economic information may not be available, simulation and heuristics can be used to determine the optimal ones. Table 2 summarizes the policy optimization between nodes. At the end of this step, the superstructure is simplified as shown in Figure 7.

In the next step, the optimization problem P_{3a} is solved for an optimal pathway of the simplified superstructure. Most of the production costs of the biomass-to-alcohol pathways were available in published technoeconomic analyses. The cost estimation from previous years was updated to year 2010 dollar value using the Producer Price Index for Chemicals and Allied Products published by the U.S. Department of Labor.[47] As all pathways start with the given feedstocks, the feedstock costs were excluded for the comparison of production costs. As different alcohols may be produced, the product price was calculated as \$/GJ to have a consistent basis. The result of this optimization step is summarized in Table 3.

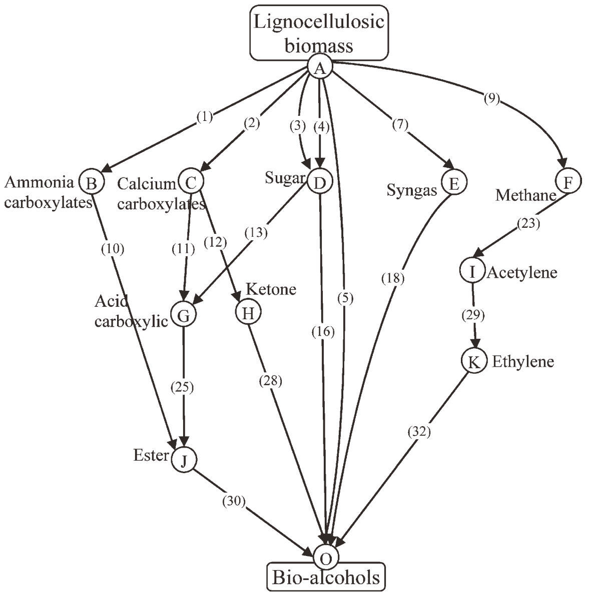

Figure 7. The synthesized superstructure after the step of optimization between nodes.

Table 3. Cost Data for the Pathway

			Base year				Year 2010			
			Capacity	Product cost†	Energy density			Alcohols cost		
Pathways	Description	Product	MMGPY[a]	$/gal	MJ/gal	Date	PPI‡	$/gal	$/GJ	References
A→B→J→O	Mixed alcohols production via acid fermentation and esterification	Mixed alcohols	45	1.21	92	2007	213.7	1.39	15.14	Granda et al.[61]
A→C→H→O	Mixed alcohols production via acid fermentation and ketonization	Mixed alcohols	35	1.44	101	2009	229.4	1.54	15.28	Pham et al.[62]
A→D→G→J→O	Ethanol production via acetongen fermentation and ester synthesis	Ethanol	n/a	n/a	n/a	n/a	n/a	n/a	n/a	The Zeachem process
A→D→O	Ethanol production via hydrolysis and yeast fermentation	Ethanol	50	1.03	79	2003	161.8	1.56	19.69	Hamelinck et al.[46]
A→O	Mixed butanol and ethanol production via ABE fermentation	Mixed alcohols	n/a	1.50	110	2007	214.8	1.71	15.47	Pfromm et al.[63]
A→E→O	Methanol production via biomass gasification	Methanol	24	0.61	59	2001	151.8	1.18	19.98	Hamelinck and Faaij[55]
A→F→I→K→O	Ethanol production via syntheses of methane, acetylene, and ethylene	Ethanol	13	2.74	79	2008	245.5	2.73	34.43	Calculation

*MMGPY: Million gallons per year of products. Online operation is 8000 hours per year.

†All the product costs exclude feedstock costs.

‡PPI: Producer Price Index for Chemicals and Allied Products. PPI in 2010 (245.1) is the average from January to July.

The calculation results show that the following pathways are the most economically attractive routes: Mixed alcohols production via acid fermentation and esterification (A→B→J→O; $15.14/GJ of products). Mixed alcohol production via acid fermentation and ketonization (A→C→H→O; $15.28/GJ). Mixed butanol and ethanol production via ABE fermentation (A→O; $15.47/GJ).

As the calculated costs of these three configurations are relatively close, additional analyses must be carried out. This is consistent with the stated objective of the devised approach, which is aimed at the quick screening of pathways to generate a set of attractive configurations that can be later screened in more details.

Conclusions

A new methodology for the synthesis and optimization of biorefinery configurations was proposed and demonstrated for a case study of producing fuel-grade alcohols from lignocellulosic biomass. The proposed forward and backward branching techniques along with matching and interception steps are used to synthesize the biorefinery pathways based on known conversion technologies. Bellman's principle of optimality can be applied to decompose the optimization problem into subproblems that can be readily solved to reduce the number of possible pathways from the synthesized ones without missing the globally optimal solution. The methodology is a systematic way to quickly synthesize and screen biorefinery pathways so as to generate promising pathways that can be assessed in more details.

Acknowledgment

Financial support by the U.S. Department of Energy is gratefully acknowledged.

Notation

Parameters

r = value of objective function
x = design parameter.

Indices

i = node adjacent to node j in the synthesized branching trees
j = node adjacent to node i in the synthesized branching trees
n = node in the synthesized branching trees
n' = node in the synthesized branching trees
N = the final (product) node.

Functional notations

f = function of objective values regarding constituent conversion steps
g = function of mass and energy balances, and other equality relations
h = function of specification and limitation constraints of the optimization problems
Y = function of design parameters.

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Manuscript received Jan. 18, 2011, and revision received Mar. 13, 2011.