Perspective

Conceptual Process Design: A Systematic Method to Evaluate and Develop Renewable Energy Technologies

Aniruddha A. Upadhye, Wei Qi, and George W. Huber
Dept. of Chemical Engineering, University of Massachusetts, Amherst, MA 01003

DOI 10.1002/aic.12733
Published online July 29, 2011 in Wiley Online Library (wileyonlinelibrary.com).

Keywords: conceptual process design, renewable energy, biofuels, engineering economics

Introduction

Since the 19th century, fossil fuels have been the major source of energy for our everyday energy requirements. However, over the past few decades, increasing energy needs from developed and developing countries, depleting fossil fuels reserves and environmental concerns over consumption of fossil fuels have necessitated our society to look for renewable, sustainable and environmental friendly sources of energy. Breakthroughs in the fields of chemistry, biology, catalysis, biochemistry, solar and wind energy technology, and fuel cell technology have been reported to show great potential toward providing viable energy alternatives to fossil fuels. Governmental funding agencies are currently putting in hundreds of millions of dollars into various types of basic research that promises to revolutionize the fields of renewable energy. The fundamental challenge with all alternative energy technologies is economics. These new breakthroughs have to be economically competitive with fuels and energy obtained from existing fossil resources if they are to have a world-wide societal impact. Unfortunately, many of these new reported "scientific breakthroughs" do not report on the economic impact of their discovery. Furthermore, scientists trained in the fields of biology, chemistry or physics do not have the technical training to evaluate the economics of new technologies.

A method for quickly evaluating "novel energy producing processes" is imperative for the rapid development of alternative energy technologies. Unfortunately many times, much money and time is lost investing in technologies that are bound to fail. Often times at the start of the project a good engineer could tell if a project has the possibility of making economic sense. A method of estimating the economic potential of a technology needs to be fast enough to provide results within a few days or weeks. Fortunately, the chemical engineering field has long recognized the importance of being able to quickly evaluate the economics of a new process or idea using conceptual process design which is a subset of process design. Conceptual process design can provide a systematic framework to rapidly evaluate new technologies.[1–3] While a detailed process design can take several engineers, several months to complete, a rapid conceptual process design can be done with one engineer working for several days.

Conceptual process design can also be used to guide future research efforts and speed up development time of a technology. Conceptual process design identifies the steps within a process that are the most expensive providing insight into how costs can be reduced and guiding where future research efforts should be directed. In this perspective we will provide some background on conceptual process design and give an example of how it can be used to estimate the economics of a simple process. While the focus of this Perspective is on using conceptual process design for evaluating biomass conversion technologies,[4] this same approach can also be adopted for other alternative energy projects. Conceptual process design is critical for using our renewable energy resources as efficiently as possible as well as reducing the development time for commercializing new technologies. It is a highly underused tool in the sciences which has led to the investment in technologies that are not economically viable and the squandering of private and public investments.

Unfortunately, process design does not receive funding from most major US research agencies. Conceptual process design has been viewed as a mature field that should primarily be funded by industry. The reason for this is probably that the petrochemical industry has matured and new petrochemical processes have not been built in the U.S in recent years. However, with the increased focus on renewable energy many new processes are being developed. For

Aniruddha A. Upadhye and Wei Qi are joint co-authors.
Correspondence concerning this article should be addressed to G. W. Huber at huber@ecs.umass.edu.

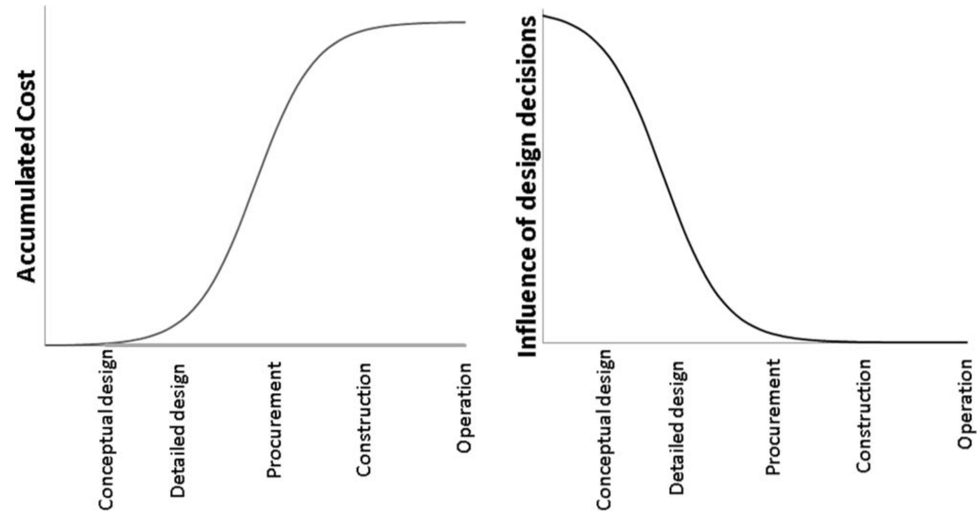

Figure 1. Accumulated cost/Influence of decisions vs. stage of process development.
(Adapted from Towler and Sinnott[11]).

example the Dept. of Energy Office of Biomass program is currently supporting 29 integrated biorefinery projects at pilot (12), demonstration (11), and commercial (4) scale to make renewable transportation fuels from biomass.[5] These new projects are causing the need for the rediscovery of conceptual process design.[6] If academics are not going to do process design then it is likely that they will not be able to invent any new technologies that will have a long term economic impact. It is also highly unlikely that industry will share their process design analysis to guide academic research. Therefore, if we are to truly tackle the challenge of replacing our fossil fuel resources then we need to clearly understand the economics of the renewable energy alternative technologies.

Energy is a commodity that has low margins and high volumes. Thus, an effective process design is necessary for the process to be economically successful, making process design even more important for the energy industry.[7] Today, about 85 million barrels of crude oil are processed every day in the world, with the largest refinery processing 1.24 million barrels per day.[8,9] Because of such high-production rates, these industries take advantage of economy of scale in ensuring the economic viability of the project. Hence, even a small change in production efficiency results into large differences in energy efficiency. In the current petroleum-based industry, raw materials (crude oil) dominate the cost of production. It is expected that as we move from the conventional sources to renewable biomass sources, the cost of processing will be more important than raw material costs.[10] Therefore, conceptual process design will be a critical tool for developing cost-effective processes to solve the problem of our ‘‘energy crisis’’. We believe that the field of process design will be of growing importance in the future as we continue to work toward reducing our dependence on fossil fuels. We recommend that all the scientists working in the area of renewable energy collaborate with engineers that have conceptual process design experience that can help guide the design of the future research efforts. Conceptual process design is a powerful tool that can be used to guide scientific discoveries and help rapidly move them toward commercial reality.

Conceptual Process Design

The design, construction and operation of any chemical process is typically done in five different stages shown in Figure 1.[11] In the first stage, the conceptual design stage, the process flow sheet is drawn, and the major types of equipment are decided upon. Most influential decisions are made at this first stage, with very little money spent. The second stage is the detailed design. In this stage most of the detailed engineering work is done including the drawing of detailed process and instrumentations, obtaining contractor estimates for the equipment fabrication, the discussion of startup and shutdown strategies, the optimization of process variables and the drawing of the ‘‘best’’ possible flow sheet. At this stage most of the engineering decisions are already made. The costs start to increase as these detailed engineering designs are completed and making changes to the process becomes increasingly more expensive. The next two stages are procurement of the equipment and construction of the facility. These are the stages with the largest cash outflows and the smallest flexibility in accommodating changes in the design; here changes in the process are extremely costly. The last stage is operation of the plant. A commonly accepted rule of thumb[12] is that $1 spent to improve the conceptual design corresponds to a cost of $100 if the same change was implemented at the detailed design stage, $1,000 after the process is constructed, and $10,000 after process failure.

In practice, very few (<1%) of the new designs ever become commercialized. Thus, there are hundreds of preliminary design alternatives for every new process. The processing costs associated with most alternatives differ by an order of magnitude or more. Therefore, we can use shortcut calculations to screen most alternatives. The profitable designs can then be assessed in terms of additional factors such as safety and environmental constraints, operational flexibility, controllability,[13] and overall economic optimization.

Conceptual design can also be used as a research tool in planning and guiding laboratory experiments. It has been argued that ''sometimes the best way to plan an experiment is to develop a design model''.[14] Laboratory chemists expend significant effort on improving conversion with a ''favorite'' solvent or with a ''favorite'' amount of solvent, which could turn out to be not economical due to the high cost of solvent separation. Integrating experiments with the conceptual design can help avoid this situation by giving guidance of the economical range of experimental parameters. Thus, doing some basic conceptual design experiments could save substantial amount of chemist's efforts, resources and time. Integrating conceptual design early in the project can help speed up development time by focusing the experimental work.

A process design problem can be solved using a variety of different approaches.[1] In the hierarchical approach[2,3] of conceptual process design by Douglas, one decomposes a very large and complex problem (e.g., a detailed design of a renewable energy refinery) into a number of smaller problems that are much simpler to handle.[2,3,15] Typically, one may decompose the conceptual process design into six hierarchical levels as listed in Table 1. In this manner, the process design proceeds with minimum added effort at each level and systematically eliminates poor designs without investing unnecessary effort to obtain a complete solution. If the results seem promising, then one proceeds to obtain the necessary information required by the next level of analysis, and add the successive layer of detail to the design.

As shown in Table, the proposed approach starts with Level-0 design where all the relevant information about the process is obtained. This information ranges from obtaining physicochemical data of the raw materials, to the market analysis of the feedstock and products. It is common to find that the available data may not be enough or accurate at early phases of the projects, especially for a biomass conversion project. In such case the designer can begin the conceptual design using the most optimistic scenarios of uncertain information, and then revise the design with updated information. At Level-1 the pivotal decision of whether to run the process in batch or continuous mode is made, using information obtained in Level-0, and that sets the framework for the development of the pertinent class of process flow sheets, which starts at Level-2. At Level-2 a box is drawn around the entire process and only the input-output structure of process flows is considered. This is the most basic flow sheet structure for the process, but some of the most important decisions regarding the raw materials and products are made at this level of design. In Level-3 the reactor and the recycle streams are added to the process description, allowing the quantification of the associated costs. Most processes use one reactant in excess or use an inert for reducing reactant concentration, thus, this becomes an important level of process design.

In Level-4, one designs the separation system which accounts for a large percentage of the total cost in a chemical process. Thus, decisions made at this level of design often determine the profitability of the project. In Level-5, heat integration, one looks to conserve energy and reduce load on utilities by integrating heat exchangers. The process flow sheet obtained at the end of this stage can then be used for detailed engineering analysis and further optimization.[16,17] Often, at the same level, different process alternatives are generated, we prefer to complete the design for the most promising alternative, and then use it as a base-case design. With the base-case as a reference we can examine a stream of alternatives better and faster. This strategy corresponds to the ''depth-first'' strategy suggested by Douglas,[8] and is viewed as a more efficient approach than the alternative ''breadth-first'' in shorting alternatives and selecting the ''best'' design.

Throughout this analysis one uses engineering economics, with progressively more detailed economic models, as a tool to evaluate the process alternatives. At each level, when economic potential becomes unfavorable, the designer must understand the underlying causes (i.e., the engineering decisions that lead to unfavorable designs), and look for alternatives. For some design decisions there are heuristics or rules of thumb available for guidance.[3,11,18] Simple correlations can be used to generate cost estimates for the equipment, operations and utilities.[3,11,18] This simple yet powerful approach enables the designers to quickly screen numerous alternatives. The methodology is extremely useful in calculating order of magnitude cost estimates and developing an effective process flow sheet, especially when it is supported by modern computer-aided engineering tools, such as Aspen Engineering Suite, which provides effective modeling of processing units, estimation of physical properties, simulation of the complete design and assessment of its economic potential, after the various designs have been composed at Levels-3, -4, and -5.

Example of Conceptual Process Design Applied to Manufacture of Tridecane from Aqueous Hemicellulose Stream

Brief description of the process

In this section, the authors will provide a brief illustration of the hierarchical approach[2,3] in conceptual process design, described in the previous section, as it was applied in the synthesis of a new process for generation of fuels from a biorenewable raw material, i.e., the conversion of aqueous hemicellulose into tridecane,[19] a chemical that has found use in jet/diesel blends.

The aqueous hemicellulose stream can be obtained as a byproduct from wood processing industry[20] and can be produced from lignocellulosic biomass via hot water extraction or acid hydrolysis process.[21,22] The hemicellulose stream consists of monomers and oligomers of xylose and other 5-carbon sugars, whose composition depends on the severity of hydrolysis conditions.[23,24] For this analysis, the hemicellulose stream is considered as a mixture of monomers and oligomers of xylose in water.

Figure 2 shows the chemistry involved in the conversion of hemicellulose to tridecane. The first step in the process is the dehydration of the xylose to furfural. Dilute HCl is used as a catalyst for the dehydration reaction. In the process, oligomers of xylose can also be hydrolyzed to xylose monomers thereby reducing the requirement on the

Table 1. A Hierarchical Approach to Conceptual Process Design

Level	Decision(s) to be made/Information required	Output(s) to process
0	**Input information**	
	1. The information about the reactions and catalysts*	1. Location of process
	2. Availability of raw materials	2. The raw materials resources and purities
	3. Product specification*	3. Process scale
	4. Processing constraints*	4. Product composition specification
	5. Potential related plant and site data*	
	6. Physical properties of all components*	
	7. Safety, toxicity and environmental concerns involved in the process*	
	8. Cost data for by-products, equipment and utilities*	
1	**Batch vs. continuous***	Operation mode
2	**Input-output structure***	Overall mass balance of the whole process
	1. Should we use a preprocess purification system to purify raw materials?	
	2. Remove or recycle a reversible by-product?	
	3. Should we consider a gas recycle and purge stream?	
	4. Should we discard some reactants?	
	5. Number of product streams?	
	6. Design variables and associated economic trade-offs?	
3	**Recycle structure***	
	1. Number of reactors, any separation required between the reactors?	Reaction system flowsheet
	2. Number of recycle streams?	1. Costs of reactors (including heterogeneous catalysts)
	3. An excess of one reactant vs. stoichiometric amount.	Gas recycle system flow sheet
	4. Number of gas compressors and associated costs?	1. Costs of gas compressors
	5. Reactors operation (adiabatically, direct heating or cooling, or required a diluent or heat carrier)	2. Electricity costs of compressors
	6. Whether to shift the equilibrium conversion and how?	
	7. Impacts of reactors and compressors costs on economic potential	
4	**Separation structure**	
	Vapor recovery system*	
	1. Do we need a vapor recovery system?	
	2. Location of vapor recovery system? (a. purge stream, b. recycle stream and c. flash vapor stream)	
	3. Type of vapor recovery system? (a. condensation (cryogenic distillation), b. absorption, c. adsorption, d. membrane and e. reaction system)	
	Liquid recovery system	Separation system flowsheet
	1. What separation can be made by L-L split?	1. Equipment and utilities costs of Vapor recovery system
	2. Methods to remove contaminating light ends,	2. Equipment and utilities costs of Liquid recovery system
	and destination of the light ends?*	3. Equipment and utilities costs of Solid recovery system
	3. What separation can be made by distillation, how we handle azeotropes in the recycle stream?*	
	4. Column sequencing of distillation system?*	
	5. If distillation is infeasible, what methods should we use for separation?*	
	Solid recovery system	
	1. Do we need a solid recovery system?	
	2. Location of solid recovery system?	
	3. Type of solid recovery system? (a. crystallization, b. filtration, c. centrifugation and e. sedimentation)	
5	**Heat generation & exchange network**	
	Heat generation	Heat generation & exchange flowsheet
	1. What resource do we have (e.g. purge steam, residues of biomass)	1. Heat required or gained
	to generate heat and how?	2. Cooling required
	Heat exchange*	3. Equipment costs of heat generation and exchange network
	1. Minimum heating and minimum cooling, minimum no. of exchangers and exchanger area required.	

*Adapted from Douglas, J.M., *Conceptual Design of Chemical Processes*, McGraw-Hill, 1998.

preceding hydrolysis step and offering further feedstock flexibility. Dehydration of xylose in pure water results in low selectivity's due to undesired side reactions.[25,26] Thus, the dehydration is carried out in a biphasic reactor system which uses tetrahydrofuran (THF) as an extractant to remove furfural from the aqueous phase. Addition of NaCl into the hemicellulose stream enhances the partitioning of furfural into the organic phase by "salting-out" the furfural.[27] The second step is aldol condensation, in which the furfural is reacted with stoichiometric amounts of acetone in the presence of basic catalyst (NaOH) to produce a furfural-acetone dimer. This is also a biphasic reaction with THF as a solvent, however unlike the first step, NaCl is not necessary. In the next step, the dimer is hydrogenated over Ru/C catalyst, which saturates the double bonds in the dimer. This stabilizes the dimer and, thus, the hydrogenated dimer can then be subjected to a higher-temperature hydrodeoxygenation. In the hydrodeoxygenation step, Pt/SiO_2-Al_2O_3 is used as a catalyst to convert the hydrogenated dimer to tridecane by removing oxygen in the form of water. In this step, some byproducts

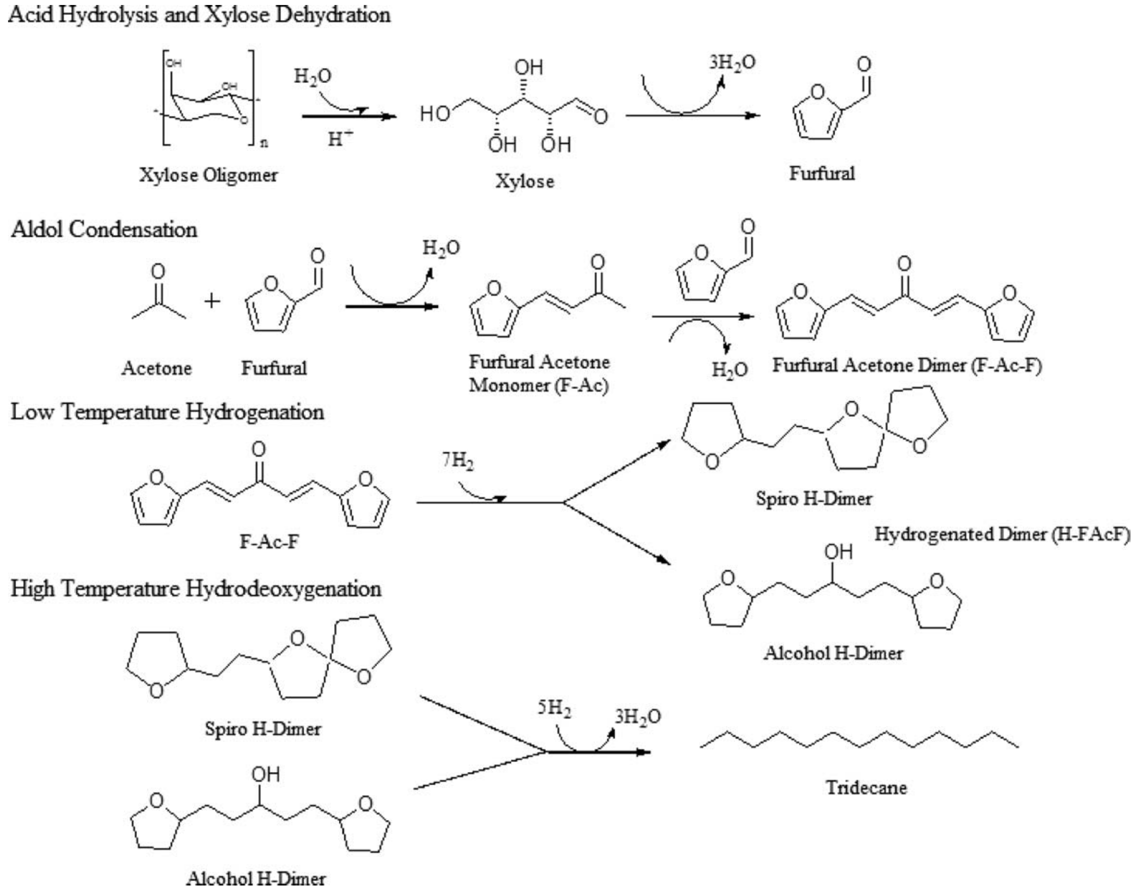

Figure 2. Reaction chemistry for the conversion of xylose oligomers into tridecane.
(Adapted from Xing et al.[19]).

(mostly smaller alkanes or isoalkanes) are identified. These byproducts are still desirable because they can also be blended into jet or diesel fuel. Some light alkane byproducts (e.g., CH_4) are also formed which exit the reactor with hydrogen in the vapor phase. If these byproducts are not removed, they will progressively increase to unsustainably large values in the hydrogen recycle loop, and eventually cause process failure.

Hierarchical Conceptual Process Design

In this section, the application of the different levels of the conceptual process design for the hemicellulose conversion process will be illustrated with a few relevant examples to biofuels industry, as an example of rapid assessment of alternative energy producing options.

Level-0 Analysis: Input Information

At Level-0, all the relevant information about the process is collected as summarized in Table 1. This information is used for determining the raw material and desired product purity, production rate and selecting plant location. The greatest distinction between biofuels projects and traditional chemical processes is raw materials. The dispersed nature of biomass increase the cost of collecting and transporting the raw materials to the process location compared to raw materials in the traditional chemical industry. From the conceptual design standpoint, this difference leads to two design decisions (1) the location of process, which is determined by availability and costs of raw materials, and (2) the scale of process, which is limited by the availability of biomass in certain biomass-captured geographic regions. As we increase the biomass capture radius, the cost of collecting and transporting the biomass will increase, and, hence, at a certain level, the increasing cost will eliminate the benefits from the economies of scale. For the hemicellulose conversion process, a plant site could be selected near a pulp and paper process to take advantage of cheap available raw materials or it could be viewed as an add-on project for an existing biorefinery for which aqueous hemicellulose streams are byproducts (e.g., cellulose conversion to jet fuel via biofine process[28,29]). The plant scale for this process will be selected based on the availability of hemicellulose, acetone or hydrogen. Also, at this level, decisions about the purities of raw materials need to be made. For example, what is the cost of using hydrogen with different levels of CH_4 and CO impurities? The answer to this question, as most questions asked in process design, can only be addressed by laboratory data. However, asking questions like this, very early, guides the experimental effort. The process designer clearly needs to work with experimentalists to help answer these questions and only long term data can truly answer questions of these types.

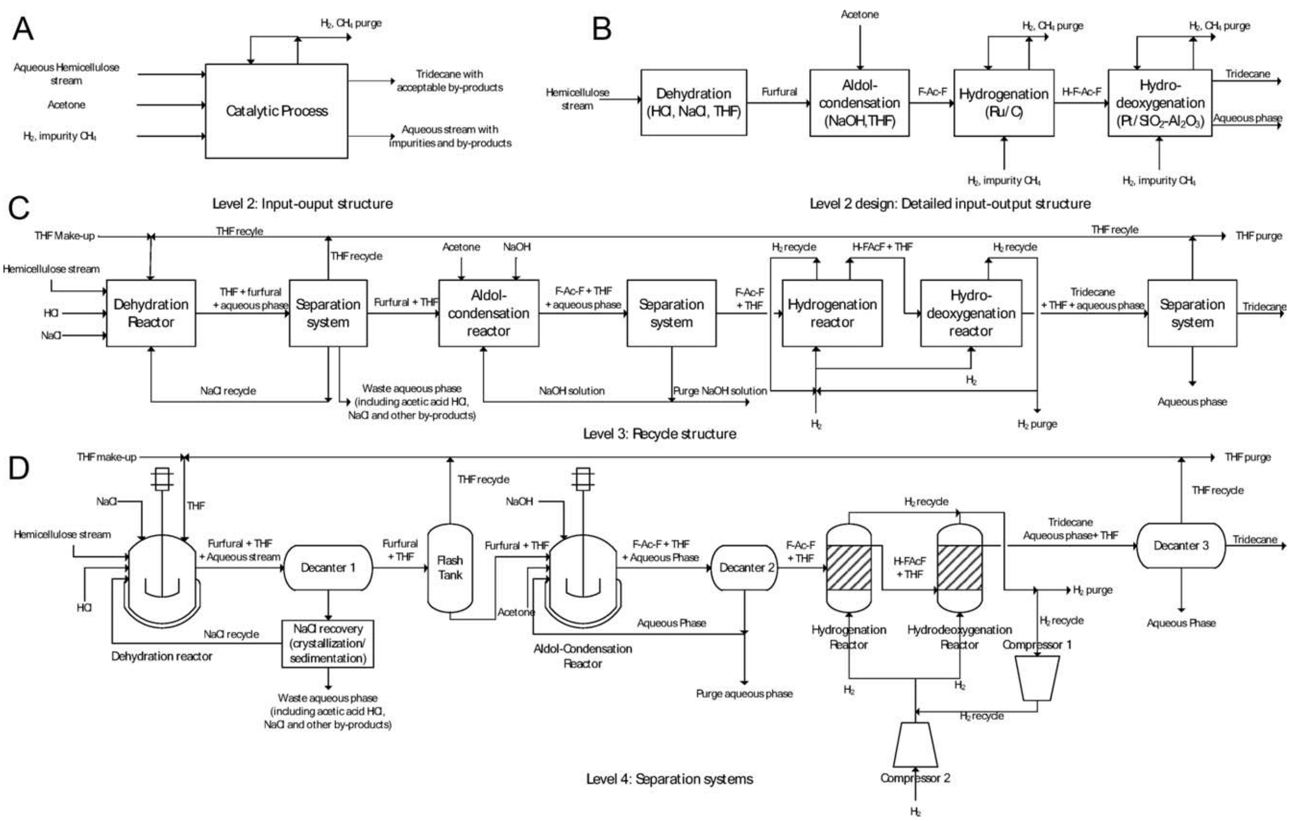

Figure 3. Hierarchical levels of design for the process of conversion of aqueous hemicellulose stream to tridecane.

Selecting the medium for gasification (air or oxygen), production of hydrogen on site/off site are some examples of Level-0 decisions in certain biofuels projects.

Level-1 Design: Batch vs. Continuous

At this level, the decision to be made is whether to design a continuous or batch process. Continuous processes are usually desired for biofuel projects due to the high volume of production. However, it is possible to have economic batch processes for other biomass conversion projects, which target the low-volume specialty chemicals. It is also possible to have some batch operation steps in a continuous process with intermediate storage tanks as buffers between batch/semibatch and continuous processing units, and continuous segments in an otherwise batch process. For the hemicellulose conversion process the large volume of processed materials dictates the use of a continuous process.

Level 2 Design: Input-Output Structure

Figure 3A and 3B shows the input-output flow diagram for the entire process. This input-output structure includes only reactants, products, byproducts, purge stream, and does not include the catalyst (NaOH and HCl), recycled solvent (THF), or promoter (NaCl). One of the process variables considered here is the feed composition, i.e., the concentration of hemicellulose in aqueous stream. Increasing the concentration of the hemicellulose reduces the total volumetric flow rate and this in turn decreases the total capital and operating costs. However, the concentration can only increase up to a certain level beyond which the gain due to the reduction in operating and capital costs is exceeded by the loss in product yield in the biphasic dehydration reactor.

The economic evaluation of the process, using an estimate of its economic potential, starts at this early stage. The process economic potential at this level is primarily the difference between the revenues from the products and the raw material costs. Some utility costs and capital costs are also incorporated for pretreating the feedstock and waste disposal, leading to the following estimate (Eq. 1) of the economic potential for Level-2 design.

$$EP_2\left(\frac{\$}{yr}\right) = \text{product value} + \text{Byproduct value} - \text{Raw Material cost} - \text{Waste Disposal Fee} \quad (1)$$

Table 2 provides the first economic assessment for the process by computing the economic potential based on a product selling price of \$3.5/gal. The largest portion of the product cost is due to acetone, despite the fact that consumption of acetone is very low compared to the hemicellulose stream. Thus, if acetone is replaced by another cheaper carbonyl compound for aldol condensation[30] or produced through different route within the project, one can decrease the product cost further. This observation suggests that significant cost reductions can be achieved by replacing acetone with another carbonyl compound. In conceptual process design, typically as we increase the complexity and detail of process design the

Table 2. Economic Analysis of the Hemicellulose Conversion Process of Production Capacity of 50 Mgal/yr at Different Hierarchical Levels of Conceptual Process Design

Raw material costs per gallon of product			Amount required per gallon product		Cost	
Level 2: Input-output structure*						
Xylose	0.66	$/gal	6.60	kg/gal	0.1	$/kg
Acetone	0.72	$/gal	1.03	kg/gal	0.7	$/kg
Hydrogen	0.41	$/gal	0.41	kg/gal	1	$/kg
Total raw material cost	1.79	$/gal				
Product selling price	3.5	$/gal	Capacity	50	Mgal/yr	
Economic potential = 1.71 $/gal						
Economic potential = 85.50 M$/yr						
Installation cost			Utilities			
Level 3: Recycle structure						
Dehydration reactor	2543	k$	Dehydration reactor	44024	k$/yr	
Aldol condensation reactor	24012	k$				
Hydrogenation reactor	5047	k$				
Hydrodeoxygenation reactor	5106	k$				
Compressor 1	559	k$	Compressor 1	74	k$/yr	
Compressor 2	3798	k$	Compressor 2	766	k$/yr	
Total installation cost	41065	k$	Total utilities cost	44864	k$/yr	
Economic potential = 7.95 M$/yr						
Sepatation units costs			Utilities			
Level 4: Separation structure**						
Decanter 1	1937	k$	Decanter 1	0	k$/yr	
Decanter 2	160	k$	Decanter 2	0	k$/yr	
Decanter 3	87	k$	Decanter 3	1535	k$/yr	
Flash	1049	k$	Flash	29171	k$/yr	
Total separation cost	3233	k$	Total utilities cost	30706	k$/yr	
Economic potential = −25.33 M$/yr						
Level 5: Heat integration						
Savings on utilities						
Dehydration reactor	7189	k$/yr				
Decanter 1	0	k$/yr				
Decanter 2	0	k$/yr				
Decanter 3	1535	k$/yr				
Flash	29171	k$/yr				
Total savings	37895	k$/yr				
Economic potential = 12.56 M$/yr						

The costs for installed equipment and associated utility costs are calculated based on the correlations described by J.M. Douglas in *Conceptual Design of Chemical Processes*, McGraw-Hill, 1998.
*Costs for HCl, NaCl, THF make-up streams are not included in the analysis.
**Separation system does not include cost for recovery of NaCl from the aqueous stream of decanter 1.

economic potential will decrease due to increase in capital and operating costs.

In biofuels projects, the feed is available in diverse and complex forms, while the products specifications are driven by the market requirements. The designer needs to evaluate the impact of the impurities on the reaction system. Usually, it is expected that use of the practical raw materials will bring more challenges than pure chemical reagents. Sometimes using the actual raw materials brings unexpected advantages. For example, Xing et al.[31] showed that use of the actual raw materials leads to much less NaCl usage in the process due to the heavy inorganic salts present in the hemicellulose steam from a paper mill.

Level-3 Design: Recycle Structure

At Level-3 more details are added to the process by considering the reactor system and its associate costs and introducing recycle streams in the flow sheet. In cases of equilibrium reactions, one would generally use one reactant in excess to increase the conversion, with the excess reactants recycled back from the product stream. With excess reactant, the reactor heat duty increases, due to the increase in throughput, leading to an increase in reactor capital and operating costs. Furthermore, the design of the heat exchanger system for the reactor becomes an important consideration due to increased heat duties. Sometimes a diluent is used to reduce the concentration of the reactant and help remove the heat of reaction. Other times a heat carrier is used to add heat to the reaction. In both cases, the diluent or heat carrier has to be recycled back to the reactor, leading to an increase in capital and operating costs of the subsequent separation subsystem. By making the decisions listed in Table 1, the block flow diagram for the hemicellulose conversion process at Level-3 is generated, as shown in Figure 3C. In this flow diagram the separation system block assumes that there exist separations technologies that can generate all the different liquid product streams shown in the process of Figure 3C. Furthermore, it has been assumed that the various gaseous products (anything that has a boiling point lower than propane) are removed as a single "gas stream". Given the fact that the separation systems at this level have not been specified their cost is not included in the computation of the economic potential.

For the hemicellulose conversion process, one important design variable is the ratio of the organic (THF) to aqueous phase-flow rate in the biphasic dehydration reactor. Experimental results have indicated that as the ratio of THF to the aqueous phase flow rate increases, the yield of furfural increases. This increase however also leads to larger reactor and higher capital and operating costs. Thus, a trade-off exists for selecting the "optimal" ratio of THF to aqueous phase flow rate. Such trade-offs are very common for biofuels projects where selectivity is highly dependent on concentrations of reactants and catalysts. Another additional design decision at this stage is how much excess hydrogen should be used in the hydrogenation and hydrodeoxygenation steps and how much gas should be recycled into the hydrotreaters. This will increase the recycle cost of hydrogen stream and the raw material costs. The reactors and compressor can be sized and costed based on the flow rate and residence time of the reactors, the gas-flow rates, and the reactor pressure. The next step is to convert the capital costs into annualized capital recovery costs, using the capital charge factor (CCF). The resulting economic potential for Level-3 is, thus, calculated by Eq. 2, assuming a CCF of 0.25

$$EP_3\left(\frac{\$}{yr}\right) = EP_2 - \text{Annualized reactor(s) cost} - \text{Annualized compressor(s) cos} \qquad (2)$$

The capital costs for the reactor are calculated based on the onsite costs by correlations presented in Douglas.[3] The results are shown in Table 2; the economic potential has decreased to about \$7.95 M/yr. The largest portion of the reactors' capital cost is associated with the aldol condensation reactor because of its large residence time. The largest contributor to the operating costs is the heating up of the dehydration reaction. This indicates that future research efforts should be focused on decreasing the size of the aldol condensation reactor.

Level-4 Design: Separation System

In Level-3 design, the separation system was represented by an abstract block performing an ideal separation. At Level-4 one designs the separation system in detail, which can be divided into three types as shown in Table 2.

1. Vapor recovery system

The purpose of the vapor recovery system is to collect any condensable products in gaseous streams and send them to the liquid recovery system. Common vapor recovery systems include condensation, absorption, adsorption, reaction or membrane separation. The vapor recovery system can be put in three different locations: on the gaseous purge stream, on the recycle stream (before reactor), or before the gaseous purge stream and the recycle stream. The selection of where to put the vapor recovery system depends on what one is trying to accomplish in the process. In the hemicellulose conversion process, there is no need to employ any vapor recovery system as no valuable or harmful product is present in the purge stream.

2. Liquid recovery system

The liquid recovery system should be structured in such a way as to generate distinct liquid streams representing the desired products and any recycles back to the reactor. Distillation is the most common mode for the separation of liquid components but one should consider first the use of a simple liquid-liquid splitter, which requires simple equipment (decanter) and consumes less energy compared to a distinct distillation unit. With the knowledge of physical properties, optimal distillation systems can be designed using different strategies[32,33] to obtain accurate estimations. If conventional distillation is not feasible, extraction, adsorption, reaction, crystallization or other form of distillation like vacuum, azeotropic,[34] extractive or reactive distillation[35] unit can be considered to carry out the desired liquid separations.

In the hemicellulose conversion process, the separation can be carried out using decanters because of the biphasic reaction scheme. In this preliminary analysis, a simplistic separation system consisting of flash columns for the THF separation after the dehydration and hydrodeoxygenation reactors has been assumed. However, it should be noted that a better design of a separation system consisting of a train of distillation units could be required to carry out the needed separations.

3. Solid recovery system

Units like crystallization, filtration, centrifugation, electrostatic precipitation and sedimentation are used for solid recovery. In biofuels projects, like catalytic fast pyrolysis,[36] the solid recovery system can be crucial to the process.

In other biofuels projects like biomass gasification, the separation of tars from the reactor or clean-up of syngas introduce large costs and often define the feasibility of the project.[37] Thus, the design of the optimum separation system is critical in the development of economically feasible biofuels processes.

By making the decisions listed in Table 1 the flow sheet of hemicellulose conversion process shown in Figure 3D is generated. The utility and capital costs required for the separations are calculated and used to estimate the economic potential as shown in Eq. 3. The economic potential for this level has been reduced to \$ -25.33 M/yr. In this preliminary analysis, the cost of NaCl recovery from the aqueous stream has not been accounted for and the recovery of acids from the waste aqueous stream has also not been considered. The largest contributors to the economic potential are the utilities cost due to the flash column and the decanter 3. We may anticipate significant cost savings from the possible energy integration of the reactor and flash column. Consequently, the analysis proceeds to the next level of design even though our process has a negative economic potential at this level.

$$EP_4\left(\frac{\$}{yr}\right) = EP_3 - \text{Annualized separation system cost} \qquad (3)$$

Level-5 Design: Heat Integration

Energy conservation is one of the important parts of process design especially in the production of commodities like fuels. A systematic method for heat integration is available in the literature,[3,38] and, thus, will not be discussed here in detail. Heat integration can also be carried out using commercial software (e.g., Aspen energy analyzer), while different algorithms are discussed in the literature for optimal heat integration process.[39,40]

In biofuels projects, heat integration is a must for designing a cost efficient process. Typically, heat is recovered from most exothermic reactions. In the case of the hemicellulose conversion process, the heat required for the decanter and the flash column is obtained by cooling the product stream. The economic potential is calculated by Eq. 4 and unlike the earlier stages of design, where the economic potential was continuously decreasing, at this stage it increases to \$12.56 M/yr as a result of the extensive savings in utilities achieved through energy integration.

$$EP_5\left(\frac{\$}{yr}\right) = EP_4 + \text{Energy savings through heat integration} \tag{4}$$

Summary

A six-level hierarchical approach to conceptual design is summarized in Table 1 with the decisions to be made and the outcomes to be expected at each level of the conceptual design. This approach has been used to systematically develop process flowsheets (Figure 3) for the hemicellulose conversion process. The process is economically attractive and the single most significant factor in its economic viability has been the reduction of utilities costs due to energy integration. The aldol condensation reactor is the unit with largest contribution to the total capital cost, suggesting that future laboratory experiments should focus on decreasing the reactor size.

Conclusion

The challenge with all renewable energy projects is one of economics. Conceptual process design is a powerful approach which can be used to generate and evaluate alternative designs for renewable energy projects. Conceptual process design can also be used to guide laboratory experiments so that research is focused and development time is shortened. This method uses engineering economics and chemical engineering heuristics to quickly screen process alternatives. The fundamentals of this method can be applied to any type of processes and it can play a pivotal role in sorting out the attractive options of the energy challenges. We recommend that all the scientists working in the area of renewable energy collaborate with engineers that have conceptual process design experience that can help guide the design of the future research efforts.

Acknowledgments

The authors would like to thank Dr. Hakan Olcay, Prof. Michael F. Malone and Prof. James M. Douglas for helpful discussions. The authors would also like to thank Prof. George Stephanopoulos for his editorial inputs toward preparing the manuscript.

Literature Cited

1. Nishida N, Stephanopoulos G, Westerberg AW. A review of process synthesis. *AIChE J*. 1981;27(3):321–351.
2. Douglas JM. A hierarchical decision procedure for process synthesis. *AIChE J*. 1985;31(3):353–362.
3. Douglas JM. *Conceptual design of chemical processes*. New York: McGraw-Hill; 1988.
4. Huber GW, Iborra S, Corma A. Synthesis of transportation fuels from biomass: Chemistry, catalysts, and engineering. *Chem Rev*. 2006;106(9):4044–4098.
5. EERE FY12 Congressional Budget. http://www1.eere.energy.gov/biomass/pdfs/fy12_congressional_budget_biomass.pdf.
6. Douglas JM. *25* The Paradigm After Next. In: Clark KC, ed. *Advances in Chemical Engineering*. Vol 16. San Diego, CA: Academic Press; 1991:535–542.
7. Huber GW. Breaking the Chemical and Engineering Barriers to Lignocellulosic Biofuels: Next Generation Hydrocarbon Biorefineries. Washington D.C.: National Science Foundation; March 2008.
8. US Energy Infromation Administration. http://www.eia.doe.gov/ipm/supply.html.
9. http://www.ril.com/html/business/refining_marketing.html.
10. Lange JP. Lignocellulose conversion: an introduction to chemistry, process and economics. *Biofuels Bioprod Bioref Biofpr*. 2007;1(1):39–48.
11. Towler G, Sinnott R. *Chemical Engineering Design: Principles, Practice and Economics of Plant and Process Design*. San Diego, CA: Butterworth-Heinemann, Elsevier, Inc.; 2008.
12. Kletz TA. Friendly plants. *Chem Eng Prog*. 1989;85(7):18–26.
13. Bahri PA, Bandoni JA, Romagnoli JA. Integrated flexibility and controllability analysis in design of chemical processes. *AIChE J*. 1997;43(4):997–1015.
14. Doherty MF, Malone MF. *Conceptual Design of Distillation Systems*. Boston: McGraw-Hill; 2001.
15. Rudd DF. The synthesis of system designs: I. Elementary decomposition theory. *AIChE J*. 1968;14(2):343–349.
16. Halemane KP, Grossmann IE. Optimal process design under uncertainty. *AIChE J*. 1983;29(3):425–433.
17. Grossmann IE, Sargent RWH. Optimum design of chemical plants with uncertain parameters. *AIChE J*. 1978;24(6):1021–1028.
18. Green DW, Perry RH. *Perry's Chemical Engineers' Handbook*. 8th ed. New York: McGraw-Hill; 2008.
19. Xing R, Subrahmanyam, AV, Olcay H, Qi W, van Walsum GP, Pendse HP, Huber GW. Production of jet and diesel fuel range alkanes from waste hemicellulose-derived aqueous solutions. *Green Chem*. 2010;12(11): 1933–1946.
20. Um BH, van Walsum GP. Mass balance on green liquor pre-pulping extraction of northeast mixed hardwood. *Bioresource Technol. Aug* 2010;101(15):5978–5987.
21. Wyman CE, Dale BE, Elander RT, Holtzapple M, Ladisch MR, Lee YY. Coordinated development of leading biomass pretreatment technologies. *Bioresource Technol*. 2005;96(18):1959–1966.

22. Liu CG, Wyman CE. Partial flow of compressed-hot water through corn stover to enhance hemicellulose sugar recovery and enzymatic digestibility of cellulose. *Bioresource Technol*. 2005;96(18):1978–1985.
23. Parajo JC, Garrote G, Cruz JM, Dominguez H. Production of xylooligosaccharides by autohydrolysis of lignocellulosic materials. *Trends Food Sci Technol*. 2004; 15(3–4):115–120.
24. Lloyd TA, Wyman CE. Combined sugar yields for dilute sulfuric acid pretreatment of corn stover followed by enzymatic hydrolysis of the remaining solids. *Bioresource Technol*. 2005;96(18):1967–1977.
25. Dias AS, Pillinger M, Valente AA. Dehydration of xylose into furfural over micro-mesoporous sulfonic acid catalysts. *J Catal*. 2005;229(2):414–423.
26. Weingarten R, Cho J, Conner WC, Huber GW. Kinetics of furfural production by dehydration of xylose in a biphasic reactor with microwave heating. *Green Chem*. 2010;12(8):1423–1429.
27. Roman-Leshkov Y, Barrett CJ, Liu ZY, Dumesic JA. Production of dimethylfuran for liquid fuels from biomass-derived carbohydrates. *Nature*. 2007;447(7147): 982–U985.
28. Fitzpatrick SW, Fitzpatrick SWFitzpatrick SWs; Biofine, Inc., assignee. Production of Levulinic Acid from Carbohydrate-Containing Materials. US patent 5,608,105. Mar. 4,1997.
29. Serrano-Ruiz JC, Braden DJ, West RM, Dumesic JA. Conversion of cellulose to hydrocarbon fuels by progressive removal of oxygen. *Appl Catal B Environ*. 2010; 100(1–2):184–189.
30. Subrahmanyam AV, Thayumanavan S, Huber GW. C-C Bond Formation Reactions for Biomass-Derived Molecules. *Chemsuschem*. 2010;3(10):1158–1161.
31. Xing R, Qi W, Huber GW. Production of furfural and carboxylic acids from waste aqueous hemicellulose solutions from the pulp and paper and cellulosic ethanol industries. *Energy Environ Sci*. 2011;4(6):2193–2205.
32. Rathore RNS, Vanwormer KA, Powers GJ. Synthesis of distillation systems with energy integration. *AIChE J*. 1974;20(5):940–950.
33. Umeda T, Niida K, Shiroko K. A thermodynamic approach to heat integration in distillation systems. *AIChE J*. 1979; 25(3):423–429.
34. Widagdo S, Seider WD. Azeotropic distillation. *AIChE J*. 1996;42(1):96–130.
35. Malone MF, Doherty MF. Reactive Distillation. *Ind Eng Chem Res*. 2000;39(11):3953–3957.
36. Carlson TR, Cheng YT, Jae J, Huber GW. Production of green aromatics and olefins by catalytic fast pyrolysis of wood sawdust. *Energy Environ Sci*. 2011;4(1):145–161.
37. Milne TA, Evans RJ. NA. Biomass Gasifier "Tars": Their Nature, Formation and Conversion. Golden, CO: NREL; 1998.
38. Nishida N, Liu YA, Lapidus L. Studies in chemical process design and synthesis: III. A Simple and practical approach to the optimal synthesis of heat exchanger networks. *AIChE J*. 1977;23(1):77–93.
39. Floudas CA, Ciric AR, Grossmann IE. Automatic synthesis of optimum heat-exchanger network configurations. *AIChE J*. 1986;32(2):276–290.
40. Townsend DW, Linnhoff B. Heat and power networks in process design. Part II: Design procedure for equipment selection and process matching. *AIChE J*. 1983;29(5): 748–771.