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Advances in Energy Systems Engineering

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ABSTRACT: Huge and ever-increasing energy consumption and consequent greenhouse gas (GHG) emissions pose unprecedented challenges to the sustainable development of the international human society. Our existing energy systems, where primary energy is converted to all sorts of final energy services, remain the major contributor to these global energy and environmental challenges. It is becoming a consensus that the conventional energy conversion and utilization mode should make place for a more sustainable one with higher energy conversion efficiency, lower air pollutions and GHG emissions, less dependence on fossil fuels, and more utilization of renewable energy. However, although there exist many technical options and technology pathways to enable this transition, they are usually treated separately by their very own technical communities and political groups without coordination with others, and the overall effect and potential is therefore greatly constrained as compared to a systematic approach where all alternatives are taken into consideration in an integrated way. Energy systems engineering provides a methodological modeling and optimization framework to address the complex energy and environmental problems existed in design and operation of energy systems in an integrated manner. This methodological framework is generic, and it can help to produce optimal design and operational plans for energy systems ranging from nanoscale, microscale, mesoscale, to mega-scale levels over operating horizons from milliseconds to months and years. This Article first gives a brief overview of typical methodologies of energy systems engineering, comprising superstructure based modeling, mixed-integer linear and nonlinear programming, multiobjective optimization, optimization under uncertainty, and life-cycle assessment. The concept of energy systems engineering and these methodologies are further illustrated via their applications in some typical real-life energy systems of very different nature and scale, ranging from polygeneration energy systems, hydrogen infrastructure planning, energy systems in commercial buildings, and biofuel supply chains.

INTRODUCTION

Energy and Environmental Challenges and Energy Systems Engineering. Sufficient energy supply and less greenhouse gas (GHG) emission are two key issues to maintain the sustainable development of the global human society. However, the existing energy systems may have problems in meeting these two targets simultaneously. Between 1997 and 2006, global energy consumption increased at an annual rate of 2.34%, from 402.0 EJ to 494.9 EJ. During the same period, global carbon dioxide emissions from energy consumption grew even faster at an annual rate of 2.59%, from 23.2 billion metric tonnes to 29.2 billion metric tonnes.[1] Without substantial improvements to the existing energy systems, it may not be possible to meet the increasing energy demand, which is projected to increase by 44% during the period between 2006 and 2030,[2] while reducing the global GHG emissions to either the 1990 level or the 2005 level.

The conventional way of energy production, conversion, and utilization should be improved to meet the targets of maintaining energy supply and reducing GHG emissions. Changes are expected to take place in the following directions:

First is improvement in energy efficiency of conventional technologies. Considering the huge capacity of the existing energy infrastructure and the fact that there is still space for further improvement of conventional technologies, this is the most effective measure in the near to midterm future.

Second is energy savings. This is the most cost-effective way to reduce energy demand from end-use sectors, although it may take place at the price of reduced human convenience.

Third is shifting from the current fossil fuel dominant energy supply mode to one with higher proportion of renewable energy. Renewable energy is expected to play an important role in the future energy supply system, but it takes time to accomplish the transition from fossil fuel-based energy systems to renewable energy-based ones.

Next is process-wide integration across sectors. Process integration provides opportunities for more efficient energy utilization than do stand-alone processes. Integrated energy systems could play an important role in the gap between fossil fuel-based energy systems and renewable energy-based ones.

Also, changes are expected in carbon dioxide capture and sequestration (CCS) technologies. Carbon dioxide, which is the main source of GHG emissions, can be separated from other gases in power plants and sequestrated in places geologically suitable for storage. However, it also brings an unaffordable efficiency penalty to the energy production sector.

Finally, we have revolutionary technological breakthroughs. Controlled nuclear fusion, cellulosic biofuels, and natural gas hydrate belong to this category. Once they take place, they can

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solve the energy and environmental problems faced by all human beings. However, we are still at a very early stage of these technologies, and there is a long way to go. Furthermore, it may take decades to build the required capacity.

These measures differ from each other in both spacial and time scale. They are usually treated separately by their own technical community or political groups, although it is becoming a consensus that a sustainable future requires all these measures to coordinate with each other. The major reason for this lack of cooperation is lack of methodologies and supporting techniques.

Energy systems engineering provides a methodological framework to address the complex energy and environmental problems by an integrated systematic approach which accounts complexities of very different scales, ranging from technology, plant, to energy supply chain, and megasystem.[3,4] Typical methodologies of energy systems engineering involve superstructure-based modeling, mixed-integer programming, multiobjective optimization, optimization under uncertainty, and life cycle assessment.

The concept of energy systems engineering was proposed by Pistikopoulos for the first time in the sixth European Congress of Chemical Engineering.[3] Since then, it has been successfully applied in the planning and design of many types of energy systems, typical ones of which are polygeneration energy systems,[5−10] energy and process integration,[11−14] hydrogen infrastructure planning,[15−18] energy systems in commercial buildings,[19] biofuel and biorefineries,[20−36] urban energy systems,[37] integration of renewable energy,[38,39] power industry,[40] pulp and paper industry,[41−44] oil and gas production,[45] wind turbines,[46] and carbon dioxide capture and sequestration.[47,48] These energy systems have very different nature and scale, but they share common design and operation problems from an energy systems engineering viewpoint.

This Article is organized as follows. First, key methodologies of energy systems engineering are briefly introduced to give a clear and whole picture of the framework of energy systems engineering. Following this, applications of energy systems engineering in polygeneration energy systems, hydrogen infrastructure planning, energy systems in commercial buildings, and biofuel supply chains are presented, respectively. Finally, future directions of energy systems engineering are discussed.

Key Methodologies of Energy Systems Engineering. The fundamental basis of energy systems engineering is the concept of superstructure, superstructure representation of energy systems, and superstructure-based modeling. The concept of superstructure has been widely used in process systems engineering, referring to an approach to simultaneously determine the optimal configuration of a process and its optimal operating conditions from all possible alternatives.[49] In a superstructure representation of an energy system, all possible technical pathways, system configuration, process integration, operating modes, and other important issues to be decided can be covered in a systematic way. Based on the superstructure representation, all these alternatives can be modeled in a mathematical way, making further quantitative systematic analysis and optimization possible. Superstructure-based modeling was first proposed to address process synthesis issues in heat exchanger networks (HEN)[50] and widely used in process design thereafter. It is regarded as one of the most significant accomplishments in process systems engineering.[51]

Superstructure-based modeling, while allowing one to cover all alternatives and options, however, also brings great challenges to the modeling side. Selections of technical choices or system configuration are discrete by nature, but the conventional modeling techniques only allow for continuous modeling. Mixed-integer programming (MIP) successfully solves the problem of mathematical representation of discrete decisions by introducing binary (0−1) variables together with continuous variables, and it is a natural tool to implement superstructure-based modeling.[52] In a MIP model, each discrete decision to be made is represented by a binary variable, and its value stands for the selection (or not) of the decision. Following this rule, any logical condition between discrete events in a superstructure representation can be expressed using a set of mathematical constraints in a MIP problem.

Solution of MIP problems pose algorithmic and computational challenges due to their discrete nature. Many approaches have been made to solve different types of MIP problems, including linear (MILP) and nonlinear problems (MINLP), convex and nonconvex problems (for nonlinear problems), regular and large-sized problems, and local and global solutions. Some of these algorithms or techniques have been commercialized as commercial solvers. They can be used directly to solve a certain type of MIP problems. Because of the high efficiency and wide coverage of problem types, GAMS[53] and its solvers are widely used to solve MIP problems.

On establishing a mathematical model of an energy system, conventional optimization techniques allow optimizing its behavior according to a specific criterion. Traditionally, this criterion is usually an indicator of energy efficiency or economic performance. As GHG emissions have drawn more and more concern, GHG emissions are becoming another important design criterion, which should be considered together with energy and economic design criteria. However, conventional optimization techniques do not provide this ability, and these problems can only be addressed using multiobjective optimization, another important methodology in the framework of energy systems engineering.

Multiobjective optimization, or multicriteria optimization, is to simultaneously optimize a problem according to two or more (conflicting) criteria subject to certain constraints. Multiobjective optimization is suitable to be applied to a problem where trade-offs exist among its objective functions and optimal decisions should be made in the presence of these trade-offs.[54] Typical algorithms for solving multiobjective optimization problems are parametric programming[55] and ε-Constraint method.[56,57] Both algorithms solve a multiobjective optimization problem by first converting it to a set of single-objective optimization problems where only one of the objective functions remains as the objective function of the consequent single-objective optimization problems while the other objective functions are converted to constraints. Based on this conversion, the parametric programming approach solves the problem as a multiparametric programming problem where the parametric space of the objective functions is explored. The ε-Constraint method solves the problem by discretizing the space of objective functions into small intervals and obtaining optimal solutions at the discretized points.

Note that GHG emissions produced by an energy system include not only those produced during its operating stage, but also those produced in the production procedure of equipment, construction of the energy system, and transportation of feedstocks and equipment. In energy systems engineering, life-cycle assessment (LCA) techniques are used to quantify and summarize all these emissions from very different sources and time periods. Life-cycle assessment, also known as life cycle analysis, is to evaluate and quantify the environmental impacts of a certain product or production procedure caused by its existence.[58] LCA has also been included by ISO (International Organization for Standarlization) as part of the standards for environmental management systems.[59,60]

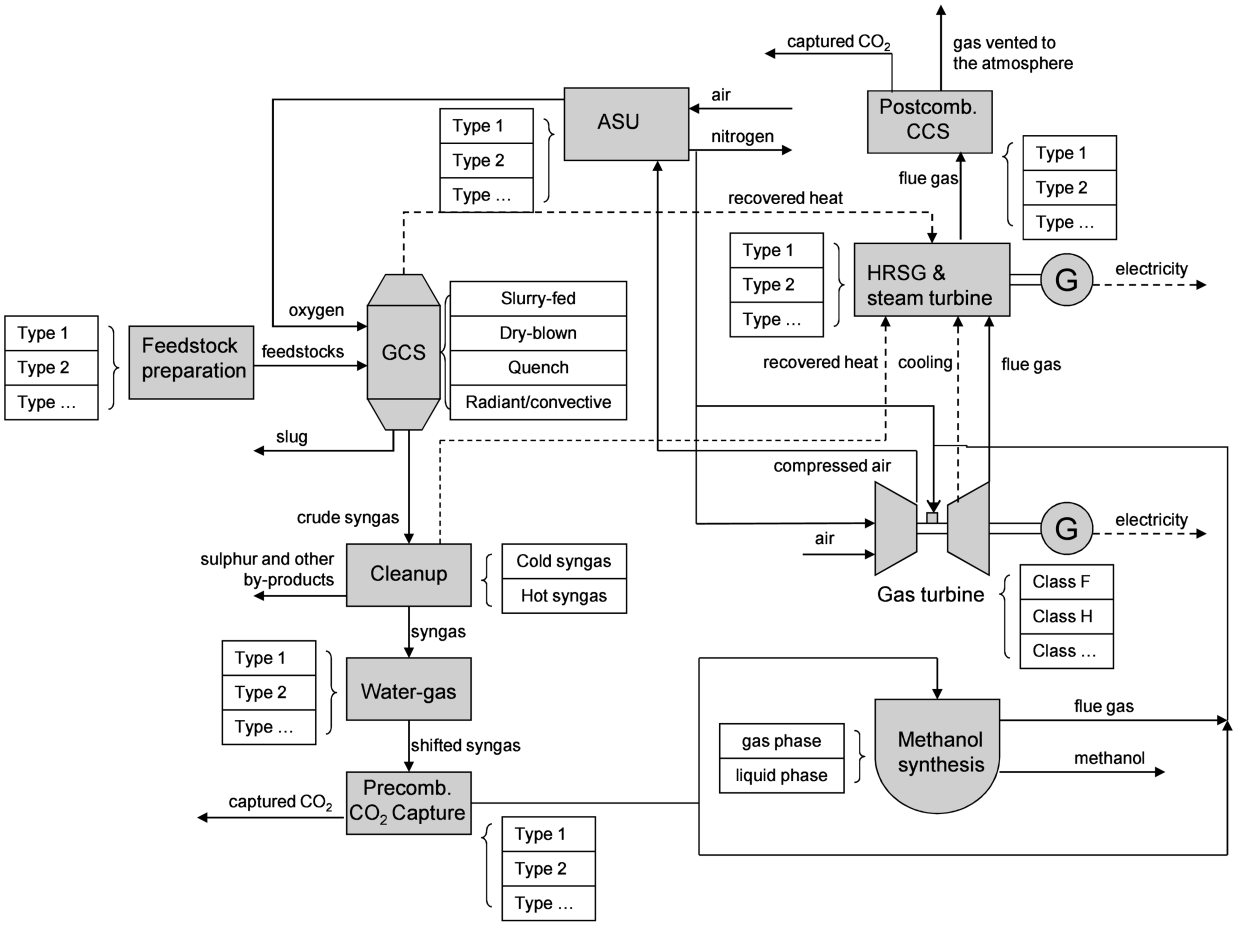

Figure 1. Superstructure representation of a polygeneration process.

Another problem involved with planning or design of energy systems is uncertainty. An energy system is usually expected to work over an operating period of many years, during which uncertain events such as fluctuation of market prices are inevitable and unpredictable. Optimization under uncertainty makes it possible to account for the impacts of uncertainty on an energy system at its planning or design stage.[61] The main approaches to optimization under uncertainty are comprised of stochastic programming, fuzzy programming, and stochastic dynamic programming. In most applications, stochastic programming has evolved as the preferred modeling framework.[33] Stochastic programming covers a wide range of approaches. According to the nature of uncertainty and the form it appears in a mathematical model, stochastic programming ranges from recourse programming, probabilistic programming, and dynamic programming, where recourse programming is regarded as an especially powerful method for sequential decision-making problems.[62]

These methodologies of energy systems engineering form a generic modeling and optimization framework to address the energy and environmental problems that exist in the planning and design of complex energy systems. Next, their applications in four real-life energy systems are presented.

POLYGENERATION ENERGY SYSTEMS

Polygeneration energy systems are multi-input and multi-output energy systems that coproduce electricity and synthetic liquid fuels. Process design of a polygeneration energy system involves several typical energy systems engineering issues, as follows:

A polygeneration energy system is a complex system that comprises many units and pieces of equipment. For each unit or piece of equipment, there usually exist many alternative technologies or types of equipment. Making the optimal selection from the many alternatives remains a challenge.

As public concern over fast increasing GHG emissions grows, the environmental impact of an energy system has become an important design criterion. Designing a polygeneration energy system according to multiple design criteria (economic, environmental, etc.) poses another challenge.

A polygeneration energy system usually has an operating horizon of several decades, over which there exist many inevitable and unpredictable uncertainties. Design of a polygeneration energy system under uncertainty makes the task further complicated.

Liu et al.[5−9] proposed a modeling and optimization framework for the optimal process design of polygeneration energy systems, based on the methodologies of energy systems engineering. First, a superstructure representation of a polygeneration energy system is constructed, shown in Figure 1, where a polygeneration energy system is divided into many functional blocks. For each functional block, all alternative technologies and types of equipment are included in the superstructure representation, and thus all possible types of process design are captured.

On the basis of the superstructure representation, a MINLP design problem is developed in the following form:

$$\begin{aligned} \min_{y,d,x} \quad & f(y,d,x) \\ \text{s.t.} \quad & h^{dc}(y,d) = 0 \\ & g^{dc}(y,d) \leq 0 \\ & h^{oc}(y,d,x) = 0 \\ & g^{oc}(y,d,x) \leq 0 \\ & d \in \mathscr{R}^l, y \in \{0,1\}^m, x \in \mathscr{R}^n \end{aligned} \tag{1}$$

where binary design variables, denoted as vector y, represent the selection (or not) of technologies or types of equipment for each functional block.

Continuous design variables, denoted as vector d, represent the capacities of the functional blocks, for instance, coal processing capacity of a gasifier, and methanol synthesis capacity of a chemical synthesis block.

Continuous operational variables, denoted as vector x, represent quantitative decisions to be made over the operating horizon, for instance, flow rates, stream compositions, and the like.

The objective function f could be a scalar or a vector involving cost, profit, energy, and environmental behavior.

Equality design constraints h^{dc} involve design variables y and d only, for instance, evaluation of initial investment costs.

Inequality design constraints g^{dc} involve design variables y and d only, for instance, logical relations between different functional blocks.

Equality operational constraints h^{oc} involve operational variables x_t and/or design variables y and d.

Inequality operational constraints g^{oc} involve operational variables x and/or design variables y and d. This category of constraints mainly comes from the mass and energy balances calculation.

In the MINLP design problem, there could be more than one objective function, that is, design criterion. Here, both the economic and the environmental behavior of a polygeneration energy system is evaluated. Net present value (NPV) is selected to be the economic design criterion, which comprises the initial capital costs and the discounted profit obtained over the entire operating horizon. A cradle-to-gate GHG emissions indicator is selected as the environmental design criterion, mainly comprising three parts: GHG emissions produced within the process during operation, GHG emissions produced throughout mining, extraction, and other processing stages of feedstocks, and GHG emissions produced during equipment production and plant construction.

On obtaining these two objective functions, a multiobjective MINLP problem is formed as follows:

$$\begin{aligned} \min_{y,d,x} \quad & U\begin{cases} f_1(y,d,x) = -NPV \\ f_2(y,d,x) = GHG \end{cases} \\ \text{s.t.} \quad & h^{dc}(y,d) = 0 \\ & g^{dc}(y,d) \leq 0 \\ & h^{oc}(y,d,x) = 0 \\ & g^{oc}(y,d,x) \leq 0 \\ & d \in \mathscr{R}^l, y \in \{0,1\}^m, x \in \mathscr{R}^n \end{aligned} \tag{2}$$

where f_1 is the objective function representing the net present value, and f_2 is the objective function representing the GHG emissions.

Problem (2) is solved using ε-Constraint method. Optimal results are presented on a Pareto curve, shown in Figure 2. For this example, there exist 18 different combinations of technologies, but only four of them appear on the Pareto curve, according to different economic and environmental design criteria. Each point on the curve represents a different process design. A decision-maker can thus pick up any point from the curve according to their specific interest or requirements.

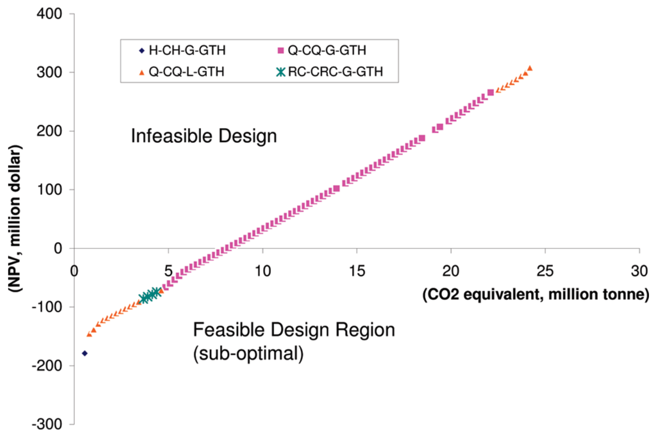

Figure 2. Pareto curve for polygeneration energy systems design.

In problem (1), all time-variant parameters are considered as piecewise constant functions over the operation horizon, which is discretized into several time intervals. However, due to the very nature of the long-term operation horizon, uncertainty is almost inevitable at the design stage, for example, due to external factors, such as market demands for products, prices of feedstocks and products, and the like. Here, we consider that all uncertain parameters can be presented as random variables following given probability distribution functions $p(x)$.

By incorporating the uncertainty into the MINLP design problem (1), the following two-stage stochastic programming problem results:

$$\begin{aligned} \min_{y,d} \quad & f_d(y,d) + E_{\theta \in \Theta}[f_s(y,d,\theta)] \\ \text{s.t.} \quad & h^{dc}(y,d) = 0 \\ & g^{dc}(y,d) \leq 0 \\ & d \in \mathscr{R}^l, y \in \{0,1\}^m \\ \text{with:} \quad & \\ f_s(y,d,\theta) = \min_x \quad & f_s(y,d,x,\theta) \\ \text{s.t.} \quad & h^{oc}(y,d,x,\theta) = 0 \\ & g^{oc}(y,d,x,\theta) \leq 0 \\ & x \in \mathscr{R}^n \\ & \theta \in \Theta \end{aligned} \tag{3}$$

where the objective function is split into a deterministic term f_d representing decisions at the design stage, and the expectation of a stochastic term f_s, which depends on the realization of uncertain parameters θ at the operation stage. Discrete variables y and continuous variables d are "here-and-now" (design) variables, which should be decided at the first-stage problem before the realizations of uncertain parameters θ occur, and x is a vector of

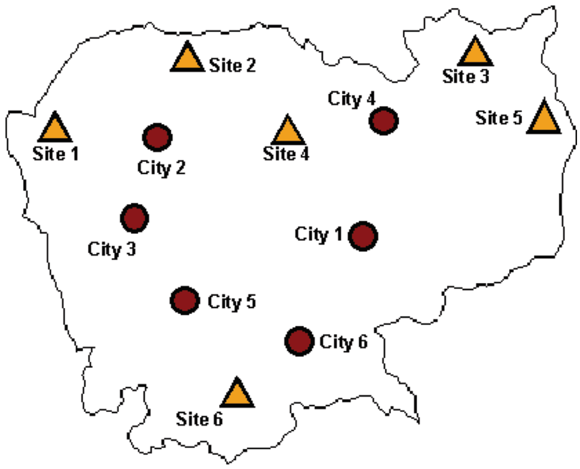

Figure 3. Illustrative representation of a hydrogen infrastructure planning problem.

"wait-and-see" (operational) variables, which can be decided over the operating horizon, that is, the second-stage problem, where all uncertain parameters have been observed. In the second-stage problem, the recourse term based on a specific realization of uncertain parameters is optimized, and corresponding corrective actions in terms of values of x are made. Problem (3) is solved using a decomposition-based solution strategy.

HYDROGEN INFRASTRUCTURE PLANNING

Energy systems engineering methodologies have been applied in hydrogen infrastructure planning in the work of Hugo et al.[15,16] The problem under study is illustrated in Figure 3: given a specific region where several potential production sites and markets (city as shown in the figure) are available, obtain the optimal infrastructure which connects the production sites to markets via a supply chain from primary feedstocks, central production, distribution, forecourt refuelling, to the final product over a long-term planning horizon.

This approach addresses the following issues involved in hydrogen infrastructure planning: planning over a long-term future horizon, geological site allocation, representing the state of existing infrastructure, especially the natural gas distribution network, electricity grid, and existing hydrogen production facilities, all types of available primary feedstocks, production, distribution, and forecourt refuelling technologies, trade-offs between large-scale centralized production and small-scale distributed production, transitions from one type of supply chain structure to another over time, and planning according to both economic and environmental performance indicators.

A superstructure representation of the modeling framework is shown in Figure 4. It captures all possible types of primary feedstocks, production sites, production technologies, distribution technologies, forecourt refilling technologies, and potential markets, and gives the optimal planning scheme over the entire future planning horizon.

Based on this modeling framework, a multiobjective optimization was conducted where net present value was selected as an economic objective and a LCA-based environmental impact factor as an environmental objective. A Pareto frontier comprising the full range of trade-offs between the economic and environmental objectives was obtained, shown in Figure 5. Any point on the Pareto frontier represents an infrastructure design with specific economic and environmental performances, and decision-makers can pick up any point from this curve as the final design according to their own specific interest and preference.

ENERGY SYSTEMS IN COMMERCIAL BUILDINGS

The applications of energy systems engineering methodologies in polygeneration energy systems and hydrogen infrastructure planning focus primarily on the energy production side. However, energy systems engineering is not confined within the scope of energy production. It can also be applied to model and optimize the energy consumption within a process or system. Liu et al.[19] have proposed an energy systems engineering approach to the energy systems design in commercial buildings, where on-site energy generation, conversion, and consumption are integrated.

The energy system in a commercial building usually comprises both an energy consumption section and an energy supply section. Energy demands usually come from requirements for lighting, HVAC (heating, ventilating, and air conditioning), and refrigeration. The energy supply is usually obtained from grid electricity, district heat, and on-site energy generation, for instance, distributed power generation and boilers. Major issues to be addressed at the design stage are summarized as follows:

First is selection of technologies. For each type of energy demand, several types of technologies or types of equipment are usually available. Selecting the optimal combination of them may become a challenging problem when faced with too many choices. This issue could be further complicated when involved with other design issues, for instance, integration between energy consumption and energy production sectors.

Second is integration. Integration among different energy consumption sectors within a system can reduce the entire energy demand of the system. For instance, heat produced in the refrigeration sector of a supermarket could be collected to heat the aisle space; otherwise, an extra amount of energy is required to meet the heating demand. The integration issue could become more complicated when on-site production technologies are also involved.

Third is building design. From an energy saving viewpoint, building design should also be involved at the design phase. For instance, sizing and positioning of windows could be considered together with the lighting requirement of a build to minimize it.

Last is GHG emissions. From an LCA point of view, emissions from a commercial building come from two sources. One source is the emissions produced over the entire operation period, and the other one is the emissions produced in manufacturing and transporting equipment and construction materials. Emissions from both categories should be considered at the design phase to give an overall environmental impact indicator.

To address these issues, a superstructure representation of the energy system in a commercial building is first constructed, shown in Figure 6. It comprises an energy supply section, an energy conversion section, and an energy savings section. The function of the energy supply section is to provide electricity and heat for the entire energy system. The energy conversion section converts electricity and heat obtained from the energy supply section to all energy demand tasks, such as refrigeration, lighting, ventilation, bakery, and space heating. The energy savings section further involves available types of energy savings technologies, such as night blind and weir screen for the refrigeration subsystem.

Based on the superstructure representation, a multiobjective MILP problem is formed and solved to obtain the Pareto curve,

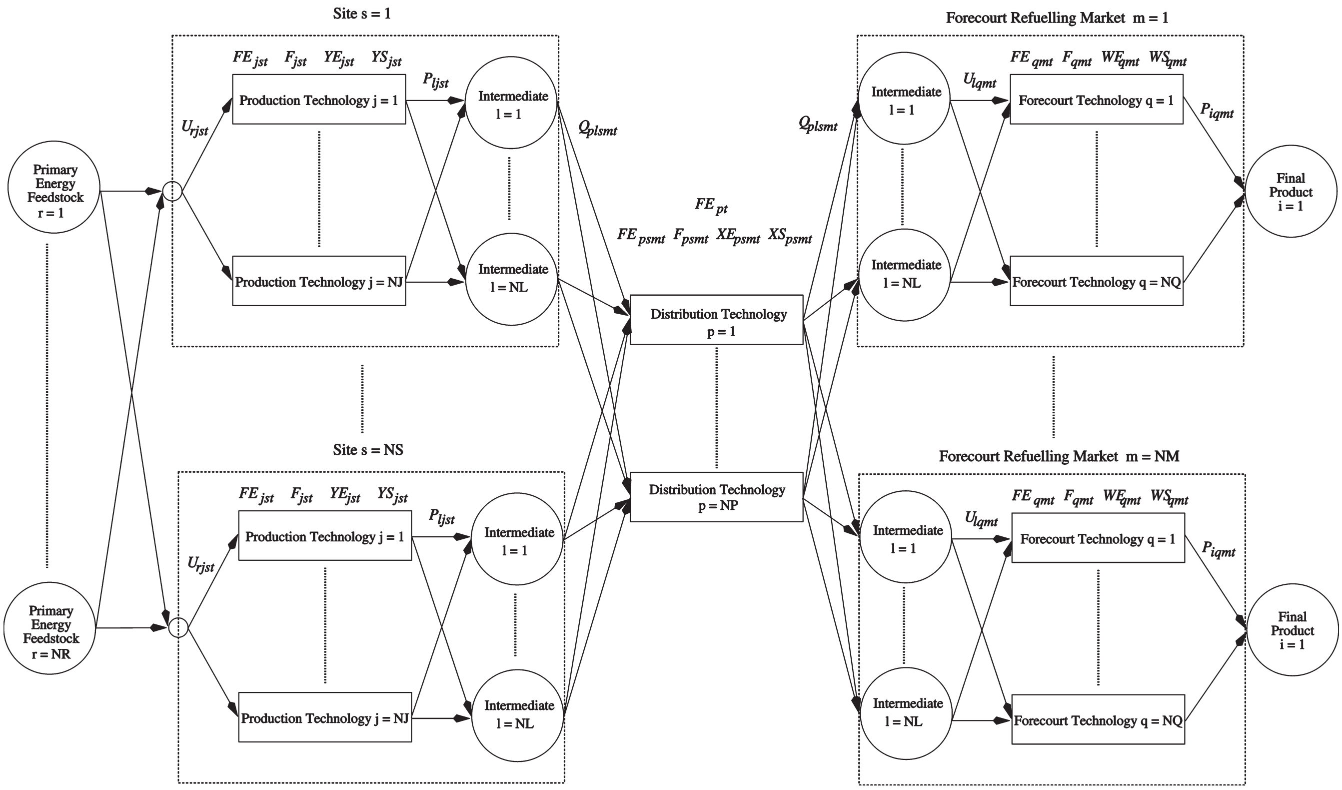

Figure 4. Superstructure representation of the modeling framework for hydrogen infrastructure planning.

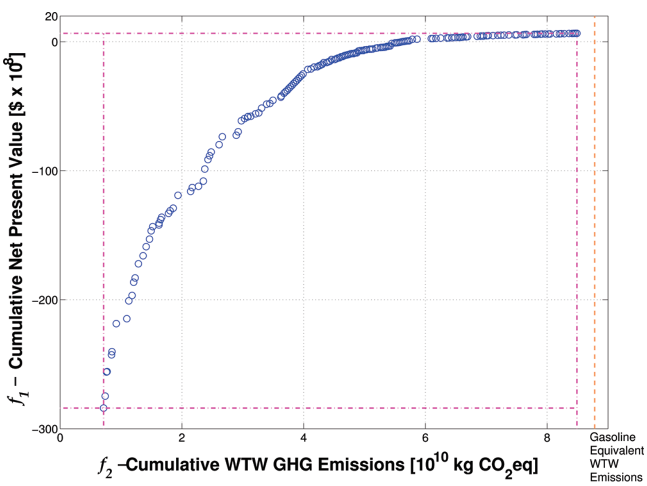

Figure 5. Pareto curve for hydrogen infrastructure planning.

shown in Figure 7. A decision-maker can pick up any point from the Pareto curve according to their specific design criteria or interest. Once a design point is selected, the system configuration behind it can be obtained directly from the model results.

BIOFUEL AND BIOREFINERIES

Biorefineries are processing facilities that use renewable plant materials as feedstocks. Raw materials comprised of carbohydrates and associated oil, protein, lignin, and other components are converted in the biorefinery into higher-value chemicals and other materials. The broad definition of biorefineries includes an initial process that utilizes renewable carbon-free feedstocks containing sucrose, starch, and cellulose as shown in Figure 8. Essential elements of a biorefinery are: multiple feedstock capability and a tolerance of a wide variation in those feedstocks, feedstock processing by enzymes to fermentable sugars (and byproduct streams), biocatalyst, which converts sugars to desired product(s), and coproducts, which are used in the process, recycled through the process, or sold.

Three basic biorefineries as depicted in Figure 9 are evolving on the basis of the nature of the feedstock, that is, sucrose, starch, or cellulose. On a fermentable-carbon-cost basis, the sucrose-based biorefinery I is currently the most competive. In recent years, however, the starch-based biorefinery II has become more cost competitive as a result of innovations in farming and milling grain like corn. In principle, the cellulose-based biorefinery III will become more competitive as technical and economic challenges are addressed in Figure 10.

The basic steps of each biorefinery are summarized as follows. In the first step, the precursor-containing biomass is separated by physical methods. The main products and the byproduct will subsequently be subjected to microbiological or chemical methods. The follow-up products of the main and byproduct can be also converted or enter the conventional refinery (Figure 10). Currently, four complex biorefinery systems are used in research and development: the lignocellulosic feedstock biorefinery, which uses "natural-dry" raw material such as cellulose-containing biomass and waste, the "whole crop biorefinery", which uses raw material such as cereals or maize, the "green biorefineries", which use "natural-wet" biomass such as green grass, clover, or immature cereal, and the "biorefinery two platform concept", which includes the sugar platform and the syngas platform.

In the realization of biobased chemical industry, two distinct approaches can be identified. In the first approach, the value chain approach, value-added compounds in biomass are identified and isolated in different processing and (bio)-conversion steps. The remaining biomass is then transformed into a universal substrate

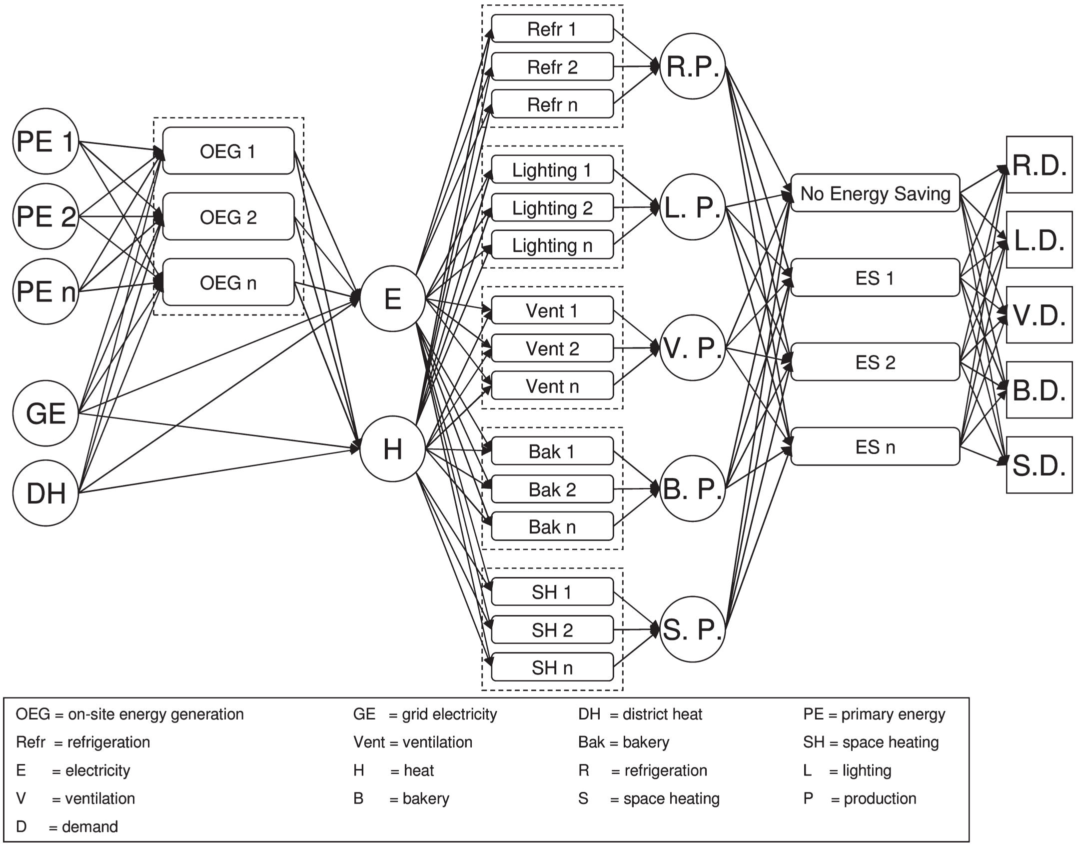

Figure 6. Superstructure representation of the energy system in a commercial building.

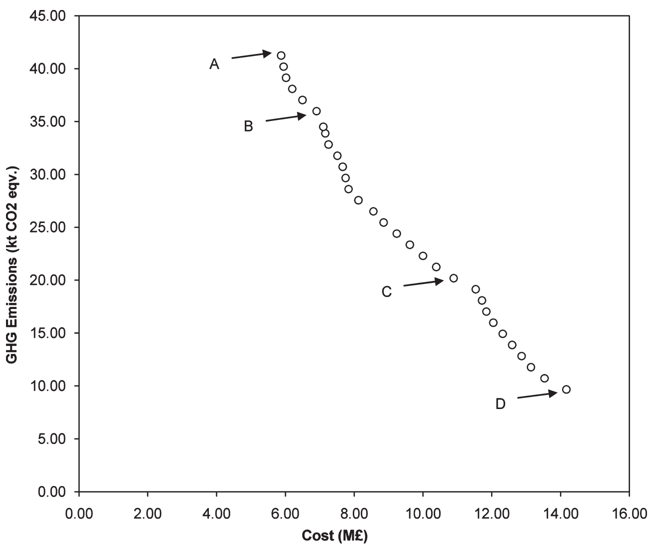

Figure 7. Pareto frontier for the energy system design in a commercial building.

from which chemical products can be synthesized. In this approach, it is thought that it is technologically and economically beneficial to extract valuable chemicals and polymers from biomass rather than building these components from universal building blocks. It can be concluded that the main technological challenges to aid the economic feasibility of this approach lie in the area of biomass refining, separation technology, and bioconversion technology. The second approach, the integrated process chain approach, follows the analogue of the petrochemical industry. In this scheme, a "universal" substrate is first transformed into universal building blocks, based on which chemical products are produced. In this approach, it is considered technologically and economically attractive to build chemicals in highly integrated production facilities. The main technological challenges for this approach lie in the high-efficiency transformation of biomass into commonly known building blocks for the petrochemical industry. The main technologies producing chemicals from biomass are: biomass pretreatment or refining, thermochemical conversion (gasification, pyrolysis, hydrothermal upgrading, etc.), fermentation and bioprocessing, and product separation and upgrading.

The integrated biorefinery is a facility that integrates in a flowsheet biomass conversion processes and equipment to coproduce fuels, power, and chemicals from diverse biomass sources. The biorefinery concept is analogous to today's petroleum refineries, which produce multiple fuels and products from petroleum (Figure 11). Industrial biorefineries have been identified as the most promising routes to the creation of a biobased economy.[20] These systems can be improved by better utilization of residues and optimization of the total added-value creation. New biorefineries can be enhanced by applying techniques, methodologies, and tools used in the traditional petroleum refinery processes.

The Process Systems Engineering Community has recently realized the significant potential offered by its computer-aided methodologies, tools, and techniques toward the synthesis, design, and optimization of economically attractive and sustainable biorefinery supply chains. Lignocellulosic bioethanol technologies exhibit significant capacity for performance improvement across the supply chain through the development of high-yielding energy crops, integrated pretreatment, hydrolysis and fermentation technologies,

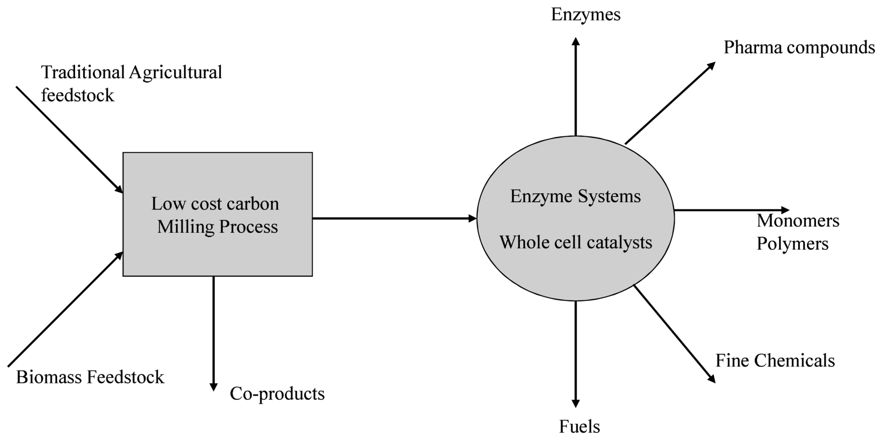

Figure 8. The overall biorefinery model.

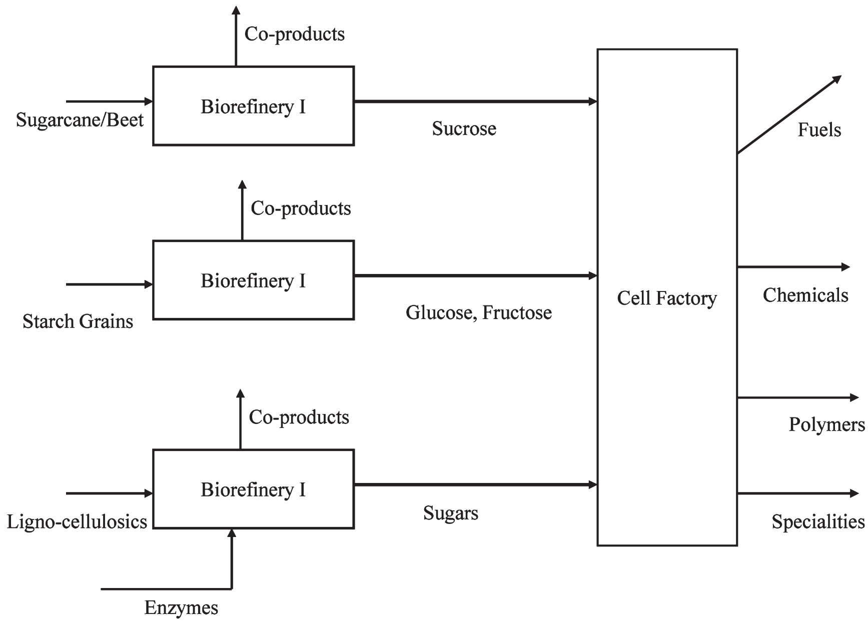

Figure 9. Biorefinery evolution.

and the application of dedicated ethanol pipelines. The impact of such developments on cost-optimal plant location, scale, and process composition within multiple plant infrastructures is poorly understood.

Dunnett et al.[21] presented a combined production and logistics model to investigate cost-optimal system configurations for a range of technological, system scale, biomass supply, and ethanol demand distribution scenarios specific to European agricultural land and population densities.

Zaboni et al.[22] presented a general modeling framework conceived to drive the decision-making process for the strategic design of biofuel supply networks. The design task is formulated as a MILP problem that accounts for the simultaneous minimization of the supply chain operating costs as well as the environmental impact in terms of GHG emissions (Zaboni et al.[23]). The model is devised for the integrated management of the key issues affecting a general biofuel supply chain, such as agricultural practice, biomass supplier allocation, production site locations and capacity assignment, logistics distribution, and transport system optimization. A spatially explicit approach has been adopted to capture the strong geographical dependence of the biomass cultivation practice performance.

Recently, Alvarado-Moralesa et al.[24] illustrated the use of a systematic methodology for design and analysis using bioethanol production as an example. More specifically, a well-known bioethanol production route was considered and analyzed with respect to cost, operation, and sustainability, and, on the basis of these, new alternatives with respect to waste reduction (water) and efficient downstream separation were generated.

Piccolo and Bezzo[25] considered and analyzed two different process alternatives (i.e., the enzymatic hydrolysis and fermentation process and the gasification and fermentation process) for the production of fuel ethanol from lignocellulosic feedstock. After a rigorous mass and energy balance, design optimization was carried out. Both processes are assessed in terms of ethanol yield and power generation as well as from a financial point of view. A sensitivity analysis on critical parameters of the processes' productivity and profitability is performed.

Franceschini and Macchietto[26] demonstrated the applicability and validity of model-based experiment design techniques through a biodiesel production process. The technique was applied to the planning of optimal experiments for complex kinetics elucidation. The need for an appropriate use of these tools, in particular a judicious problem formulation, was highlighted. A trade-off was found between the predicted precision of the estimates and important experimental aspects (for example, times and costs of the analytical work). The intelligent application of these techniques allows finding experiments that are suitable for the collection of data for complex kinetic networks. A methodology capable of dealing with experiment design problems that involve complex reaction mechanisms was also presented, and advantages and limitations of this procedure were discussed in the light of the results obtained from the parameter estimation.

Karuppiah et al.[27] addressed the problem of optimizing corn-based bioethanol plants through the use of heat integration and mathematical programming techniques. The goal was to reduce the operating costs of the plant. A limited superstructure of alternative designs was first proposed including the various process units and utility streams involved in ethanol production. The objective is to determine the connections in the network and the flow in each stream in the network such that the energy requirement of the overall plant is minimized. This is accomplished through the formulation of a mixed-integer nonlinear programming problem involving short-cut models for mass and energy balances for all the units in the system, where the model is solved through two nonlinear programming subproblems. The results indicate that it is possible to reduce the current steam consumption required in the transformation of corn into fuel grade ethanol by more than 40% as compared to initial basic design.

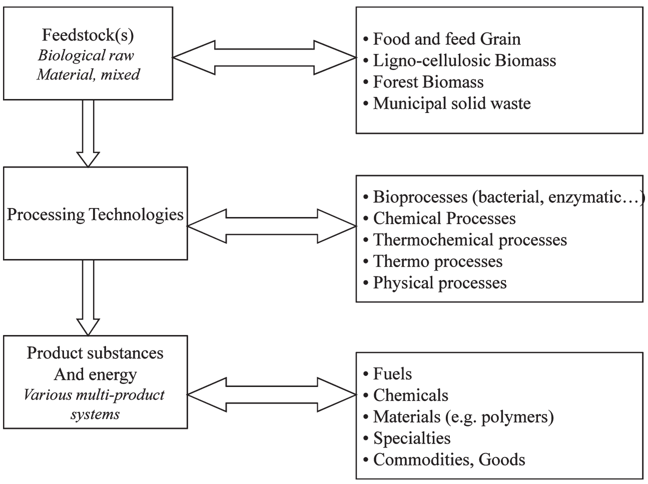

Figure 10. Basic principles of generation III biorefinery.

Gassner and Marechal[28] presented a detailed thermo-economic model considering different technological alternatives for thermochemical production of synthetic natural gas (SNG) from lignocellulosic biomass. First, candidate technology for processes based on biomass gasification and subsequent methanation was discussed and assembled in a general superstructure. Both energetic and economic models for biomass drying with air or steam, thermal pretreatment by torrefaction or pyrolysis, indirectly and directly heated gasification, methane synthesis and carbon dioxide removal, physical absorption pressure swing adsorption, and polymeric membranes were then developed. Based on this work, a future thermo-economic optimization will allow for determining the most promising options for the polygeneration of fuel, power, and heat from these systems.

From a process systems engineering perspective, the design, optimization, and synthesis of biorefineries are challenging problems as biorefineries, to compete with conventional processes, should achieve maximum efficiencies with economically attractive design, improved sustainability performance, better control, and process integration. Kokossis and Yang[29] presented an excellent review of the research challenges to be addressed by process systems engineering approaches and tools in the context of biorefinery design and synthesis. Klatt and Marquardt[30] highlighted the optimal processing of renewable feedstocks as one of the emerging application domains in process systems engineering. The development of biorefineries has to follow an integrated design approach, with new challenges to account for the wide range of feedstocks and their uncertainty and a need to formulate local and regional patterns of solutions. Unlike the case of fossil oil and gas as they are produced and processed on a global basis, the sustainable utilization of biomass requires production plants to be allocated close to the raw material resources.

From a systems perspective, biorefineries represent ordered combinations of feedstocks, processing pathways, processing technologies, and products.[29] At least in reference to the biochemical transformations, early developments actually addressed a limited number of biofuel products (mainly ethanol and

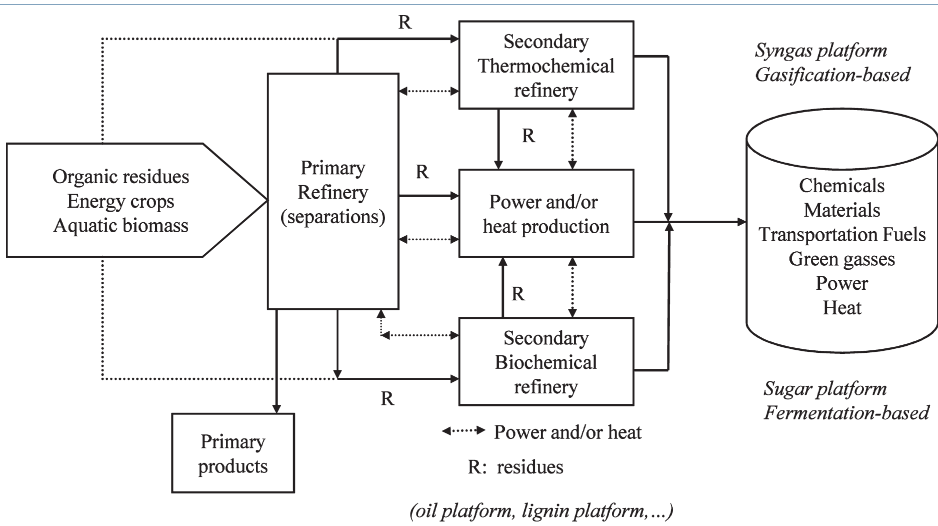

Figure 11. Detailed overview of an integrated biorefinery process.

biodiesel), well-known processing pathways, a limited number of processing technologies, and a variety of different feedstocks. Still, process systems engineering technology can offer powerful methods and tools to systematical improve biorefinerey supply chains by: designing the biorefinery supply chain network utilizing mixed-integer programming techniques and formulations similar to the supply chain production networks,[21,22] employing superstructure optimization-based or target-based techniques to derive optimal biorefinery design options,[24,28,32] systematically considering the impact of variability and uncertainty in the feedstocks by using parametric programming and other uncertainty techniques,[33] applying model-based experiment design techniques to derive unknown reaction schemes,[26] exploring energy and process integration opportunities,[27] applying advanced process control techniques to ensure operable biorefinery design options, and designing biorefineries under sustainability criteria.[34]

As pointed out by Kokossis and Yang,[29] in biodiesel processes, similar challenges relate to the selection of pretreatment stages, the design and the selection of reactors and reaction conditions, and the potential to integrate adjacent processes (i.e., reaction and separation). Thermochemical paths offer more aggressive routes to energy (through higher temperatures) and alternative processes to use (gasification, pyrolysis, methanol synthesis, Fischer–Tropsch), with some processes still developing (especially the ones involving catalysis) and others already developed.

Aside an apparent interest in new developments, an equally interesting aspect is the appropriate selection and integration of the available technologies. Superstructure methods can provide significant insight into a systematic screening of technological options for the pretreatment stages or a rigorous assessment of performance limits for reactors and separators. Multiparametric programming techniques could have systematically assessed the variability in raw materials and compositions,[3] whereas Pinch Analysis could have determined quick targets for energy and water use, setting incentives for better integration.

■ CONCLUSIONS AND FUTURE DIRECTIONS FOR ENERGY SYSTEMS ENGINEERING

Methodologies of energy systems engineering are introduced in this Article to guide the planning and design of energy systems. These methodologies involve superstructure based modeling, mixed-integer programming, multiobjective optimization, optimization under uncertainty, and life cycle assessment. These methodologies cooperate with each other and provide a systematic solution strategy for the planning and design issues involved with any energy system. These methodologies are illustrated via their applications in real-life energy systems of very different nature and scale. It shows that energy systems engineering is of tremendous importance to guide the transition from our existing generation of energy systems to a more energy efficient and environmentally benign one. It is certain that research in this field will continue and prosper. Systems engineering tools, particularly those in synthesis, optimization, and modeling, could have a huge impact on the development of units, processes, supply chains, and the biorefinery concept itself. Some recommendations for future research directions are summarized as follows:

The generic modeling and optimization methodologies presented in this Article can serve as a starting point, and more methodologies that are suitable for energy systems could be added into the scope of energy systems engineering. This would certainly extend its applicable fields and enhance its capability.

Modeling at a microlevel could be explored. The methodologies introduced here enable modeling at strategic planning and process design levels, which can be regarded as modeling at mega-level and macro-level, respectively. Modeling at a microlevel, for instance, at the molecular level for biodiesel production, would give a much better insight to these systems.

The generic modeling and optimization methodologies introduced in this Article could be used in the control field. First, it can be used in an integrated design and control scheme where both operational and control requirements are taken into consideration at the design stage. Second, the framework can be also used in the context of model predictive control.

Applications could be made in energy value chain modeling and optimization. For instance, bioenergy is expected to play an important role in the ongoing transition from conventional energy system to a more sustainable and environmentally benign one. There also have been many controversies around bioenergy about its capability to ameliorate energy security and climate change, concerning its life cycle GHG emissions and competition on land use with food crops. The modeling and optimization methodologies developed in this framework could be used to guide the planning and design of a bioenergy value chain in terms of analyzing and quantifying net profit of bioenergy, producing methodologies and tools for the optimal design of bioenergy value chains with the right technologies at the right scale, and providing policy suggestions to direct the development of bioenergy.

The incorporation of uncertainty in the design and operation of future energy supply chains and energy systems could be done. Here, uncertainty in energy prices seems to significantly affect optimal investments decisions for new energy supply chains as well as their future operation. A scenario-based approach for uncertainty modeling, similar to the manufacturing supply chains,[63] provides a simple and effective way to systematically assess the impact of uncertainty on the design and operation of future energy systems.

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