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Sustainable design and synthesis of energy systems

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This paper provides an overview of sustainable design and synthesis of energy systems. We review recent progress and present major research challenges of the superstructure optimization based approach in terms of: (1) systematic generation of comprehensive process superstructures; (2) building optimization models that integrate techno-economic assessment with life cycle sustainability analysis while addressing uncertainty issues; (3) efficient computational algorithms for solving the resulting mixed-integer nonlinear optimization problems. Process integration and process intensification are briefly outlined as alternative approaches to sustainable design and synthesis of energy systems. This paper identifies several future research directions for sustainable design of energy systems, such as broadening the scope of sustainable design with a consequential perspective, handling uncertainties using multi-stage robust optimization techniques, and integrating standalone energy systems through multi-scale optimization.

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Introduction

Energy systems involve a broad range of systems that are related to the generation and consumption of energy [1,2]. This paper focuses on systematic methods for sustainable design and synthesis of such systems as they relate to chemical engineering. Energy production is integral to our society both now and in the future. As nonrenewable sources diminish, it will be critical to design and synthesize sustainable energy systems to meet future energy demands. In previous years, process systems engineering has expanded to incorporate sustainability issues in energy systems design. Accordingly, methods such as superstructure optimization, process integration, process intensification, among others, and their applications to sustainable design and synthesis of energy systems have become an active research area [3•].

This paper reviews recent progress in this area and presents three major research challenges of the superstructure optimization based approach for energy systems design. The first challenge is to generate comprehensive process superstructures in a systematic manner; the second challenge involves developing optimization models based on the superstructure and integrating techno-economic assessment and life cycle sustainability analysis methodology with the model while also addressing uncertainty issues; the third challenge lies in the development of efficient computational algorithms for solving the superstructure optimization problem to obtain the sustainable design and synthesis decisions. Additionally, to address these research challenges we identify future research directions, including the introduction of a consequential perspective into sustainable design, the application of multi-stage robust optimization techniques to hedge against uncertainties, and the utilization of multi-scale optimization to determine the best integrated energy systems.

The rest of this article is organized as follows. The next section briefly outlines three approaches to process synthesis. Later, we review recent contributions and present research challenges in sustainable design and synthesis of energy systems, followed by other approaches to sustainable design and synthesis of energy systems. Future research directions are discussed in the penultimate section. The article is concluded in the last section.

Approaches to process synthesis

Several systematic methods have been developed to search among technology and process alternatives [4••]. The first one is total enumeration, which simply evaluates every alternative and selects the one with the best performance [5]. This method is straightforward in principle but demands large amounts of computational or labor resources unless the number of alternatives is considerably small. The second method, referred to as the evolutionary method, begins with a feasible base-case design and makes incremental improvements to part of the system in each iteration [6]. This method cannot guarantee that the final design decisions represent the optimal design in the corresponding design space. A hierarchical decomposition method was developed to address process synthesis problems through a sequence of design decisions at different levels [7]. Even though this method could handle complex systems, optimal solutions are not assured because it does not consider interactions between different decision levels [8].

Assisted directly by mixed-integer programming techniques, superstructure optimization enables simultaneous evaluation of process/technology alternatives and automatic generation of the globally optimal configuration [9]. In virtue of this advantage, the superstructure optimization approach has received much research attention over the past thirty years [10–14]. Specific applications of superstructure optimization can be found for heat integration [15,16], bioethanol production [17], hybrid feedstock systems [18•], polygeneration systems [19,20], and multi-product biorefinery systems [21].

Sustainable design and synthesis of energy systems based on superstructure optimization

Sustainability has recently emerged as an important consideration in the design and synthesis of energy systems [22••]. Evaluating sustainability metrics during the conceptual design phase provides a straightforward method to assess the sustainability of an energy system. However, this static method does not support the search for the most sustainable design, even though arduous, iterative evaluations can improve the sustainability of a design gradually. A trending systematic method for sustainable design and synthesis of energy systems evolves from superstructure optimization and dynamically integrates the tenets of techno-economic and life cycle sustainability analyses into a multi-objective framework [23••,24]. As opposed to other methods, this method enables systematic generation and automatic evaluation of design candidates with the best process economics and highest levels of environmental sustainability. Recently this method has been actively applied to optimally designing and synthesizing various energy systems, including hydrocarbon biorefineries [25••,26,27,28••,29], algal systems [30–33], polygeneration systems [34–36], shale gas processes [37–39], and network systems [40].

As illustrated in Figure 1, there are three stages in sustainable design and synthesis of energy systems based on superstructure optimization: superstructure generation, optimization model development, and optimal design decision determination. The remainder of this section describes each stage in detail and presentspertinent challenges.

Superstructure generation

The success of the superstructure optimization approach relies on generating a complex superstructure a priori. With increasing knowledge of new technologies and processes, we have access to a large number of process/technology alternatives for the same unit operation in energy systems. If a wide array of candidate operating units are given and the connections between these units are not restrictive, there will be a large number of combinatorially possible network structures to produce certain end-products from given feedstock materials. In such cases, a process-graph approach has been proposed for the generation of a maximal structure (superstructure) [41] and corresponding feasible structures [42]. If we are given alternative processes instead of isolated operating units or the sequence of technologies applied in the entire process is predetermined, the following three steps can be considered to generate a superstructure from scratch: (1) Define design targets. This step determines the types and quantities of accessible feedstocks and desired products, as well as possible process restrictions. This information helps reduce the size of a superstructure and computational resources needed for optimization. (2) Establish a preliminary superstructure. In this step, a preliminary superstructure is established by dividing a process into sections and filling each section with multiple alternative unit operations or technologies. General technology and process information can be retrieved from literature. (3) Specify alternatives. Once the preliminary superstructure is created, specific process details are added and corresponding process data can be collected from experimental literature and simulation works. Extracting data plays a central role in this step since the data directly determine the type of model to be used in mass and energy balances. It is common that a set of data are beyond the scope of the existing contributions, or multiple data are available for the same parameter. In these cases, justifiable assumptions, simulation, and/or experiments can be employed to eliminate the data gap or to choose the correct data. If these methods fail to collect adequate data, the corresponding technologies must be abandoned in the superstructure so as not to identify unjustified optimal solutions.

Research challenges of superstructure generation

The above steps are helpful and effective especially when abundant process details are specified and many process restrictions are imposed. For example, if we intend to develop a superstructure for the conversion of shale gas to hydrocarbon fuels via Ficher-Tropsch synthesis, we may consider alternatives for reforming reactions [43], and Ficher-Tropsch synthesis [25••], respectively. In this example, it is not a difficult task to exhaust available technologies in literature. However, generating a comprehensive superstructure becomes a challenging task when more degrees of freedom are granted. For example, if we intend to develop a sustainable energy system for the production of hydrocarbon fuels and no restrictions are imposed on technology or process selection, the corresponding superstructure could be much more difficult to generate. A hypothetical strategy in this case is to incorporate as many technology alternatives as possible so that the resulting superstructure optimization does not miss the optimal design. Unfortunately, there is not yet a quantitative guarantee for the completeness of a comprehensive superstructure. There are two reasons for the challenge in