Energy 73 (2014) 145–159

Contents lists available at ScienceDirect

Energy

journal homepage: www.elsevier.com/locate/energy

Technology analysis of integrated biorefineries through process simulation and hybrid optimization

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ARTICLE INFO

Article history:
Received 6 January 2014
Received in revised form
29 May 2014
Accepted 31 May 2014
Available online 4 July 2014

Keywords:
Process synthesis
Hybrid optimization
Process integration
Renewable energy
Lignocellulosic biorefinery

ABSTRACT

This work investigates the design and modeling of fully integrated processes which utilize renewable feedstocks as raw materials by evaluating alternative technology options and possible process integrations to select the optimal configuration according to calculated process yields and economic profit criteria. The analysis is carried out by exploiting the advantages of process simulation and a novel hybrid optimization framework which includes a two layer optimization strategy composed of strategic and operational level decisions. Additionally, an integrated software platform is developed to incorporate experimentally-derived kinetics of complex biological reactions in process simulation. To demonstrate the effectiveness of the proposed approach, an advanced biofuel production facility which has alternative technology choices for each section of the plant is utilized. The results prove the efficiency of the proposed approach, and an optimal configuration for a lignocellulosic biorefinery is obtained.

1. Introduction

As the world has recognized the importance of diversifying its energy resource portfolio away from fossil resources and more towards renewable resources such as biomass, there arises a need for developing strategies which can design renewable sustainable value chains that can be scaled up efficiently and provide tangible net environmental benefits from energy utilization [11,13,23,24,37]. Biobased fuels and chemicals can be derived from any form of biomass such as plants or organic wastes. After a boom in the U.S. corn-based ethanol (first-generation biofuel) in the early part of the 21st century [48], the interest has gradually shifted towards more viable renewable resources such as lignocellulosic feedstocks since the viability and sustainability of first generation biofuels are uncertain and questionable [33,43]. Negative impacts of first generation biofuels might lead to the risk of deforestation by overuse of lands, environmental risks by the widespread use of fertilizers and pesticides, and decreasing food security by the risk of creating a competition between food and fuel production.

Cellulosic ethanol is an example of such alternative fuel which is considered as a second-generation biofuel and is derived from cellulose instead of starch. The fuels and chemicals produced from lignocellulosic feedstocks are extremely attractive owing to the fact that the raw materials can be composed of “left-over” wastes of food crops and forest harvests that do not interfere with the human food chain. It also can provide new income and employment opportunities in rural areas. Further, due to the large variety of lignocellulosic materials and their abundance, these types of produced fuels and chemicals (second-generation) can overcome the challenge of limited feedstock availability that first generation biorefineries have to contend with.

There are two main conversion platforms in a biorefinery process: (1) the biological conversion pathways based on fermentation, and (2) thermo-chemical conversion pathways based on heat-based technologies such as gasification and pyrolysis. The main difference between these two conversion mechanisms is the primary catalysis system [9]. In biological conversion pathways, biocatalysts such as enzymes and microorganisms are utilized. However, in thermochemical production routes, heat and physical catalysts are utilized to convert biomass to biofuels and chemicals.

By considering the fact that conversion technologies in second generation biorefineries are relatively immature and recalcitrance of lignocellulosic materials can cause major barriers to the economical production of biofuels [6,18], process synthesis by analyzing alternative technology options, considering possible process integrations, and developing mathematical optimization methodologies can be useful for designing more cost-effective configurations with improved techno-economic and environmental characteristics. Many frameworks have been proposed for designing technological flowsheets with improved performance. Some research studies

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http://dx.doi.org/10.1016/j.energy.2014.05.114

focused on analyzing the performance of alternative technology options for a section of biorefinery plant [35,51,56]. These studies provide a good insight for the performance and optimal operating conditions of that particular section. However, conversion of biomass to biofuels and biochemicals is a complex process which includes different processing steps; for example in biochemical route, pretreatment, hydrolysis, fermentation and purification are required to produce fuels and chemicals from biomass; there are many tradeoffs in the commercial scale design of these sections owing to their interdependency, which are often overlooked when each section is analyzed independently.

Additionally, several research studies considered single-product endeavors that produce low margin fuels like ethanol [7,12,28,41,53]; with low-margin products, slight changes in input costs, process yields, or markets (prices) can have a major impact on project profitability. With this in mind, it is important to analyze a mix of high and low margin products and optimize the production volume of them to maximize the long term value of a biorefinery.

Finally, several approaches have been developed for selecting optimal feedstocks, technological superstructures and product portfolios in the biorefinery process [3,26,28,45,61]. Most of these studies have focused on using single values for process parameters (including reaction conversion rates) that may or may not be true in real operations of the plant. Further, most of these studies considered linear methods or shortcut equations for modeling the integrated biorefinery process to allow for large model development with relatively short computational times. However, conversion mechanisms in biorefinery processes are inherently non-linear in nature.

In this study, we incorporate solutions for the aforementioned shortcomings in order to develop a more robust framework that can mimic the actual design methodology that planners, developers, and enterprises should follow for designing sustainable biorefineries of the future:

1. To achieve a cost-effective design of commercial-scale biorefineries, it is crucial to understand the entire integrated biorefining process and how one stage of the process can impact the performance of the others. Therefore, these tradeoffs should be incorporated in the process by developing detailed fully integrated models which include all the process units from feedstock to products.
2. Ethanol as a fuel and succinic acid as a high value chemical are the main products of the biorefinery in our current study and their production rates can be varied to optimize plant margins based on input costs and product markets.
3. To impart a greater degree of realism to biorefinery design, true estimates of process parameters are crucial. Consequently, nonlinear process dynamics that are inherent in complex bioprocesses should be incorporated while modeling the plant.
4. Operational level optimization should be included in the optimization framework to design a comprehensive optimization strategy which considers the impact of- and the tradeoffs between long and short term decisions into a single framework.

By considering the challenge of integrating process dynamics, nonlinear optimization and strategic planning, different software platforms need to be interlinked in a novel fashion to execute the framework seamlessly. Our analysis is performed by exploiting the advantages of a novel hybrid optimization framework which incorporates a two layer optimization strategy including strategic planning and operational optimization using rigorous nonlinear process simulations as well as metaheuristic optimization. At this stage of model development, the focus of our current study is analyzing the profitability of the process based on production yields, operating costs, and energy consumptions. Detailed cost estimation of all the unit operation at different capacities will be done as the next step to expand our proposed framework and add more flexibility into it. The case study considered in this work is an advanced biorefinery which has different technology options for each section of the process, and the ability to produce multiple products from lignocellulosic raw materials.

2. Hybrid optimization methodology

The proper choice of optimization methodology depends on the complexity of the problem. To design an optimal biorefinery different aspects including strategic and operational level decisions should be considered. Strategic decisions are the longer term decisions which have an extended impact on the economic, environmental and social value of an enterprise, while operational level decisions focus on daily/weekly management of plant operation. In a previous publication [10] a framework was proposed to maximize the economic value of renewable energy systems with decision tasks that included feedstock selection, product portfolio design, technology superstructure design, strategic capacity planning, and optimization of operating conditions.

Following is the brief description of the hybrid optimization algorithm, with considering some modifications to the previously proposed framework. LP (linear programming) models are suggested for the purpose of strategic capacity planning. However, there will be a mismatch between the real (nonlinear) mechanism of the plant and the LP-based optimization model. To overcome the mismatch and also for incorporation of nonlinear operational level optimization in one framework, a two-level approach is proposed as shown in Fig. 1. This two level approach combines NPV (net present value) optimization for long term planning with rigorous nonlinear operational level simulation and optimization. In the upper level, the capacity is designed strategically by maximizing the NPV of the plant. Then this capacity is sent to the lower level of the optimization algorithm. First the process is simulated in the simulation software (Aspen Plus) based on the optimal capacity plan and results are utilized in the process optimization model in MATLAB to optimize the decision variables by maximizing the

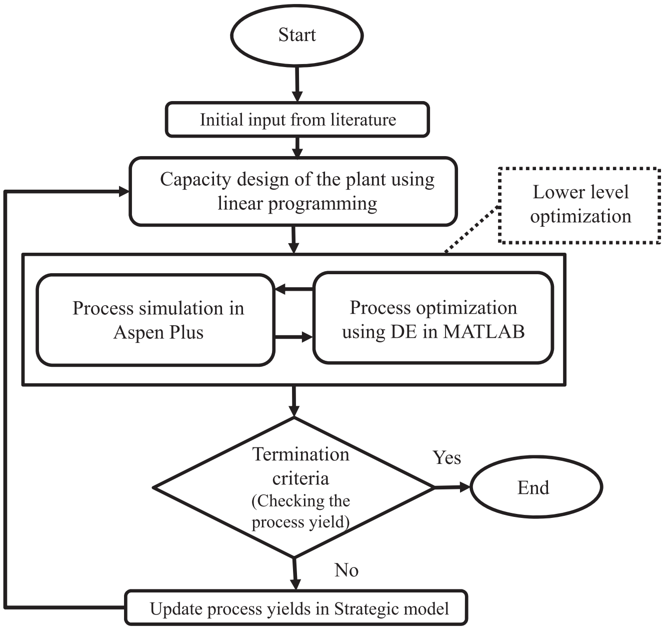

Fig. 1. Structure of the proposed hybrid methodology.