A modeling framework for design of nonlinear renewable energy systems through integrated simulation modeling and metaheuristic optimization: Applications to biorefineries

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ABSTRACT

This study presents the development and implementation of a novel framework for optimal design of new and emerging renewable energy production systems by considering an iterative strategy which integrates the Net Present Value optimization along with detailed mechanistic modeling, simulation, and process optimization which yields optimal capacity plan, and operating conditions for the process. Due to the non-linear nature of process conversion mechanisms, metaheuristic algorithms are implemented in the framework to optimize operating conditions of process. Further, to apply complex kinetics in the process, we have made a linkage between process simulator (Aspen Plus) and Matlab. To demonstrate the effectiveness of the proposed methodology, a hypothetical case study of a lignocellulosic biorefinery is utilized. The proposed framework results reveal a deviation in optimal process yields and production capacities from initial literature estimates. These results indicate the importance of developing a multi-layered framework to optimally design a renewable energy production system.

1. Introduction

Over the past decade, world energy consumption has increased progressively owing to the growing demand by burgeoning industrial societies in emerging markets and the rising world population. The current global state of energy supply is highly dependent on fossil fuels. Owing to finite nature of fossil fuels, rapid increase in their prices and concerns about their environmental impact, efforts around the world to develop and commercialize renewable transportation fuels and biobased chemicals have intensified (Cardona & Sanchez, 2007). As the world has recognized the importance of diversifying its energy resource portfolio away from fossil resources and more toward renewable resources, the focus has shifted from recognizing the importance of the renewable resources sector toward designing sustainable value chains that can be scaled up efficiently and provide tangible net environmental benefits from renewable energy utilization. Still, the commercialization of conversion technologies has been hampered by a multitude of endogenous and exogenous factors including unavailability of appropriate feedstock supply systems, lack of capital and investment risk appetite, and inefficient feedstock conversion systems. Out of all issues mentioned, optimizing conversion systems can have a tremendous impact on the overall profitability of renewable transportation fuels and biobased chemical value chains.

Renewable energy in its broad sense is energy that is derived from natural resources such as sunlight, wind, water, and geothermal heat; these resources have shorter cycles of replenishment and are provided by nature on a “near-continuous” basis. Renewable energy, as a final product, comes in 2 essential forms; (1) electricity that is transported geographically using fixed transportation mediums such as utility grids and wires, and (2) transportation fuels, such as biodiesel, ethanol and butanol, whose mediums (vehicles) are mobile in nature. Once we have categorized the type of renewable energy, we can start to focus on the renewable resources that are currently utilized to produce these energies. Solar, wind, water, and hydrothermal sources in their native forms are used mostly to produce electricity. In order to democratize the use of renewable energy specifically as transportation fuels, a seamless transformation where the renewable resources are converted from their native forms to a more usable and convertible form, is necessary. Fortunately nature provides such a transformative process through the use of photosynthesis, where carbon inputs are chemically altered into organic compounds using energy from sunlight. These compounds, primarily in the form of sugars and lipids, are used to form the structure and backbone of almost all plants and trees we see around us. The question then becomes, what processes and technologies are needed to harvest this natural energy and convert them into usable forms for use as portable,
transportation fuels in an economically viable and environmental and socially responsible manner.

The concept of a biobased facility had been prevalent in the United States and the world in general, for hundreds of years. Paper and sugar mills are quintessential examples of bio-facilities where renewable raw materials such as wood pulp and sugarcane are converted to value-added products. The use of composting facilities and waste digesters in farms and rural areas around the world has been a source of sustainable generation of electric power from renewable resources for decades. In recent times, the emphasis on biobased production using renewable resources has significantly broadened its footprint to incorporate production of fuels, power and chemicals derived from a wider variety of renewable resources. Some renewable transportation fuels that are already in the commercial production phase include first generation ethanol (corn ethanol) and biodiesel (from vegetable oils and animal fats).

Recent ventures into renewable energy have been fraught with corporate failures. A driving reason for these unsuccessful ventures, in part governed by the lack of proper planning in designing renewable energy plants and supply networks. Often exuberant forecasts of market evolution and insufficient levers in plant and supply chain design for risk mitigation have led to companies failing to maintain solvency when lab- and bench-scale innovations are commercialized for the production of renewable products. An essential part of the planning process is garnering sufficient decision support to guide long-term strategic actions in the face of process and policy uncertainty, and market and competitive risks.

Decision modeling frameworks are ubiquitously classified as decision support systems in a variety of industry verticals. In its most basic form, a decision support system is used to help value chain actors make mission-critical decisions that have an economic, social, or environmental impact on the stakeholders of the value chain. Additionally, the nature of the decisions can be (1) strategic in nature leaning toward longer term decisions that will have an extended impact on stakeholders, (2) tactical which help stakeholders develop tactics to execute the strategies that are developing through strategic planning, or (3) operational in nature where the daily or weekly management of value chain functioning is emphasized.

Within the renewable products industry, decision support systems are relatively new, somewhat driven by the nascent of the industry itself. Owing to the complex nature of supply chains, conversion processes, and product markets, the use of decision support to aid in decision-making seems appropriate and in many cases it does lead more sound actions being taken by stakeholders based on a more complete picture of what is actually happening around them. Most decision support systems use complex mathematical formulations to model the interactions and interplay of actual physical phenomena that may go unaccounted for in case of ad-hoc decision making; consequently they are considered a valuable tool for any decision maker to compliment the “due diligence process” that they would go through before finalizing and executing critical decisions that would impact stakeholders over the short, medium, and long terms. Table 1 shows a list of renewable product industries and corresponding support functions for a prototypical decision support framework.

From the perspective of new renewable product value chains, we have to be cognizant of the fact that most of these endeavors are still in their design and pre-feasibility study phase, wherein, the processes that execute the purpose of the value chain are still nonexistent. For example, 2nd and 3rd generation biofuels including cellulosic ethanol and butanol, and algae oil are still in the research, development and demonstration (R&D) phase in their commercialization cycle, where feedstock supplies, processing technology yields, and product markets are still being studied and developed. When developing a decision support framework for such enterprises, the initial functions of the framework should therefore focus on aiding stakeholders in the intelligent design of the supply and production chains that will impact all actors and participants over strategic time horizons (10–30 years).

The inception of decision support tools and frameworks is a relatively new concept in the field of renewable energy and biochemicals and is gaining attention. Ramachandra, Jha, Krishna, and Shruthi (2005) presented a model based decision support tool that helped solar power companies estimate the probable amount of solar energy regionally. Ouammi, Ghiglotti, Robba, Mimet, and Sacile (2012) published a model based environmental decision support system that stressed optimal technology selection and site location for wind power generation. In recent times, several analytical models have been suggested to study the effect of biomass species, technology choices, plant capacities, and process operating conditions on the production and profitability of cellulosic ethanol. The National Renewable Energy Laboratory (NREL) has developed several analytical models (Aden, 2008; Dutta & Phillips, 2009; Kazi, Fortman, & Anex, 2010) that analyze different process configurations for the production of cellulosic ethanol. A technical report by Minnesota Technical Assistance Program (2008) investigates ethanol production and introduces potential improvements in energy and water requirement as well as environmental impacts reduction. In this report a comparison of newer and older facilities in Minnesota for ethanol production is also provided. Sammons, Eden, Yuan, Cullinan, and Aksoy (2007) developed a general systematic framework for optimizing product allocation and process configuration for a flexible biorefinery. Their methodology provides a framework for process design and product selection based on optimization. In their model, process integration methods such as pinch analysis are employed to optimize the plant. Production pathway and product portfolio are selected based on economic and environmental criteria. Zondervan, Nawaz, de Haan, Woodley, and Gani (2011) proposed a model to compute the optimal processing routes in a biorefinery by considering different feedstock and products. Bao, Ng, Tay, Jimenez-Gutierrez, and El-Halwagi (2011) developed a systematic optimization framework by integrating multiple conversion technologies. In this model the optimization problem is formulated as a linear program. Karuppiah et al. (2008) and Martin and Grossmann (2011) showed a superstructure optimization model which incorporates heat integration inside the plant. The optimization problem is formulated as a mixed-integer non-linear programming problem involving short-cut models for all the units in the system that consist of mass and energy balances, and design equations. Pham and El-Halwagi (2012) proposed a systematic two-stage approach to the synthesis and optimization of biorefinery configurations with the available feedstocks and desired products. A “forward–backward” approach is introduced for synthesizing possible pathways. An increased emphasis on efficient supply chain management and Net Present Value optimization has yielded substantial literature concerning supply chain

<table>
<thead>
<tr>
<th>Renewable energy sub-industry</th>
<th>Decision support functions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solar</td>
<td>Solar resource assessment; Power market analysis (supply, demand, price), load forecasting</td>
</tr>
<tr>
<td>Wind</td>
<td>Wind resource assessment, load and power forecasting, discrete parts’ inventory management</td>
</tr>
<tr>
<td>Biomass (electricity)</td>
<td>Regional feedstock inventory analysis (GIS), feedstock logistics management, emissions management</td>
</tr>
<tr>
<td>Hydropower</td>
<td>Water resource assessment and planning, Hydropower forecasting, environmental management</td>
</tr>
</tbody>
</table>
modeling and strategic value optimization (Lainez, Puigjaner, & Reklaitis, 2009; Naraharisetty, Karimi, & Srinivasan, 2008; Puigjaner & Lainez, 2008). Eksioglu, Acharya, Leightley, and Arora (2009) developed a MILP model to design the supply chain and manage the logistics of a biorefinery. In their multi-period model, the supply chain problem is described as a network design problem to determine the optimal number, size, and location of biorefineries. Mansoornejad, Chamboiost, and Stuart (2010) suggested and exemplified a strategy for hierarchical product, process, and network design for biorefining systems. Girola, Zamboni, and Bezzo (2011) developed a multi-objective optimization model by considering financial and environmental performances simultaneously to design optimal hybrid first and second generation biorefineries. The problem is formulated as a multi-period mixed-integer linear model. Mansoornejad, Pistikopoulos, and Stuart (2013), suggested metrics to analyze the flexibility and robustness of biorefining supply chains, which evaluate their performance against volatility.

Developing an optimal biorefinery plant depends on many factors including strategic and operational level decisions. Although various decision support models have been developed, in most of these studies, strategic, tactical, and operational decision tasks are not considered together, even though there is significant interdependence between them. Furthermore, most of the considered optimization problems are linear models, which do not take into account the inherently nonlinear mechanism of conversion processes. The complexity of these types of processes reveals the need for developing a comprehensive framework, which can support a multitude of strategic, tactical, and operational tasks by integrating the nonlinearities involved in the process.

In this paper we present the development and implementation of a novel multi-layered decision support tool for the optimal design of new and emerging renewable energy production systems which can integrate the aforementioned aspects, i.e., strategic, tactical, and operational tasks. The methodology is developed using a hypothetical case study that involves a multi-product biorefinery producing bio-ethanol, bio-succinic acid, and bio-electricity from lignocellulosic energy crops. The proposed methodology is based on an iterative framework that utilizes systems-based strategic planning and optimization in conjunction with detailed mechanistic modeling, simulation and optimization of non-linear systems. The framework builds up on our previous work (Sharma, Sarker, & Romagnoli, 2011; Sharma, Vlosky, & Romagnoli, 2013) where a techno-economic, strategic decision optimization framework is used to select an optimal technological platform, a feedstock portfolio, and a product portfolio for the conversion of lignocellulosic resources to biofuels and value-added biochemicals. Further, an optimized long-term capacity plan for the resultant configuration was also developed. In this paper, the resulting large scale linear programming (LP) model for strategic planning is integrated into bi-layered modeling and optimization framework for designing non-linear renewable energy systems.

2. Design of a decision support methodology for renewable energy systems

In order to create long-term value, a renewable energy enterprise has to carefully design, scale up, and operate its processing plant(s). From a modeling perspective, strategic planning models are characterized by a few salient features including inherently long planning horizons and intrinsic relationships between process variables (such as processing capacity and production rates) and economic parameters such as sales, revenue, costs, and value. In order to mathematically optimize the long term value of a renewable energy enterprise, these complex relationships have to be represented accurately without impacting the model performance significantly. While process conversion mechanisms are inherently non-linear in nature, owing to complex kinetic and thermodynamic relationships, non-linear strategic optimization models can quickly become complex to solve with solution performance suffering as more nonlinearities are added to a model. Consequently, LP models are suggested in this paper for the purpose of strategic planning. To overcome the mismatch between nonlinear process mechanisms and LP-based strategic optimization, a decomposition strategy is proposed that combines Net Present Value (NPV) optimization for long term planning with rigorous non-linear process modeling and process-level optimization. The proposed strategy has the advantage of not only being able to integrate long term planning based on financial optimization with nonlinear process mechanisms, but also optimize process operating conditions, using metaheuristic algorithms for non-linear optimization.

Fig. 1 shows a general schematic structure of the proposed iterative decision support strategy. The proposed framework utilizes iterative process to obtain a piecewise linear approximation of the nonlinear reaction- and thermo-dynamics; the nonlinear dynamics are simulated and their linear approximations are used during strategic planning and optimization. The following steps are performed in sequence:

(1) Strategic optimization: A linear programming (LP) model is proposed to optimize the project value of a renewable energy production system with decision tasks that can include feedstock selection, product portfolio design, technological superstructure design, supply chain design, and strategic capacity planning. At this stage, linear black box models can be utilized to represent the core technologies in a renewable process system in terms of process yields, raw material inputs, and energy loads for each technology; each one of these inputs can then be used to generate material and energy balances (linear) for the system being studied. These mass and energy balances can be integrated with financial variables through the use of cost functions (for raw material inputs), revenues (for production rates), capital investments (for capacity design), and cash balances. Readers are referred to (Sharma et al., 2011, 2013) for a detailed investigation of these linkages.

(2) Process simulation: The optimized design from strategic planning can then be utilized to simulate the renewable process in detail using rigorous mechanistic models. Process simulations can be carried out in standard simulation software packages (like Aspen Plus), and can be used to represent complex nonlinear processes at a plant level (operational versus strategic); additional linkages can also be made between simulation software and other mathematical packages (like Matlab) in order to completely specify a non-linear plant model.

(3) Operational level optimization: In the next layer of this methodology, operating conditions of the process are optimized using metaheuristic algorithms implemented in mathematical software packages that can solve large scale, non-linear mathematical problems. These mathematical optimization models are integrated with process simulation; the optimal operating conditions along with the simulated process yields (nonlinear) are then fed back into the strategic decision optimization model for comparison of results. Process yields are calculated based on the amount of products obtained in each unit operation from simulation results. In fact, calculated process yields from simulation results incorporate the nonlinearities of process mechanisms in strategic model and overcome the mismatch between process mechanisms and strategic planning decisions. This process is carried out iteratively until the capacity plan (from 1st Layer) and the process yields (from 2nd Layer) remain unchanged through consecutive iterations.
3. Application case study: Lignocellulosic biorefinery

In order to demonstrate the utility of the proposed framework, the aforementioned decision support system (DSS) is applied to a hypothetical biorefinery that utilizes lignocellulosic feedstock(s) to produce bio-based fuels and chemicals. Readers should note that while we are utilizing a lignocellulosic process to demonstrate the DSS, the applicability of the framework transcends just biorefineries (other processes can include algae process design, solar and wind processes, and even oil and natural gas processing plants).

3.1. Lignocellulosic biorefinery description

The biofuels and biochemicals produced from renewable raw materials can replace fossil-based transportation fuels like gasoline and petrochemicals and work to reduce the net carbon that is released into the atmosphere through human consumption. The CO\textsubscript{2} released during biofuel and biochemical production and consumption is biogenic carbon (derived from plant material) which is initially sequestered from the atmosphere by photosynthetic processes occurring during plant growth; this closed carbon cycle implies that, unlike fossil-based fuels and chemicals, bio-based fuels and chemicals have little impact on the carbon balance in the atmosphere (Naik, Goud, Rout, & Dalai, 2010). Various sources of biomass can be utilized to produce bioproducts: cellulosic wastes like tree thinning and yard waste, forest wood and residues, agriculture residues, and dedicated energy crops (Saxena, Adhikari, & Goyal, 2009). Based on production technologies, the bioproduct can be classified under one of two categories: (1) first-generation bioproducts derived from food crops and forest wood, and (2) second-generation bioproducts derived from lignocellulosic waste materials, residues and energy crops. Some concerns exist about the production of first-generation bioproducts, like corn ethanol and soy-based biodiesel, due to the impact that it has in the land use for food crop production and decreasing the ratio of food-crop-to-land area, consequently putting an upward pressure on food pricing. Lignocellulosic feedstocks, or feedstocks derived from agriculture, forest and municipal waste material (organic waste) can be utilized to produce second-generation bioproducts (Naik et al., 2010). These bioproducts have the advantage of being derived from waste materials that do not compete with the food value chains.

The lignocellulosic materials-based fuel and chemical conversion platforms can broadly be subdivided into 2 major pathways: (1) the biological conversion pathways based on fermentation, and (2) thermo-chemical conversion pathways based on heat-based technologies like gasification and pyrolysis. Each pathway has been shown to have great promise, but each suffers from separate issues that prevent their commercial scale up (Foust, Aden, Dutta, & Phillips, 2009). Thermo-chemical pathways require a large investment of capital, energy optimization and heat integration of process operations, and efficient downstream clean up and conversion processes to convert gasification/pyrolysis effluents to bio-based fuels and chemicals in a profitable manner. Biological conversion pathways suffer from issues including large capital requirements for plant establishment, and inability to replicate lab-scale process yields on a commercial scale, especially yields that involve biological technologies such as enzymes and micro-organisms.

Specifically, for the sugar-based fermentation conversion pathway, there are few known commercial plants, with most demonstration scale facilities suffering from inconsistent product yields. In addition to these technical challenges, a large number of sugar platforms are essentially single-product endeavors that produce low margin fuels like ethanol (Cardona & Sanchez, 2007; Humbird, Tao, Kinchin, Hsu, & Aden, 2011; Kim & Dale, 2004; Sun & Cheng, 2002); with low-margin products, slight changes in input costs, process yields, or markets (prices) can have a major impact on project profitability. We believe that a truly sustainable biorefinery of the future will require a portfolio of products whose production rates can be varied to optimize plant margins based on input costs and product markets.

The lignocellulosic biorefinery, used in this study to validate the proposed DSS framework, is a multiproduct plant that uses a fermentation-based sugar conversion platform, with 3 products: cellulosic ethanol, biosuccinic acid, and bioelectricity. Although, a number of possible feedstocks can be used to provide lignocellulosic material for conversion, our application assumes a sample feedstock whose chemical composition resembles that of switchgrass; its composition is presented in Table 2.

It is also assumed that there is limited land available within a 100-mile radius of the plant, which can be used for the production of switchgrass for feedstock to the plant. The production chain comprises of 6 major systems: feedstock pretreatment, sugar hydrolysis, sugar fermentation, product purification, heat and power generation, and wastewater treatment. The systems superstructure is shown in Fig. 2. In each stage of the process system, there may be different technologies that can be investigated for finding the optimal technological superstructure. Pretreatment technologies break down the matrix of biomass polymeric

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Fig. 1. Decision support strategy representation.
compounds to facilitate the enzymatic hydrolysis of cellulose and solubilize the hemicellulose. Among potential technologies, the two most promising candidates for cellulosic biofuel pretreatment are dilute acid and ammonia fiber explosion (AFEX). There are multiple configurations of hydrolysis and fermentation that can be considered in technology selection for hydrolyzing and fermenting lignocellulosic materials, such as separate hydrolysis and co-fermentation (SHCF), and simultaneous saccharification and co-fermentation (SSCF). The products in the fermentation effluent need to be recovered and purified; the technologies for this will depend on the type of products that are being recovered and purified.

Due to the availability of detailed process and economic data, for our case study, we will select a fixed configuration composed of:

1. Dilute acid pretreatment.
2. Separate hydrolysis and co-fermentation (SHCF).
3. Ethanol recovery using a configuration with distillation columns followed by molecular sieve purification.
4. Succinic acid recovery using a configuration based on cell filtration followed by crystallization.

Table 2

<table>
<thead>
<tr>
<th>Component</th>
<th>wt%</th>
</tr>
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<tbody>
<tr>
<td>Glucan</td>
<td>37.00</td>
</tr>
<tr>
<td>Xylan</td>
<td>22.80</td>
</tr>
<tr>
<td>Lignin</td>
<td>15.76</td>
</tr>
<tr>
<td>Ash</td>
<td>4.93</td>
</tr>
<tr>
<td>Protein</td>
<td>3.10</td>
</tr>
<tr>
<td>Arabinan</td>
<td>3.10</td>
</tr>
<tr>
<td>Galactan</td>
<td>1.43</td>
</tr>
<tr>
<td>Mannan</td>
<td>0.30</td>
</tr>
<tr>
<td>Extractives</td>
<td>9.00</td>
</tr>
<tr>
<td>Sucrose</td>
<td>0.77</td>
</tr>
<tr>
<td>Acetate</td>
<td>1.81</td>
</tr>
</tbody>
</table>

Fig. 2. Block diagram for the multiproduct biorefinery plant.

4. Framework details

In this section, each component of the proposed framework (Fig. 1) is described in some detail with the lignocellulosic biorefinery being featured in order to apply framework design components to a case study. While the description of the framework is based on the design of the case study presented in Section 3, each component, and the framework, can readily be adapted to other process value chains also.

4.1. Strategic optimization

The strategic optimization model is derived from previously published journal paper (Sharma et al., 2013); salient components of the strategic optimization model are discussed here to give the readers a feel for the model structure and decision tasks.

4.1.1. Process model

All major processes described in Fig. 2 are represented as linear black boxes in the planning model for the technology set (fixed) considered for framework demonstration (see Section 3). The major equations that are approximated linearly in the planning models and modeled nonlinearly during simulation and optimization include unit operations’ yield and unit operations energy balances. These equations are provided in a condensed form below:

\[ RM_{r,t} = \sum_{j} R_{r,j,t}^{reqd} \times I_{j,t} \]

\[ P_{p,t} = \left( \prod_{j=1}^{n} Y_{LD_{j,p}} \right) \times BM_{j=1,t} \]

\[ E_{j,t}^{load} = E_{j,t}^{reqd} \times I_{j,t} \]

\[ E_{j,t}^{prod} = \eta \times \sum_{j} F_{j,t} \times LHV_{j} \]

Here, \( RM \) is the raw material of type \( r \) required during time \( t \), \( R_{r,j,t}^{reqd} \) is the raw material required per unit of input \( I_{j,t} \), where \( j \) is a process unit operation. Additionally, \( P_{p,t} \) is the annual production rate of product \( p \), \( Y_{LD_{j,p}} \) is the process reaction yield, \( BM_{j=1,t} \) is the feedstock input, \( E_{j,t}^{load} \) is the energy load of unit operation \( j \), \( E_{j,t}^{prod} \) is the total energy produced, \( F_{j,t} \) is the fuel output of each unit operation, \( LHV_{j} \) is the heating value of the fuel from \( j \), and \( \eta \) is the heat transfer efficiency. The per unit requirements (\( RM_{r,j,t}^{reqd}, Y_{LD_{j,p}}, E_{j,t}^{reqd} \)) are obtained iteratively from the process simulations. Readers are directed to Sharma et al. (2013) for a complete description of the strategic optimization model. For this case study, the set of raw materials, \( r \), includes:
(1) Cellulosic feedstock (Switchgrass)
(2) Sulfuric acid
(3) Water
(4) Corn steep liquor (CSL)
(5) Diammonium phosphate (DAP)
(6) Hydrolyzing enzymes (cellulase and hemicellulase)
(7) Ammonia
(8) Fermentation microbes

4.1.3. Components:

Additionally, the strategic planning model is utilized in this demonstration for strategic capacity planning; the following equations are used to model capacity design for each unit operation in Fig. 2.

\[ BVCI \times Cap_{inf} \geq CapExp \] (5)
\[ BVCI \times Cap_{inf} \leq CapExp \] (6)
\[ Cap = Cap_{inf} + CapExp \] (7)
\[ Cap_{min} \times Cap \leq SystemInput \] (8)

The first two equations provide bounds to capacity expansion (CapExp), where BVCI is the capacity increment binary variable that is 1 when capacity is incremented and 0 otherwise. Eq. (7) is used to update the processing capacity (Cap) of each operating system, adjusting for a construction delay (CD) of 2 years. Eq. (8) provides a lower bound to total established capacity based on the respective input to the operating system (SystemInput), and Eq. (9) imposes minimum equipment utilization bound (MinUtil) on the established capacity. The capacity plan is then passed on to the process simulator (Aspen Plus) and the process optimizer (Matlab) in order to determine optimal operating conditions.

4.1.3. Financial model

The financial model is broken into 5 salient aspects that describe the financial impact of resource procurement, technology selection, network design, production of final products, and sales:

(1) Capital costs (CAPEX);
(2) Financing costs of CAPEX;
(3) Operating expenses and revenues;
(4) Calculation of income and cash flow statement line items;
(5) Calculation (optimization) of the objective function (Net Present Value).

The methodology for deriving the capital cost structure was adapted from Kazi et al. (2010) that exemplified NREL’s nth plant cost analysis. The capital expenses are broken up into six components:

(1) Land acquisition charges for facility establishment,
(2) Equipment costs for processing,
(3) Construction and engineering costs,
(4) Legal and permitting costs,
(5) Contingency fund,
(6) Working capital investments.

The operating costs for the value chain were broken into 7 parts that utilize system outputs from each node in the value chain to calculate the total cost of operation:

(1) Feedstock costs including establishment, opportunity, harvesting and logistics costs
(2) Water purchase and treatment costs
(3) Process chemical costs for pretreatment
(4) Enzyme, nutrient, and micro-organism costs for fermentation
(5) Operating charges for steam and power plant operation
(6) Labor costs for the entire processing facility
(7) Selling, general and administrative costs for product distribution

Following the calculation of these costs, the income statement of a general enterprise was stated in equation form to calculate line items such as gross profit, earnings before interest taxes and depreciation (EBITDA), earnings before interest and taxes (EBIT), earnings before taxes (EBT), taxes, operating profit after taxes (NOAPAT), and net income (NI). Additionally, the cash flow statement of an enterprise was derived (in equation form) using the outputs of the income statement along with capital investment charges. The financial model was designed to assess the impact of project operation on the enterprise’s capital structure; specifically, the cash balance of the enterprise was assumed to be composed of operating (CFO), financing (CFF), and investment cash flow (CFI). The capital structure of the enterprise was represented as the debt and equity capital that can be raised in order to fund current operations and further network capacity growth. The objective function (Net Present Value, NPV) was calculated as the sum of the discounted values (20 years) of the difference between CFO and CFI. Readers are referred to Sharma et al. (2013) for a complete description and statement of the financial model and its equations, respectively.

4.2. Process simulation

Aspen Plus was utilized to simulate the multiproduct biorefinery with the optimal capacity plan obtained from strategic optimization. Additional process data for pretreatment, hydrolysis and ethanol fermentation and purification are based on the NREL reports Kazi et al. (2010) and Humbird et al. (2011), and for succinic acid fermentation and purification the data are obtained from Li et al. (2010) and Vlysidis et al. (2011). To better estimate the nonlinear reaction dynamics of enzymatic hydrolysis and fermentation, experimentally derived kinetic models are utilized to simulate the reactions in enzymatic hydrolysis, ethanol fermentation and succinic acid fermentation. Each kinetic model is briefly explained below:

4.2.1. Enzymatic hydrolysis

A multi-reaction kinetic model (Kadam, Rydhholm, & McMillan, 2004) is implemented to describe the enzymatic hydrolysis of switchgrass. The mathematical representation of the kinetics is presented in Appendix A, Table A.1. This model includes reactions for:

(1) Substrate reactivity (Eq. (A.1)), which considers the reduction in the rate of hydrolysis as saccharification progresses because of the change in crystalline structure of cellulose or substrate accessibility.
(2) Decomposition of cellulose to cellobiose (Eq. (A.2)) and glucose (Eq. (A.3)), which happen on the surface of cellulose.
(3) Cellobiose hydrolysis to glucose (Eq. (A.4)), which occurs in the solution and is a homogenous reaction, which follows Michaelis–Menton kinetics.
(4) Enzyme adsorption (Eq. (A.5)), which follows the Langmuir type isotherms.
(5) Temperature effects on hydrolysis (Eq. (A.6)) based on Arrhenius model, which is valid in a limited range of temperature where the enzyme is active.

Cellulose is hydrolysed to glucose and cellobiose by utilizing the combination of endo-β-1,4-glucanase (EC), exo-β-1,4-cellobiolydrolase (CBH), and cellobiose is hydrolysed to glucose by the action of β-glucosidase. Langmuir isotherms are used to explain the adsorption of cellulose enzyme and the model distinguishes between the CBH/EC and β-glucosidase enzymes. Sugar inhibitions considered in this model assumes that the hydrolysed sugars can bind to the active site of the substrate and decrease the formation rate of enzyme–substrate complex which is a competitive mode of inhibition.

4.2.2. Ethanol fermentation

The kinetic model implemented in this study for ethanol production (via sugar fermentation) is based on the two-substrate developed model of Leksawasdi, Joachimsthal, and Rogers (2001), by consuming a recombinant bacterium Z. mobilis ZM4 (pZBS), which is capable of fermenting glucose and xylose simultaneously (co-fermentation). The mathematical representation of the fermentation kinetics is presented in Appendix A, Table A.2. The model is based on the following reactions:

1. Cell growth on glucose (Eq. (A.7)) and xylose (Eq. (A.8)) which incorporates the Monod kinetic model for substrate limitation and product inhibition.
2. Glucose and xylose consumption (Eqs. (A.10) and (A.11)) which are considered in separate equations by incorporating the inhibition effects.
3. Ethanol production (Eq. (A.14)), which incorporates the production from glucose (Eq. (A.12)) and xylose (Eq. (A.13)) by considering the weighting factor ($\alpha$).

Due to simultaneous cell growth on both of the substrates (glucose and xylose), there is competition to contribute (via cell growth) to produce ethanol. The weighting factor ($\alpha$) represents the relative consumption rates of the two sugars (Eqs. (A.9) and (A.14)). The best value for the weighting factor ($\alpha$) was determined to be $\alpha = 0.65$ (Leksawasdi et al., 2001).

4.2.3. Succinic acid fermentation

A kinetic model developed by Song, Jang, Park, and Lee (2008) which models the conversion of glucose to succinic acid using M. succiniciproducens MBEL55E is implemented in this study. While the main product of this model is succinic acid, the other acids such as acetic, formic and lactic acids are also produced as by-products of the fermentation process. The mathematical representation of the fermentation kinetics for succinic acid is presented in Appendix A, Table A.3. The model is based on the following reactions:

1. Cell growth on glucose (Eq. (A.15)) which is based on a modified Monod equation model that incorporates excess substrate inhibition on the growth of bacteria. Product concentration and critical product concentrations are sum of the amounts of succinic and other acids produced in the process (Eq. (A.22)).
2. Cell death model (Eq. (A.16)); which is based on the equation suggested by Levenspiel (1980) to model the cell death caused by produced organic acids accumulated during fermentation in the culture broth and cause cell death after reaching a predetermined concentration of the total acid ($P_{\text{tot}}$).

(4) Glucose consumption (Eq. (A.21)) based on the carbon mass balance in the fermentation process.

The proposed model considers the conversion of glucose to organic acids; additionally we assume that 10% of xylose is also converted to succinic acid based on the following chemical reaction:

$$3 \text{Xylose} + 5\text{CO}_2 \rightarrow 5 \text{Succinic acid} + 2.5\text{O}_2$$

4.3. Process optimization

The simulated process (Aspen Plus) with optimized capacity plan from strategic planning is linked to a metaheuristic optimization model that is implemented in Matlab to optimize the process operating conditions. A simplified version of the financial model presented in Section 4.1 is used to design the objective function that is optimized here. The objective function used for optimization is the annual cash flow, $CF$, which takes into account the revenue generated from the sale of products, $P_r$, (where $r$ represents the type of product produced including ethanol, succinic acid, and excess electricity), the direct costs of raw materials, $RM_{r,p}$ (where $r$ represents the type of raw materials including feedstock, enzymes, nutrients, chemicals, make-up water), and the labor, maintenance and transportation costs (annual fixed costs, $FC$). Additionally, tax credits ($Tax^{\text{credits}}$) and liabilities ($Tax^{\text{liability}}$) are also modeled to yield the after tax cash flow, $\text{Eq. (14)}$ (objective function). The costing data are obtained from Kazi et al. (2010), Vlysidis et al. (2011) and Laser et al. (2009). Ethanol price is assumed to be $2 per gallon, Succinic acid price is assumed to be $6000 per ton and electricity prices are set at $0.05 per kilowatt-hour. Production capacities obtained from strategic planning are incorporated during process optimization as constraints (Eq. (A.15)) to control the switchgrass throughput and production rates. The following equations represent the objective function calculations.

$$CF^{\text{Before Tax}} = \sum P_r \times \text{Price}_{p} - \sum r_p \times \text{RM}_{r,p} \times \text{Cost}_{r} - FC$$

(10)

$$Tax^{\text{liability}} = CF^{\text{Before Tax}} \times tax^{\text{Rate}}$$

(11)

$$Tax^{\text{credits}} = \sum P_r \times \text{Credit}_{r}$$

(12)

$$Tax^{\text{net}} = \max(0, Tax^{\text{liability}} - Tax^{\text{credits}})$$

(13)

$$CF^{\text{After Tax}} = CF^{\text{Before Tax}} - Tax^{\text{net}}$$

(14)

$$P_{\text{simulation}} \leq P_{\text{strategic optimization}}$$

(15)

For solving optimization problems deterministically, analytical properties of the problem such as convexity of the objective function should be utilized to generate a deterministic sequence of points in the search space. Additionally, in many real-world problems such as biorefinery processes, complex mass and energy constraints are involved in the optimization problem. To solve these large scale nonlinear problems deterministically, constraint equations should be incorporated into the objective function (Lagrangian relaxation). However, in our study, the process simulator (Aspen Plus) is utilized to model the biorefinery. All the mass and energy balances are embedded in the simulation and constraints are satisfied when simulation is converged. Furthermore, since the process model is comprised of non-convex functions, many deterministic optimization methods will fail to find global optima. To overcome these problems, metaheuristic approaches are implemented for process optimization as they do not require
manipulation of the mathematical structure of the objective function and the constraints (Mariano, Costa, de Toledo, Melo, & Maceiê, 2011). In fact, the optimizer treats the process simulations in Aspen Plus as a black box. The optimized decision variable values from Matlab are sent to Aspen Plus where the process is simulated for these values. The simulated results are then passed back to the optimizer to re-solve the objective function. Two alternative meta-heuristic algorithms were implemented and tested for efficiency in the optimization of the selected bioengineering process: (1) differential evolution, and (2) simulated annealing. These algorithms are discussed in detail in the next 2 sections.

4.3.1. Differential evolution algorithm

Differential evolution method (DE) was first proposed by Storn and Price (1997); this method is a parallel direct search method and is often considered as an evolution-based method. The initial population of n vectors, which are the decision variables, is randomly selected and covers the entire parameter space. Each vector serves as the target vector alternatively. For each vector in generation G, xG, DE generates a new parameter vector, xG+1, by adding the randomly selected vector, xG1, to the weighted difference between two other randomly chosen vectors (Eq. (16)), xG2, xG3, (mutation operation). The mutated vector’s parameters are then mixed with the parameters of another predetermined vector, to yield the trial vector (Eq. (17)); this operation is called the crossover operation. If the trial vector yields a higher objective function than the target vector, the trial vector replaces the target vector; this is called the selection operation. The vector population is updated in each iteration according to the target vectors. This iterative process is carried out until the convergence criteria are satisfied. In this study, the DE algorithm is terminated when (1) there is no significant improvement in the best value of the objective function after a predetermined number of iterations is reached, or (2) the maximum number of function evaluations, nfe, is reached. A flow chart of the utilized DE algorithm is presented in Fig. 3.

\[
\begin{align*}
    v^{G+1} & = x_G^1 + F \cdot (x_G^2 - x_G^3) \\
    u^{G+1} & = \begin{cases} 
        v^{G+1} & \text{if rand}(i) \leq CR \\
        x_G^i & \text{if rand}(i) > CR
    \end{cases}
\end{align*}
\]

(16)

(17)

4.3.2. Simulated annealing algorithm

Simulated annealing is a stochastic local search algorithm initially proposed by Kirkpatrick, Gelatt, and Vecchi (1983). The key feature of simulated annealing is its ability to escape local optima by allowing hill-climbing moves that worsen the objective function value in hopes of finding global optima. This optimization algorithm is based on Metropolis acceptance criteria, which governs how a thermodynamic system moves from its current state to a new state where its internal energy content is being minimized. The candidate solution (Y) is accepted based on the acceptance probability (Eq. (18)). In this equation Tk is the temperature at iteration k (outer loop). Based on this equation, a worse solution, in maximization problem, might be accepted with some probability, as a hill-climbing move in order to escape a local maximum. The Tk value is determined by a cooling schedule; in this study we utilized a geometric law to describe the temperature reduction (Eq. (19)); as Tk decreases the probability to accept a worse solution also decreases.

\[
P(\text{accepting } Y \text{ as next solution}) = \begin{cases} 
    \exp \left[ \frac{-f(Y) - f(X)}{T_k} \right] & \text{if } f(Y) - f(X) < 0 \\
    1 & \text{else}
\end{cases}
\]

(18)

\[
T_{k+1} = \alpha T_k
\]

(19)

A flow chart of the utilized simulated annealing algorithm is presented in Fig. 4.

Simulated annealing starts with an initial solution vector, X, that is randomly generated in the solution space and evaluated to find the objective function (f(X)) value. A neighboring solution is then generated (Y) as a new candidate, by choosing a random point in the search that defines the random direction and the step size, \( \Delta r \). We used an adaptive step size change, which implies that as the number of iterations increase in inner loop, the new selected candidate’s deviation from the previous point decreases. This iterative process is carried out until the convergence criteria are satisfied. In this study, the SA algorithm is terminated when (1) there is no significant improvement in the best found solution after a predetermined number of iterations, or (2) the calculated temperature in the outer loop reaches the predetermined Tmin.

4.3.3. Penalty function

For both of these algorithms the inequality constraints, which are the production capacities that obtained from strategic planning, are handled by utilizing the penalty function method. In this approach for handling inequality constraints, the modified objective function \( F(\bar{x}) \) is defined as sum of original objective function \( f(x) \) and a penalty term \( g(\bar{x}) \), which depends on the constraint violation.

\[
F(\bar{x}) = f(\bar{x}) + \sum_{j=1}^{f} R_j \cdot (g_j(\bar{x}))
\]

(20)

The parameter \( R_j \) is the penalty parameter of the jth inequality constraint to make the constraint of the same order of magnitude as the original objective function value.

5. Results and discussion

To demonstrate the proposed methodology, the assumed process technology superstructure (Dilute Acid—SHCF—Distillation—Sieves—Crystallization) is used for strategic design of processing and product recovery capacities (Results provided later). During strategic planning, data utilized for process yields and costing parameters for each technology is based on National Renewable Energy Laboratory reports and literature data (Humbird et al., 2011; Kazi et al., 2010; Li et al., 2010; Vlysidis et al., 2011).

Dilute acid pretreatment breaks down the cellulose structure of biomass and converts the xylose polymer to xylose sugar. Enzymatic hydrolysis then converts cellulose to glucose by utilizing cellulase enzyme which is a mixture of enzymes that work together to break down complex cellulolic polymers to simpler sugars like glucose. The sugars produced from hydrolysis and pretreatment are then fermented to ethanol and succinic acid. We utilized a process configuration where hydrolysis and fermentation are carried out in separate tanks; when hydrolysis and fermentation occur separately, the sugar stream sent to enzymatic hydrolysis reaction can be at an elevated temperature allowing for faster and more efficient conversion of cellulose (due to higher activity of enzymes at higher temperatures). Ethanol production occurs by simultaneous fermentation of two sugars, glucose and xylose. The microorganism proposed by Leksawadi et al. (2001), recombinant Z. mobilis, is capable of fermenting both of the sugars to produce ethanol. Additionally, M. succiniciproducens, an organism, which utilizes glucose to produce succinic acid is assumed to be added to fermentation reactor to produce succinic acid. In this study, we additionally assume that 10% of xylose is also converted to succinic acid. A beer column followed by a rectification column is designed to purify ethanol up to its azetropic boiling point, followed by sieve-based purification to reach fuel grade purity (99.5% by mass). For succinic
acid purification, a one-step crystallization recovery model, developed by Li et al. (2010), which is based on the variation of succinic acid solubility at different PHs, is selected.

The entire process is simulated in Aspen Plus for the capacities that are designed during strategic optimization. The process conditions for dilute acid pretreatment, and ethanol purification are based on the process design data obtained from National Renewable Energy Laboratory (NREL) report (Humbird et al., 2011). For simulating enzymatic hydrolysis, and ethanol- and succinic acid fermentation, kinetic models described in Section 4.2 are implemented in Matlab and linked with Aspen Plus to obtain precise conversions of each reaction by solving a system of differential equations in Matlab.

For succinic acid purification, cellular debris is separated from the fermentation effluent by centrifugation, which is followed by an evaporator that vaporizes most of the water and organic acids that have lower boiling points than succinic acid. The concentrated stream obtained from bottom of the evaporator is sent to a crystallizer that separates succinic acid from other organic acids and trace water based on differential solubilities. While formic, acetic and lactic acids are water-miscible at pH from 1 to 14 at temperatures above 0 °C, succinic acid solubility decreases sharply when the temperature decreases (Li et al., 2010). Therefore, succinic acid can be selectively separated from other acids using solubility-driven crystallization. Pure succinic acid crystals are obtained via another centrifugation operation, and finally a dryer is used to reduce the moisture in the crystals to purify it to acceptable end use purity (>90% by mass).

Process integration suggested by Zeikus, Jain, and Elankovan (1999) and Nghiem, Hicks, and Johnston (2010) is utilized in this work to capture the carbon dioxide produced during ethanol fermentation and use it in succinic acid fermentation (as a carbon source). We assumed that CO$_2$ produced from ethanol fermentation has a high purity and is siphoned from the ethanol fermentation tank to succinic acid fermentation tank. This can have a 2-fold benefit on plant economics and emissions – (1) it reduces the carbon footprint of the biorefinery as it permanently sequesters ethanol-derived CO$_2$ into succinic acid molecules, and also (2) it reduces the amount of carbon dioxide that is required as a purchased input for succinic acid production. The process flowsheet for succinic acid production is shown in Fig. 5.

During process optimization, the following operating variables are manipulated in order to optimize annual operating cash flows for the biorefinery: (1) temperature in enzymatic hydrolysis, (2) sugar allocation (from hydrolysis) between ethanol and succinic acid fermentation, and (3) enzyme (cellulase) loading during hydrolysis.

Enzyme activity is correlated with reaction temperature, through the Arrhenius model (Eq. [A.6]); temperature plays an important role in increasing or decreasing the rate of enzymatic
reactions, and thus impacts the overall cellulose (to glucose) conversion yield. Decreasing reaction temperature below a certain threshold can also result in a dramatically reduced rate of reaction, while increasing it above a threshold can result in protein denaturation; consequently the search space for optimal temperature determination is limited between a range (Humbird et al., 2011). In this study, we assumed that the acceptable range for temperature (T) is between 40 °C and 50 °C. The hydrolyzed sugar stream, mainly glucose and xylose, is split in 2 before fermentation; one stream is sent to ethanol fermentation reactors while the other is used for succinic acid fermentation. These allocated sugar streams impact the fermentation reaction kinetics and consequently the product yields in the fermentation effluent. The manipulated decision variable during optimization is the fraction of total sugar that is used for ethanol fermentation (X). The amount of enzyme used in hydrolysis is determined by a ratio based on the amount of cellulose present

Fig. 4. Flow chart for simulated annealing algorithm.

Fig. 5. Process flowsheet for succinic acid production.
Table 3
Lower and upper bound for optimization variables.

<table>
<thead>
<tr>
<th>Optimization variable</th>
<th>Lower bound</th>
<th>Upper bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrolysis temperature (°C)</td>
<td>40</td>
<td>50</td>
</tr>
<tr>
<td>Sugar allocation ratio (sugar to ethanol)</td>
<td>0.1</td>
<td>1</td>
</tr>
<tr>
<td>Enzyme load (g enzyme/kg Cellulose)</td>
<td>5</td>
<td>50</td>
</tr>
</tbody>
</table>

Table 4
Differential evolution and simulated annealing parameters.

<table>
<thead>
<tr>
<th>Parameters/operators</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simulated annealing</td>
<td></td>
</tr>
<tr>
<td>Iteration per temperature</td>
<td>40</td>
</tr>
<tr>
<td>(T_\text{max})</td>
<td>400</td>
</tr>
<tr>
<td>(\alpha)</td>
<td>0.01 ((T_\text{max}))</td>
</tr>
<tr>
<td>Cooling rate (\alpha)</td>
<td>0.8</td>
</tr>
<tr>
<td>Initial step size</td>
<td>0.3 ((\text{upper bound} - \text{lower bound}))</td>
</tr>
<tr>
<td>Penalty coefficient (K_j)</td>
<td>100,000</td>
</tr>
<tr>
<td>Differential evolution</td>
<td></td>
</tr>
<tr>
<td>Maximum number of function evaluation (\text{MAXNF})</td>
<td>500</td>
</tr>
<tr>
<td>Population size (\text{NP})</td>
<td>30</td>
</tr>
<tr>
<td>Weighing coefficient (F)</td>
<td>0.5</td>
</tr>
<tr>
<td>Crossover rate (\text{CR})</td>
<td>0.95</td>
</tr>
<tr>
<td>Penalty coefficient (K_j)</td>
<td>100,000</td>
</tr>
</tbody>
</table>

Table 5
Optimal values for decision variables and objective function.

<table>
<thead>
<tr>
<th></th>
<th>DE</th>
<th>SA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>44.00 °C</td>
<td>47.00 °C</td>
</tr>
<tr>
<td>Sugar allocation</td>
<td>0.40 (ethanol), 0.60</td>
<td>0.40 (ethanol), 0.60</td>
</tr>
<tr>
<td>(succinic acid)</td>
<td>(succinic acid)</td>
<td></td>
</tr>
<tr>
<td>Enzyme loading ratio</td>
<td>20 (g enzyme/kg Cellulose)</td>
<td>24 (g enzyme/kg cellulose)</td>
</tr>
<tr>
<td>Cash flow</td>
<td>$70 million per year</td>
<td>$69 million per year</td>
</tr>
</tbody>
</table>

in the sugar stream to hydrolysis reactor and the specific activity of the enzyme. Based on the kinetic models implemented in Matlab for hydrolysis and fermentation, sugar yield and ethanol production generally increase with higher enzyme loading (Fig. 6a and b). However, additional enzyme increases direct costs and furthermore, as shown in Fig. 6c, there is an optimal enzyme loading rate for succinic acid production beyond which product yield decreases with increasing enzyme concentration. The initial glucose concentration in succinic acid fermentation depends on the amount of sugar allocated to its production and also the amount of sugar that is produced during hydrolysis; therefore, enzyme loading, sugar allocation and temperature have a complex set of impacts on process yields and consequently, on process economics.

The lower bound and upper bound of the optimization variables are set as shown in Table 3.

As described before, simulated annealing (SA) and differential evolution (DE) optimization algorithms are implemented separately in Matlab and linked to the simulations in Aspen Plus. The parameter settings for DE and SA are shown in Table 4.

The average number of function evaluations required to find the optimal values for decision variables are 200 (DE algorithm) and 300 times (SA algorithm). In our case, DE algorithm is also able to find a better objective function value (average). The comparison between the results is shown in Table 5. These results show that DE has better performance characteristics compared to the SA algorithm for this specific application. Therefore, DE is chosen to implement the iterative optimization framework (Fig. 1). The convergence behavior of the DE algorithm is plotted in Fig. 7. It can be seen that the convergence is steady and stable. The iteration results are presented in Table 6.
Table 6

<table>
<thead>
<tr>
<th>Parameters and variables</th>
<th>Iteration 1</th>
<th>Iteration 2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Step 1</td>
<td>Step 2</td>
</tr>
<tr>
<td></td>
<td>Step 1</td>
<td>Step 2</td>
</tr>
<tr>
<td>Capacity constraints</td>
<td>–</td>
<td>333.3</td>
</tr>
<tr>
<td>Feedstock (1000 ton/yr)</td>
<td>–</td>
<td>333.3</td>
</tr>
<tr>
<td>Ethanol (MM gal/yr)</td>
<td>–</td>
<td>10.082</td>
</tr>
<tr>
<td>Succinic acid (1000 ton/yr)</td>
<td>–</td>
<td>15.6</td>
</tr>
<tr>
<td>Process variables</td>
<td>–</td>
<td>0.52</td>
</tr>
<tr>
<td>Sugar allocation</td>
<td>–</td>
<td>0.40</td>
</tr>
<tr>
<td>Yield parameters</td>
<td>–</td>
<td>0.52</td>
</tr>
<tr>
<td>Sugar (kg/kg)</td>
<td>0.87</td>
<td>–</td>
</tr>
<tr>
<td>Ethanol fermentation</td>
<td>0.85</td>
<td>–</td>
</tr>
<tr>
<td>Succinic acid fermentation</td>
<td>0.25</td>
<td>–</td>
</tr>
<tr>
<td>Ethanol purification</td>
<td>0.99</td>
<td>–</td>
</tr>
<tr>
<td>Succinic acid purification</td>
<td>0.78</td>
<td>–</td>
</tr>
</tbody>
</table>

Table 6 shows that during the first iteration, yield data obtained from literature (Step 1) is utilized for strategic capacity planning (LP). The optimal plant capacities (Step 2) are passed to the process simulation and optimization steps in order to find the optimal operating conditions by using non-linear optimization technique. Yields calculated from the results of optimal simulation are passed to strategic model (Step 3). To check the convergence, these yields are compared with the ones used in Step 1–iteration 1. As the difference between the values is greater than the threshold, the strategic optimization solves the LP model again, based on new yield values (Step 1–iteration 2). The new capacity plan is again sent to process simulation and optimization module to find the optimal operating conditions and calculate process yields accordingly (Step 2–iteration 2). Major changes from the literature derived yield values (Step 1, Iteration 1) are noticed in Table 6, as non-linear kinetic models are utilized as opposed to linear yield equations, in order to estimate the dynamics of the reactions (Step 3–Iteration 1, Step 2–Iteration 2). This demonstrates the utility of the proposed methodology to reconcile nonlinear process models with LP-based economic optimization (strategic planning). While feedstock capacities remain the same throughout the framework demo, the optimal product recovery capacities are reduced successively as the actual process yields (obtained from our ASPEN simulations) are shown to be much lower than assumed (linear) conversion yields in literature (also utilized during initial strategic optimization). Fig. 8 presents the optimal process configuration and the main process specifications.

Fig. 7. Convergence history for DE algorithm.

Fig. 8. Optimal process configuration.
This Figure shows that the main sections requiring energy are the fractionation and recovery; during co-generation, by burning combustible by-products from the biorefinery, such as lignin and biogas, the steam and electricity demand for the plant is supplied internally. Furthermore, additional revenues are generated by selling excess electricity as a by-product. Fig. 9 shows the final simulated concentration profiles of the reactants and products in enzymatic hydrolysis and ethanol and succinic acid fermentations obtained by solving the system of differential equations for the kinetic models implemented in Matlab. Final configuration of the proposed framework for the biorefinery process is shown in Table 7 which represents the optimized variables in strategic planning and process modeling and optimization sections and final yields calculated for each section of the plant accordingly.

6. Conclusion

We developed a framework to optimally design renewable energy production systems that are governed by nonlinear process dynamics. The framework focuses on integrating strategic planning tasks with operational tasks such as plant operations and the optimization of process conditions. Our methodology focuses on integrating simulation and optimization of nonlinear processes with LP-based optimization of strategic planning decisions. The framework takes a distributed modeling approach, wherein, strategic planning decisions are optimized separately from process optimization, and the nonlinear process dynamics (during strategic planning) are represented using an iterative algorithm. Standard simulation and mathematical software packages are utilized to represent nonlinear processes and optimize their operating conditions; the optimized results are passed back and forth between the LP and the nonlinear simulation/optimization until optimal results do not change through consecutive iterations.

The strategic planning LP focuses on optimizing the long term value (NPV) of a renewable energy enterprise by manipulating decisions such as technology selection, feedstock and product portfolio design, strategic capacity planning, and supply chain design. In this paper, we presented a detailed development of the operational simulation and optimization component of the framework. We utilized a hypothetical case study of a lignocellulosic biorefinery that produces bioethanol, bio-succinic acid, and bioelectricity from switchgrass. For the sake of demonstration, the technology
superstructure for the biorefinery was assumed to be fixed and the LP was used to optimize strategic capacity plans for the plant. Further, the operational modeling and optimization of the plant utilized Aspen Plus for nonlinear simulations and Matlab for nonlinear process optimization. Kinetic process models were implemented in Matlab to impart greater fidelity to the simulation in Aspen Plus. Metaheuristic optimization algorithms were employed in order to optimize process conditions including temperature (hydrolysis), raw material loading (enzymes for hydrolysis), and flow rates (sugar allocation). The final results included an optimal capacity plan for the biorefinery, the optimal NPV, and the optimal operating conditions for the hydrolysis reactor. The framework shows a deviation in process yields, and a deviation in the production capacities and operating conditions, from initial literature estimates. This is attributed to the framework’s use of nonlinear modeling and optimization strategies, which served to impart a greater degree of realism to the representation of the actual biorefining process.

Future work will include incorporating more nonlinear process variables within the proposed framework, incorporating uncertainty analysis in the framework by analyzing different scenarios based on changes in the market condition, strategically designing the supply chain and technology superstructures, modeling environmental and social characteristics of a system during design, and applying the methodology to different renewable energy systems.

Appendix A.

The kinetic models implemented in the proposed framework are represented in the following tables and the parameters definition and values for these models are shown in Appendix B:

### Table A.1
Kinetic model for enzymatic hydrolysis (Kadam et al., 2004).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>( R_0 )</td>
<td>[ \frac{dC_G}{dC_S} = \frac{K_{H_G} + C_S}{K_{H_G} + C_S} ] (A.1)</td>
</tr>
<tr>
<td>( r_1 )</td>
<td>[ \frac{dC_G}{dC_S} = \frac{K_{H_G} + C_S}{K_{H_G} + C_S} ] (A.2)</td>
</tr>
<tr>
<td>( r_2 )</td>
<td>[ \frac{dC_G}{dC_S} = \frac{K_{H_G} + C_S}{K_{H_G} + C_S} ] (A.3)</td>
</tr>
<tr>
<td>( r_3 )</td>
<td>[ \frac{dC_G}{dC_S} = \frac{K_{H_G} + C_S}{K_{H_G} + C_S} ] (A.4)</td>
</tr>
<tr>
<td>( C_G )</td>
<td>[ \frac{dC_G}{dC_S} = \frac{K_{H_G} + C_S}{K_{H_G} + C_S} ] (A.5)</td>
</tr>
<tr>
<td>( k_{ir}(2) )</td>
<td>[ \frac{dC_G}{dC_S} = \frac{K_{H_G} + C_S}{K_{H_G} + C_S} ] (A.6)</td>
</tr>
</tbody>
</table>

### Table A.2
Kinetic model for ethanol fermentation (Leksawasdi et al., 2001).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>( r_4 )</td>
<td>[ \frac{dC_G}{dC_S} = \frac{K_{H_G} + C_S}{K_{H_G} + C_S} ] (A.7)</td>
</tr>
<tr>
<td>( r_5 )</td>
<td>[ \frac{dC_G}{dC_S} = \frac{K_{H_G} + C_S}{K_{H_G} + C_S} ] (A.8)</td>
</tr>
<tr>
<td>( r_6 )</td>
<td>[ \frac{dC_G}{dC_S} = \frac{K_{H_G} + C_S}{K_{H_G} + C_S} ] (A.9)</td>
</tr>
<tr>
<td>( r_7 )</td>
<td>[ \frac{dC_G}{dC_S} = \frac{K_{H_G} + C_S}{K_{H_G} + C_S} ] (A.10)</td>
</tr>
<tr>
<td>( r_8 )</td>
<td>[ \frac{dC_G}{dC_S} = \frac{K_{H_G} + C_S}{K_{H_G} + C_S} ] (A.11)</td>
</tr>
<tr>
<td>( r_9 )</td>
<td>[ \frac{dC_G}{dC_S} = \frac{K_{H_G} + C_S}{K_{H_G} + C_S} ] (A.12)</td>
</tr>
<tr>
<td>( r_{10} )</td>
<td>[ \frac{dC_G}{dC_S} = \frac{K_{H_G} + C_S}{K_{H_G} + C_S} ] (A.13)</td>
</tr>
<tr>
<td>( r_{11} )</td>
<td>[ \frac{dC_G}{dC_S} = \frac{K_{H_G} + C_S}{K_{H_G} + C_S} ] (A.14)</td>
</tr>
</tbody>
</table>

### Table A.3
Kinetic model for succinic acid fermentation (Song et al., 2008).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>( r_1 )</td>
<td>[ \frac{dC_S}{dt} = \frac{P_x}{P_{C_{G},d}} ] (A.15)</td>
</tr>
<tr>
<td>( r_2 )</td>
<td>[ \frac{dC_S}{dt} = -K_dC_S + P_p + P_{C_{G},d} ] (A.16)</td>
</tr>
<tr>
<td>( r_3 )</td>
<td>[ \frac{dC_S}{dt} = \alpha r_x + \beta_0 C_S ] (A.17)</td>
</tr>
<tr>
<td>( r_4 )</td>
<td>[ \frac{dC_S}{dt} = \alpha r_x + \beta_0 C_S ] (A.18)</td>
</tr>
<tr>
<td>( r_5 )</td>
<td>[ \frac{dC_S}{dt} = \alpha r_x + \beta_0 C_S ] (A.19)</td>
</tr>
<tr>
<td>( r_6 )</td>
<td>[ \frac{dC_S}{dt} = \alpha r_x + \beta_0 C_S ] (A.20)</td>
</tr>
<tr>
<td>( r_7 )</td>
<td>[ \frac{dC_S}{dt} = \alpha r_x + \beta_0 C_S ] (A.21)</td>
</tr>
</tbody>
</table>

### Appendix B.

Nomenclature: parameter definition for the kinetic models

**Enzymatic hydrolysis**

- \( R_c \): substrate reactivity
- \( \alpha \): relating substrate reactivity with degree of hydrolysis, dimensionless = 1
- \( C_G \): substrate concentration at a given time, g/kg
- \( S_0 \): initial substrate concentration, g/kg
- \( r_1 \): cellulose to cellubiose reaction rate, g/kg h
- \( K_{fr} \): reaction rate constant 1, g/kg h = 22.3
- \( C_E \): bound enzyme concentration type i, g/kg
- \( C_{G2} \): cellulose concentration, g/kg
- \( C_G \): glucose concentration, g/kg
- \( C_S \): xylose concentration, g/kg
- \( K_{Ib} \): inhibition constant for cellulose i, g/kg = 0.015
- \( K_{Ig} \): inhibition constant for glucose 1, g/kg = 0.1
- \( K_{Ib} \): inhibition constant for xylene i, g/kg = 0.1
- \( K_{2b} \): inhibition constant for cellubiose 2, g/kg = 132
- \( K_{2g} \): inhibition constant for glucose 2, g/kg = 0.04
- \( K_{2b} \): inhibition constant for xylene 2, g/kg = 0.2
- \( r_3 \): cellulose to glucose reaction rate, g/kg
- \( K_{fr} \): reaction rate constant 3, h−1 = 285.5
- \( K_{fr} \): substrate (cellulose) saturation constant, g/kg = 24.3
- \( K_{fr} \): inhibition constant for glucose 3, g/kg = 3.9
- \( K_{fr} \): inhibition constant for xylene 3, g/kg = 201.0
- \( E_{lim} \): maximum enzyme 1 that can be adsorbed on substrate, g/g = 0.06
- \( E_{lim} \): maximum enzyme 2 that can be adsorbed on substrate, g/g substrate = 0.01
**Ethanol fermentation**

- $r_4$: cell growth rate on glucose, g/kg h
- $\mu_{m,g}$: maximum specific growth rate in cell growth (glucose as substrate), 1/h = 0.31
- $C_G$: glucose concentration, g/kg
- $K_{g}$: monod constant for growth on glucose, g/kg = 1.45
- $CE_t$: ethanol concentration, g/kg
- $CE_{tmax}$: threshold ethanol concentration in cell growth (glucose as substrate), g/kg = 28.9
- $CE_{tmax}t$: maximum ethanol concentration in cell growth (glucose as substrate), g/kg = 57.2
- $K_{d,t}$: inhibition constant for growth on glucose, g/kg = 200
- $r_5$: cell growth rate on xylose, g/kg h
- $\mu_{m,xy}$: maximum specific growth rate in cell growth (xylose as substrate), 1/h = 0.1
- $C_{xy}$: xylose concentration, g/kg
- $K_{s,xy}$: monod constant for growth on xylose, g/kg = 4.91
- $CE_{tmax,xy}$: threshold ethanol concentration in cell growth (xylose as substrate), g/kg = 26.6
- $CE_{tmax,xy}$: maximum ethanol concentration in cell growth (xylose as substrate), g/kg = 56.3
- $K_{S,xy}$: inhibition constant for growth on xylose, g/kg = 600
- $r_6$: total cell growth rate, g/kg h
- $C_{y}$: cell concentration, g/kg
- $\alpha$: weighing factor for glucose consumption, dimensionless = 0.65
- $r_7$: glucose consumption rate, g/kg h
- $q_{smax,g}$: overall maximum specific glucose utilization, g/g h = 10.9
- $K_{S,g}$: substrate limitation constant in glucose consumption, g/kg = 6.32
- $CE_{tmax,gl}$: threshold ethanol concentration in glucose consumption, g/kg = 42.6
- $CE_{tmax,gl}$: maximum ethanol concentration in glucose consumption, g/kg = 75.4
- $K_{S,gl}$: substrate inhibition constant in glucose consumption, g/kg = 186
- $r_8$: xylose consumption rate, g/kg h
- $q_{smax,xy}$: overall maximum specific xylose utilization, g/g h = 3.27
- $K_{S,xy}$: substrate limitation constant, g/kg = 0.03
- $CE_{tmax,xy}$: threshold ethanol concentration in xylose consumption, g/kg = 53.1
- $CE_{tmax,xy}$: maximum ethanol concentration in xylose consumption, g/kg = 81.2
- $K_{S,xy}$: substrate inhibition constant in xylose consumption, g/kg = 600
- $r_9$: ethanol formation rate by glucose fermentation, g/g h
- $q_{pmax,g}$: overall maximum specific ethanol production by glucose fermentation, g/g h = 5.12
- $K_{S,g}$: substrate limitation constant in glucose fermentation, g/kg = 6.32
- $CE_{tmax,g}$: threshold ethanol concentration in glucose fermentation, g/kg = 42.6
- $CE_{tmax,gl}$: maximum ethanol concentration in glucose fermentation, g/kg = 75.4
- $K_{S,gl}$: substrate inhibition constant in glucose fermentation, g/kg = 186
- $r_{10}$: ethanol formation rate by xylose fermentation, g/g h
- $q_{pmax,xy}$: overall maximum specific ethanol production by xylose fermentation, g/g h = 1.59
- $K_{S,xy}$: substrate limitation constant in xylose fermentation, g/kg = 0.03
- $CE_{tmax,xy}$: threshold ethanol concentration in xylose fermentation, g/kg = 53.1
- $CE_{tmax,gl}$: maximum ethanol concentration in xylose fermentation, g/kg = 81.2
- $K_{S,gl}$: substrate inhibition constant in xylose fermentation, g/kg = 600
- $r_{11}$: total ethanol production rate, g/g h

**Succinic acid fermentation**

- $r_9$: cell growth rate, g/kg h
- $C_{S,X}$: cell dry weight in glucose fermentation, g/kg
- $\mu_{m,sg}$: maximum specific growth rate in glucose fermentation, 1/h = 1.324
- $C_{S,G}$: glucose (substrate) concentration, g/kg
- $K_{s,g}$: inhibition constant for growth on glucose, g/kg = 88.35
- $K_{S,g}$: glucose saturation constant, g/kg = 1.123
- $P_{E}$: total product concentration from fermentation glucose, g/kg
- $P_{Crit,g}$: critical product concentration at which cell growth fully stops, g/l = 17.23
- $i$: degree of product inhibition, dimensionless = 1.30
- $K_{d}$: specific death rate, 1/h = 0.010
- $r_{s,SA}$: formation rate of succinic acid, g/kg h
- $C_{s,SA}$: succinic acid concentration, g/kg
- $\alpha_{SA}$: growth-associated parameter for succinic acid formation, dimensionless = 1.619
- $B_{AA}$: non-growth-associated parameter for succinic acid formation, 1/h = 0.355
- $r_{R,AA}$: formation rate of acetic acid, g/kg h
- $C_{R,AA}$: acetic acid concentration, g/kg
- $\alpha_{AA}$: growth-associated parameter for acetic acid formation, dimensionless = 0.626
- $B_{AA}$: non-growth-associated parameter for acetic acid formation, 1/h = 0.124
- $r_{F,AA}$: formation rate of formic acid, g/kg h
- $C_{F,AA}$: formic acid concentration, g/kg
- $\alpha_{FA}$: growth-associated parameter for formic acid formation, dimensionless = 0.665
- $B_{FA}$: non-growth-associated parameter for formic acid formation, 1/h = 0.105
- $r_{L,AA}$: formation rate of lactic acid, g/kg h
- $C_{L,AA}$: lactic acid concentration, g/kg
- $\alpha_{LA}$: growth-associated parameter for lactic acid formation, dimensionless = 0
- $B_{LA}$: non-growth-associated parameter for lactic acid formation, 1/h = 0.210
- $r_{SC}$: glucose consumption rate, g/kg h
- $Y_{SA}$: stoichiometric yield coefficient of cell on glucose = 0.765
- $Y_{SA}$: stoichiometric yield coefficient of succinic acid on glucose = 1.31
- $Y_{AA}$: stoichiometric yield coefficient of acetic acid on glucose = 0.999
- $Y_{FA}$: stoichiometric yield coefficient of formic acid on glucose = 1.532
- $Y_{LA}$: stoichiometric yield coefficient of lactic acid on glucose = 0.999
- $m_{SG}$: specific maintenance coefficient, 1/h = 0.061


