A Multiobjective Optimization Framework for Design of Integrated Biorefineries Under Uncertainty

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DOI 10.1002/aic.14849
Published online May 13, 2015 in Wiley Online Library (wileyonlinelibrary.com)

A systematic approach for development of a reliable optimization framework to address the optimal design of integrated biorefineries in the face of uncertainty is presented. In the current formulation, a distributed strategy which is composed of different layers including strategic optimization, risk management, detailed mechanistic modeling, and operational level optimization is applied. In the strategic model, a multiobjective stochastic optimization approach is utilized to incorporate the tradeoffs between the cost and the financial risk. Then, Aspen Plus models are built to provide detailed simulation of biorefineries. In the final layer, an evolutionary algorithm is employed to optimize the operating condition. To demonstrate the effectiveness of the framework, a hypothetical case study referring to a multiproduct lignocellulosic biorefinery is utilized. The numerical results reveal the efficacy of the proposed approach; it provides decision makers with a quantitative analysis to determine the optimum capacity plan and operating conditions of the biorefinery. © 2015 American Institute of Chemical Engineers *AIChE J*, 61: 3208–3222, 2015

Keywords: strategic optimization, operational level optimization, stochastic programming, risk management, integrated biorefinery

Introduction

Currently, chemical and energy industries are heavily reliant on fossil fuels such as petroleum, coal, and natural gas. As fossil fuel supplies are expected to be less available, more expensive, and a leading source of air and water pollution, the needs for alternative production chains in energy and chemical sectors become more urgent. Renewable energy sources are expected to play an important role in the supply of the future energy demand. In the quest for sustainable alternatives, the industry is experiencing a steady growth in the production of bio-based fuels and chemicals that are developing the emerging concept of biorefining.[1] Biorefineries appear to be a promising avenue for energy and chemical production from biomass as part of the solution to climate change and the heavy dependence on fossil fuels[2]; this emerging industry can also enhance energy security and create job opportunities.

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 prefeasibility study phase, wherein, the processes that execute the purpose of the value chain are still nonexistent. 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 impact all actors and participants over strategic time horizons (10–30 years). Value chain actors should make mission-critical decisions that have economic, social, and environmental impacts on the stakeholders of the value chain. The nature of these decision tasks can be strategic, tactical, or operational. Hence, there is a need for development of efficient strategies to analyze these emerging technologies and yield optimal trade-offs between performances of different criteria.

To manage the complexity of the decision-making process for designing renewable energy production systems, several contributions have appeared over the last few years where mathematical programming techniques have been exploited by taking into account process and economic modeling. The National Renewable Energy Laboratory (NREL) has developed detailed analytical models to analyze different process configurations for cellulosic ethanol production.[3–5] Furthermore, many multiechelon and multiperiod models for biorefinery design and planning have been employed.[6–16] For instance, in the work by Sammons et al.,[6] a general systematic framework is proposed to optimize product allocation and process configuration for a flexible integrated biorefinery through utilization of process integration methods such as pinch analysis. This work covers the overall process design on the basis of sustainability metrics.

Additionally, multiobjective approaches have also been proposed to optimize several conflicting objectives simultaneously (such as net present value (NPV) vs. environmental impact).[17–21] These programming approaches offer the most powerful tool for the exploration of the balanced trade-offs between conflicting objectives.[22] For instance, in the work by You et al.,[18] a multiobjective mixed integer linear programming (MILP) model is proposed to address the optimal design and planning of cellulosic ethanol supply chains

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under economic, environmental, and social objectives. In this study, Pareto-optimal designs reveal the trade-off between the three main dimensions of the sustainable biorefinery supply chain. As algorithms still struggle with the size and nonconvexity of the resulting models for complex chemical processes such as integrated biorefineries, optimization problems usually incorporate simplified process descriptions and shortcut methods. A broad discussion of the challenges and opportunities in the development of biorefineries and the advantages of applying systems engineering tools in various levels of decision making has been presented in Daoutidis et al.[23] Detailed overview of recent advances in the optimization of energy systems are reviewed by Connolly et al.[24] and Shabani et al.[25]

The aforementioned studies use deterministic modeling approaches, which assume that all the model parameters that influence the optimization task are known in advance. However, common to early stages of process design is the lack of certain information that will introduce variability into the decision-making problem. Uncertainty affects the system efficiency and may lead to either infeasible design or suboptimal performance. Product prices and demands are exogenous parameters set in the open market, which propose a great challenge for the management to control their evolution during the planning horizon of the plant. These factors have hampered investment capital formation in the renewable sector and have deterred prospective entities from undertaking commercialization of labscale and demonstration scale projects. Thus, market uncertainty is a significant factor which should be incorporated into the optimization framework to add additional value and granularity to the decision-making process. Widely used methodologies developed for solving optimization problems under explicit consideration of uncertainties are reviewed by Sahinidis,[26] which includes stochastic programming,[27] chance constraint programming,[28] and robust optimization.[29]

A number of contributions addressed the presence of uncertainties in optimization of biorefineries. For example, Kim et al.[30] proposed a two-stage mixed integer stochastic programming model to determine the number, location, and size of production units by maximizing the overall expected profit while incorporating the uncertainty of parameters. In this model, global sensitivity analysis is utilized to understand the influence of various uncertain parameters and identify the parameters that have the greatest impact on the optimization problem. Dal-Mas et al.[31] proposed an MILP model for corn-based ethanol supply chain design which considers the market value fluctuation of corn and ethanol. A stochastic formulation is implemented to handle the effect of uncertainty. Gebreslassie et al.[32] developed a bicriterion, multiperiod MILP model for optimal design of hydrocarbon biorefinery supply chains under supply and demand uncertainties that simultaneously minimizes the expected annualized cost and financial risk. Tong et al.[33] presented a two-stage stochastic MILP model for optimal design and strategic planning of an advanced hydrocarbon biofuel supply chain integrated with existing petroleum refineries based on scenario generation for uncertain parameters. In this model, biomass availability, production and capital costs, crude oil price, and government incentives are introduced as uncertain parameters.

Although several decision-making frameworks have been developed for optimal design and operations of biorefineries, in most of the studies mentioned above, strategic, tactical, and operational decision tasks are not addressed within a single optimization model, even though there is a significant interdependence between them. Integration of multiple levels of systems tasks requires specialized software infrastructure that enables decision-making across different time and length scales involved. Furthermore, the aforementioned studies consider linearization assumptions and simplifications for modeling the process in order to keep the model tractable and allow large model development with relatively short computational time. However, conversion mechanisms in biorefining processes are inherently nonlinear in nature. Moreover, the risks associated with the uncertainties potentially involved in biorefineries may significantly affect the optimal performance of the plant and cause extra expenses to accommodate unexpected events.[34]

Therefore, this work aims to fill these research gaps by proposing a novel decision support tool based on a hybrid simulation and optimization approach. Recently, there have been some strategies suggested in literature which demonstrate the utility of the hybrid modeling methods that effectively combine both optimization and simulation modeling approaches[35–38]; these methods aim at combining the merits of both approaches. The work proposed by Lee et al.[38] is a notable contribution to this field that proposes a hybrid approach combining the analytic and simulation models for obtaining more realistically optimal production-distribution plans for the integrated supply chain systems. However, even though rapid progress is being made in this area, most of the proposed approaches involve long-term decisions (strategic decisions) rather than simultaneous optimization of all the three levels of decision tasks, that is, strategic, tactical, and operational decisions.

In the proposed framework, the optimization of long and short decisions is integrated seamlessly in the face of uncertainty. Given the challenge of integrating process simulation, nonlinear optimization and strategic planning, different software platforms are interlinked in a systematic procedure to execute the framework. In conjunction with the simulation and optimization studies, the proposed framework will develop quantitative metrics to associate economic values with technical barriers. A previous article by the authors[39] proposed a methodology to generate and identify optimal configuration and operating conditions for a biorefining enterprise with very promising results in terms of energy consumption and production cost. In this study, we expand the scope of the framework by incorporating market uncertainty through stochastic optimization. This iterative framework is based on a distributed, systematic approach, which is composed of different layers including systems-based strategic optimization, detailed mechanistic modeling, and operational level optimization. In the stochastic optimization model, scenario-based formulation is utilized to transform the original strategic optimization problem under uncertainty into a deterministic approximation by discretizing the uncertain market parameters.[40] Explicit risk measure is also added to the model as a new objective to allow the management of financial risk according to the decision maker's attitude; risk management formulation is introduced to the model to reduce the economic losses due to unfavorable scenarios and to simultaneously improve the economic performance, thus leading to a multiobjective optimization problem. A hypothetical case study, multiproduct lignocellulosic biorefinery that converts biomass to value-added biofuels (cellulosic ethanol) and bio-based chemicals (succinic acid), is presented to

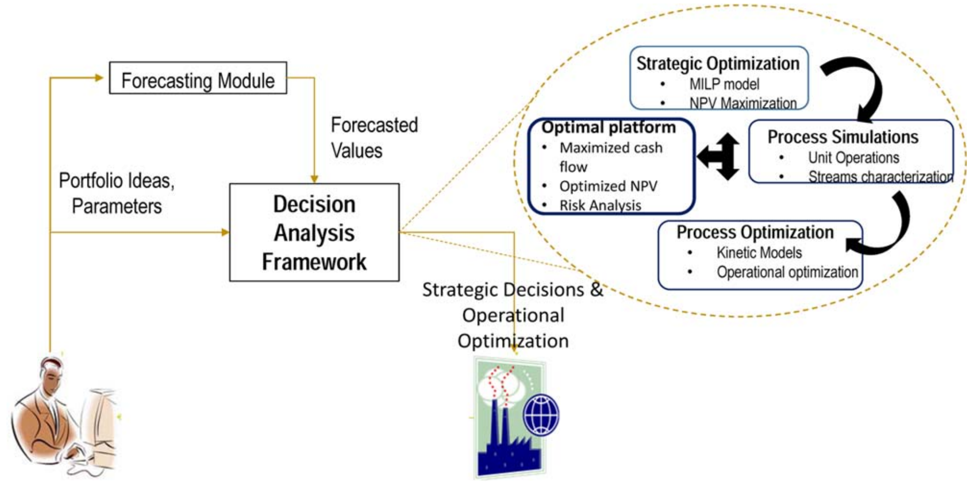

Figure 1. Structure of the proposed decision support strategy.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

exemplify the efficacy of the proposed framework. This article is organized as follows. The proposed optimization framework is presented in the next section. After a general description of the integrated biorefining case study, details of the proposed strategy and its application to biorefinery are presented. The optimization results are then presented and discussed to demonstrate the effectiveness of the proposed framework as a decision-making strategy. Lastly, concluding remarks and future directions are presented in Conclusion Section.

Decision Support Framework

The proposed framework aims to develop an innovative, model-based decision support system in order to investigate the inherent collaborative relationships between different decision layers of a renewable energy enterprise, and how these relationships can be exploited in order to improve their commercial viability and sustainability. This framework utilizes a distributed architecture to model decision making for renewable energy operations with several key features. The renewable energy enterprise will be represented as a real entity with different interdependent and functional layers in its decision hierarchy—the Corporate Planning Layer (Strategic) and the Production Planning Layer (Operational). The strategic and operational layers will consist of several sectors that will coordinate activities within a particular division. Both layers will reciprocally interact in an effort to work toward a common and specific corporate goal. A general schematic structure of the proposed iterative decision support strategy is presented in Figure 1.

The layered decomposition does not necessarily imply a hierarchy; each layer is functionally dependent on the others for information to complete its model. This information can be used in the form of constraints or parameters by other models, the idea being that the optimized solutions from one layer should not violate physical constraints in other layers. A major component of any decision support system is a forecasting module that estimates the future parameters that will impact the enterprise performance. In our study, product supplies, demands, and prices are deemed uncertain parameters; once the requisite parameters are forecasted over the desired time scales, these parameters are inserted into the decision analysis framework. During the first stage, strategic decision making will be formulated as an MILP model. The model is represented by linear equations for mass and energy balances to describe physical flow of materials across the system nodes, and financial flows that result from the system design and material movements. These mass and energy balances that dictate core technologies in the energy production system are integrated with cost and revenue functions through a techno-economic model. In this layer of the optimization framework (strategic planning), the operating conditions of each section in the plant are selected based on the literature estimates. Different scenarios are developed based on stochastic forecasts for uncertain market parameters. The strategic model will determine the optimal design of production capacity of the plant for the planning horizon by maximizing the expected NPV. Management of risk due to uncertain parameters is explicitly addressed in the strategic model by adding a criterion to control the variability of the performances associated with each specific scenario; in fact, the trade-off between risk and profitability of the plant will be incorporated to strategic decision making process.

The capacity plan is then sent to the lower level of the optimization algorithm, which optimizes the operating conditions of the plant. The production layer will contain an iterative strategy to integrate detailed process simulation of production facilities in the network with plant-wide optimization models. Process simulation will enhance our understanding of the complex process, help identify potential improvements that can be made in the configuration and operation, and incorporate much realism to the computer representation of the process (including nonlinear thermodynamics and biological kinetics). For the purpose of nonlinear plant-wide optimization, a stochastic algorithm will be integrated with simulations; these novel algorithms are especially robust in solving nonlinear optimization problems such as the optimization of a renewable energy process.

Economic optimization and risk analysis will provide users with visual tools that merge decision-making intuition with mathematical rigor; using an iterative framework implementation and real-time information exchange between each decision layer, we may potentially overcome the mismatch between nonlinear process mechanisms and linear estimations used during linear programming optimization of strategic decisions. Each component of the proposed algorithm (Figure 1) is described in greater detail within Framework Details Section.

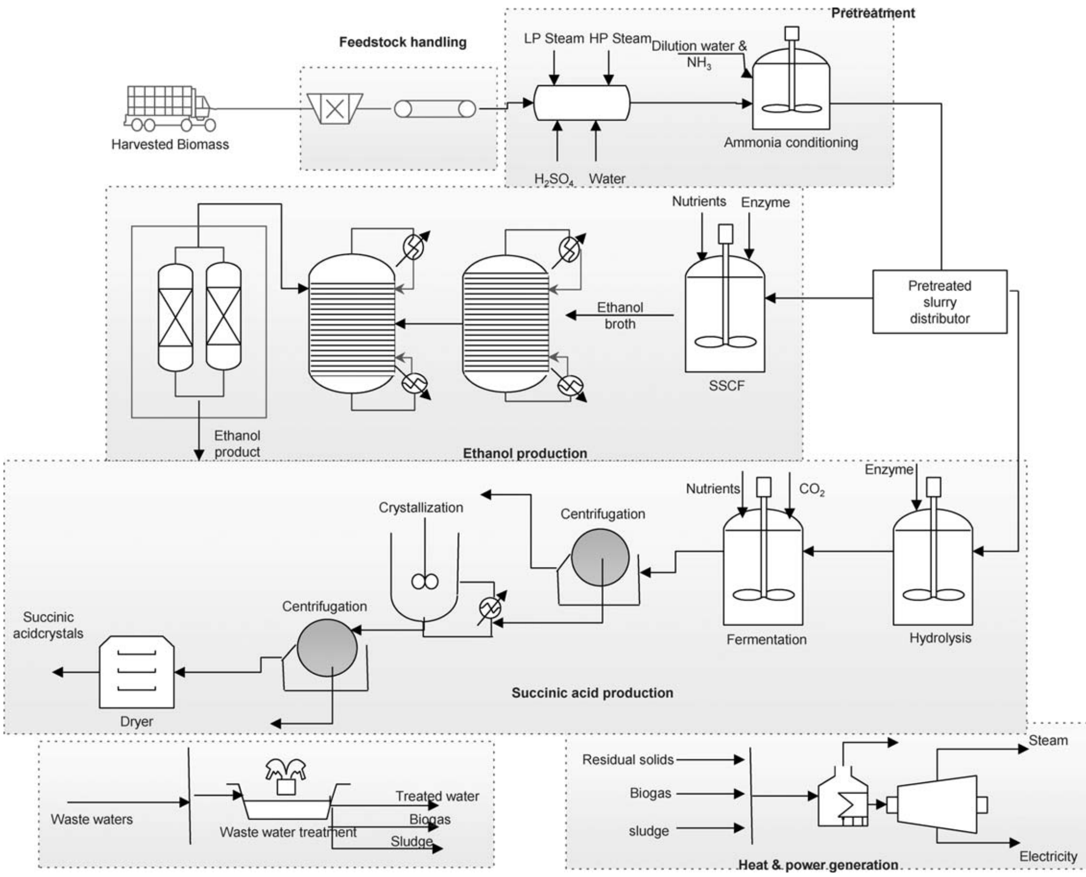

Figure 2. Process flow diagram.

Process Description

To demonstrate the utility of the proposed framework, the aforementioned optimization strategy 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, the applicability of the framework transcends just biorefineries (other processes can include algae process design, and even oil and natural gas processing plants).

Lignocellulosic biorefinery

The conversion platforms of lignocellulosic biorefinery can broadly be subdivided into two major pathways: (1) the biological conversion pathways based on fermentation and (2) thermochemical conversion pathways based on heat-based technologies like gasification. The lignocellulosic biorefinery used in this study is a multiproduct plant that uses a fermentation-based sugar conversion platform with three products: cellulosic ethanol, biosuccinic acid, and bioelectricity. We assume that the prospective biorefinery is located in the southwest region of Louisiana and utilizes biomass crops sourced from limited land available within a 100 mile radius of the plant.

Switchgrass serves as the selected feedstock for the biorefining process. The production chain comprises of six major systems: feedstock pretreatment, sugar hydrolysis, sugar fermentation, product purification, heat and power generation, and wastewater treatment. Operating conditions for each section of the plant are obtained from the data suggested in literature which are determined based on the detailed dynamic modeling of the process. The systems superstructure is shown in Figure 2. Pretreatment technologies break down the matrix of biomass polymeric compounds to facilitate the enzymatic hydrolysis of cellulose and solubilize the hemicellulose. Biomass is exposed to dilute sulfuric acid (0.05–5 wt %) at a high temperature (140–190°C) and moderate solids concentration (30 wt %) for a short time to solubilize hemicellulose and lignin and increase the digestibility of cellulose in enzymatic hydrolysis. During this process, xylose degradation products such as furfural, inhibitors such as acetic acid, and corrosion products are produced. Ammonia (NH_4OH) conditioning technology is selected for detoxification of pretreated biomass based on the work of Alriksson et al.[41] and Jennings and Schell.[42] In the conditioning reactor, mixture of ammonia and water is used to raise the pH from 1 to 5–6 and dilute the slurry to 20 wt % total solids. The resulting pretreated slurry is split into two streams: one stream that is allocated for the production of ethanol and the other stream that is sent to succinic acid production. In ethanol production, sugars produced in saccharification are simultaneously cofermented to ethanol. Purchased cellulase enzyme and nutrients for cofermentation of sugars are added to the reactor at a compromise temperature for hydrolysis and ethanol fermentation. This process is known as simultaneous saccharification and cofermentation which has been shown to help to reduce the inhibition impact of sugars in hydrolysis.[43] The pretreated slurry allocated to succinic acid production is first hydrolyzed by utilizing the purchased enzymes and the produced sugar is fermented to succinic acid and other acids such as acetic, formic, and lactic acid as by-products of fermentation by utilizing genetically engineered strain *Mannheimia succiniciproducens MBEL55E* developed by Song et al.[44]

The products in the fermentation effluent need to be recovered and purified; the purification technologies will depend on the type of products that are being recovered. Ethanol recovery is accomplished with employing two distillation columns and a sieve-based purification to obtain ethanol with fuel grade purity (99.5 wt %). In succinic acid purification, most of the water and organic acids with boiling points lower than succinic acid are vaporized in the evaporator. The concentrated stream is sent to a crystallizer which selectively separates succinic acid based on its solubility behavior. Finally, to purify succinic acid crystals to an acceptable end use purity (>90 wt %) a centrifuge and a dryer are utilized.

To reduce make-up water requirement, a sequence of anaerobic and aerobic digesters are considered in process modeling to digest organic materials contained in the waste waters coming from different sections of the plant. Anaerobic digestion produces a biogas which is rich in methane and is considered as a fuel source in combustion section. Aerobic digestion is carried out in lagoons to produce a clean water stream that is recycled to the plant. Additionally, sludge which is primarily composed of cell mass is also produced in aerobic digestion that is used to produce steam and power in combustion section. Recycled water is introduced into different areas of the plant such as pretreatment to minimize the purchased fresh water consumption. Solids from recovery sections (mainly lignin), biogas from anaerobic digestion, and sludge from aerobic digestion are considered as the combined solid feed in the combustion section to produce high pressure steam, electricity, and process heat. Combustion section is composed of combustor, boiler, and turbogenerator.

To better estimate the nonlinear reaction dynamics of enzymatic hydrolysis and fermentation, experimentally derived kinetic models are utilized in process simulation. All operational and economic data for our case study is obtained from Kazi et al.,[5] Humbird et al.,[45] Li et al.,[46] and Vlysidis et al.[47]

Framework Details

Our proposed systematic framework consists of three main steps which guide the user in solving the stochastic optimization problem (Figure 1). This iterative framework includes the methods and tools such as linear modeling of the process, uncertainty analysis, risk management, process simulation (nonlinear modeling), and stochastic optimization. In this section, each component of the proposed framework is described in some detail with the lignocellulosic biorefinery being featured in order to apply the framework design components to a case study.

Strategic model

This section presents the model that is used to describe the capacity design problem. The model is formulated as a stochastic mixed integer-based linear program (MILP) with a 14-year planning horizon and biannual time steps, yielding a total of 7 time steps. Special emphasis is laid on the strategic capacity planning leading to a long-term planning horizon. Biannual time steps were chosen to keep the computations manageable in the model and represent a full business cycle (shorter term fluctuations in market conditions are averaged out). The mathematical formulation of the strategic planning model is broken into submodels for ease of description, which include a production model, flexible capacity design model, financial model, and a risk management model. A list of parameters, variables, and subscripts is given in Notation section preceding References at the end of the article.

Production model

All major process systems are represented as linear black boxes in the planning model for the technology set considered for the framework demonstration. The major equations that are approximated linearly in the planning model and modeled nonlinearly during process simulation and optimization include unit operations' yield and unit operations' energy balances. These equations are given in the following form:

Biomass Feedstock Production. The biomass production formulation is developed to model plant's decisions for calculating the acreage of land harvested and the total amount of produced biomass to be utilized as the feedstock

$$\mathrm{BM}_{t,s}^{\mathrm{hvst}} = \mathrm{land}_{t,s}^{\mathrm{hvst}} \times \mathrm{BYLD}_t \tag{1}$$

$$\mathrm{land}_{t,s}^{\mathrm{hvst}} = \mathrm{land}_{t-1,s}^{\mathrm{hvst}} + \mathrm{land}_{t-\mathrm{GD},s}^{\mathrm{new}} - \mathrm{land}_{t,s}^{\mathrm{release}} \tag{2}$$

$$\mathrm{land}_{t,s}^{\mathrm{release}} = \mathrm{land}_{t-\mathrm{GC},s}^{\mathrm{new}} \tag{3}$$

$$\mathrm{land}_{t,s}^{\mathrm{hvst}} \leq \mathrm{Maxland}_t \tag{4}$$

The mass balance for biomass production is represented in Eq. 1, where $\mathrm{BM}_{t,s}^{\mathrm{hvst}}$ is the amount of produced biomass in time period t for scenario s based on total harvested land $\mathrm{land}_{t,s}^{\mathrm{hvst}}$ and the expected biomass yield BYLD_t from harvesting operation. Equation 2 is the area balance on land which ensures that steady feedstock is supplied to the plant at each time period t by contracting new lands, $\mathrm{land}_{t-\mathrm{GD},s}^{\mathrm{new}}$. Additionally, the growth delay of harvesting GD is introduced to the model by considering the availability of new contracted land, $\mathrm{land}_{t-\mathrm{GD},s}^{\mathrm{new}}$, after the defined growth delay. To model the growth cycle of the biomass, GC, Eq. 3 is introduced which mandates the release of the land when it has run the course of its production cycle. Harvested land is also constrained by the total amount of available land $\mathrm{Maxland}_t$ at each time period t for each scenario s based on Eq. 4 to ensure that it does not exceed its available amount.

Integrated Biorefining Process Model. The mass balance is performed for each node in the conversion chain of the integrated biorefinery; these nodes include pretreatment, hydrolysis, fermentation, product recovery, and product sales in end-use markets. These material balances should take into account the theoretical yield and the actual yield to adjust the theoretical amount to an actual yield which can be obtained from each of unit operations. The material balance is given by

$$\mathrm{SystemInput}_{\mathrm{eqp},t,s} \times \mathrm{YLD}_{\mathrm{eqp},t}^{\mathrm{theoretical}} \times \mathrm{YLD}_{\mathrm{eqp},t}^{\mathrm{actual}} = \mathrm{SystemOutput}_{\mathrm{eqp},t,s} \tag{5}$$

Here, $\mathrm{SystemInput}_{\mathrm{eqp},t,s}$ is the input to the unit operation eqp (nodes in the conversion chain) at time period t for scenario s, $\mathrm{YLD}_{\mathrm{eqp},t}^{\mathrm{theoretical}}$ is the theoretical amount of product that is expected from unit operation eqp at time period t, and $\mathrm{YLD}_{\mathrm{eqp},t}^{\mathrm{actual}}$ is utilized to adjust the amount of product from each unit operation eqp to an actual recoverable amount at time t, and $\mathrm{SystemOutput}_{\mathrm{eqp},t,s}$ represents the amount of product of node eqp during time t for scenario s. Actual yield, $\mathrm{YLD}_{\mathrm{eqp},t}^{\mathrm{actual}}$, is the parameter which is used to incorporate the nonlinearities of the process to the MILP formulation of the proposed strategic optimization model by updating its value iteratively based on the results from process simulation in Aspen Plus.

Demand constraints are introduced by the following equations to model the sale levels for each product

$$\mathrm{Sales}_{p,t,s} + \mathrm{PI}_{p,t,s} = \mathrm{Product}_{p,t,s} + \mathrm{PI}_{p,t-1,s} \tag{6}$$

$$\mathrm{Sales}_{p,t,s} \geq \mathrm{CSL}_{p,t} \times \mathrm{Demand}_{p,t,s} \tag{7}$$

$$\mathrm{Sales}_{p,t,s} \leq \mathrm{Demand}_{p,t,s} \tag{8}$$

Equation 6 is the material balance for the flow of final products to end-use markets. Where $\mathrm{Sales}_{p,t,s}$ is the amount of product p sold to the market during time t for scenario s, $\mathrm{PI}_{p,t,s}$ represents the inventory of product p at time t for scenario s which is maintained on site. It is assumed that at each time period, a certain percentage of demand, $\mathrm{Demand}_{p,t,s}$, has to be satisfied based on the customer service level CSL (Eq. 7). Sales are further constrained by the maximum demand that is available to be fulfilled at each time period t and scenario s (Eq. 8).

Capacity design

Flexible designs can add great improvements in overall expected benefits by enabling the managers to adjust to new circumstances and flexible adaption to a long-term market development. They can avoid bad circumstances for unfavorable future and when the future offers new opportunities, flexibility in design will enable them to take advantage and benefit from those possibilities. In the proposed framework, a flexible capacity design is incorporated based on the following equations. This formulation is utilized to incrementally expand the capacity (small increments) for each operating system. Additional costs incurred related to capacity expansion investments are calculated based on the financial model explained in the next section

$$0 \leq \mathrm{CapExp}_{\mathrm{eqp},t,s} \leq \mathrm{BVCI}_{\mathrm{eqp},t,s} \times \mathrm{CAP}_{\mathrm{eqp}}^{\mathrm{UB}} \tag{9}$$

$$\mathrm{Cap}_{\mathrm{eqp},t,s} \geq \mathrm{SystemInput}_{\mathrm{eqp},t,s} \tag{10}$$

$$\mathrm{Cap}_{\mathrm{eqp},t,s} = \mathrm{Cap}_{\mathrm{eqp},t-1,s} + \mathrm{CapExp}_{\mathrm{eqp},t-\mathrm{CD},s} \tag{11}$$

Equation 9 provides bounds to capacity expansion ($\mathrm{CapExp}_{\mathrm{eqp},t,s}$) of each operating system (eqp) at time period t and scenario s, where $\mathrm{BVCI}_{\mathrm{eqp},t,s}$ is the capacity increment binary variable of operating system eqp at time period t for scenario s which is 1 when capacity is incremented and 0 otherwise. Constraint in Eq. 10 ensures that total established capacity of each operating system $\mathrm{Cap}_{\mathrm{eqp},t,s}$ for each time period and each scenario is sufficiently large to satisfy the input to that operating system $\mathrm{SystemInput}_{\mathrm{eqp},t,s}$. Equation 11 is used to update the processing capacity $\mathrm{Cap}_{\mathrm{eqp},t,s}$ of each operating system, adjusting for a construction delay (CD) of 2 years. Construction delay term is utilized to force the optimizer that no production can occur while the facility is under construction. Optimized capacity plan is then passed on to the process simulator (Aspen Plus) and the process optimizer (MATLAB) in order to determine optimal operating conditions.

Financial model

The financial model is broken into three salient aspects that describe the financial impact of network design, production of final products, and sales

1. Market model
2. Calculation of capital costs, operating expenses, and revenues
3. Calculation (optimization) of the objective function (NPV).

Market Model. Market model describes price and demand evolution of the products in the integrated biorefinery. We assume that market of bioproducts is impacted primarily by oil prices as oil is the primary determinant of alternative transportation fuel markets. The price of crude oil is represented as a stochastic input following Geometric Brownian Motion (GBM), based on which the bioproduct market parameters are derived, yielding stochastic price-demand sets. GBM assumption implies a high degree of volatility in predicted prices and embeds a high level of uncertainty. As stochastic variables following GBM are lognormally distributed, oil prices can be represented by a continuous lognormal distribution characterized by the expected value and standard deviation at any time. Natural logarithm of the oil price has the standard deviation of $\sigma\sqrt{\Delta T}$. Where σ indicates the constant volatility in the GBM representation of oil price and ΔT shows the time interval considered in discretization of the stochastic model.

Scenario Generation. The most widely employed approach for optimization under uncertainty is the stochastic programming method. A stochastic program is a mathematical program in which some of the parameters defining a problem instance are random. The uncertain parameters are commonly assumed to follow discrete probability distributions and a planning horizon consisting of a fixed number of decision points. Therefore, the stochastic process can be represented with scenario trees. Scenario-based stochastic programming is an approximation approach to transform the intractable stochastic problem into a tractable one. This strategy avoids high-dimensional numerical integration in the solution of the problem, as the expected NPV (objective function) can be calculated as finite sums and each constraint can be duplicated for each scenario. The main idea is to address only a finite number of selected realizations of uncertainty in the optimization. Each realization is regarded as one scenario and is assigned with a probability. In the proposed framework, average biannual crude oil prices can move up or down with a given probability from the current time period to the next, yielding a Markov chain-based decision tree. Each node in the decision tree is represented as a price scenario for crude oil (and consequently for bioproduct markets) and over the 7 time periods this yields a total of 64 oil price scenarios.

Binomial lattice generation approach which was suggested by Cox et al.[48] is utilized to discretize the continuous stochastic model of oil price. A binomial lattice can be thought of as a time-varying probability tree. The stochastic variables are assumed to move up or down sequentially over time with estimated probabilities (P^{up} and P^{down}) obtained by the following equations

$$u = e^{\sigma\sqrt{\Delta T}}, \ d = \frac{1}{u} \tag{12}$$

$$P^{\mathrm{up}} = \frac{e^{r\sqrt{\Delta T}} - d}{u - d}, \ P^{\mathrm{down}} = 1 - P^{\mathrm{up}} \tag{13}$$

Here, u and d represent up and down movements in oil price and r is the risk-free discount rate equal to the yield on

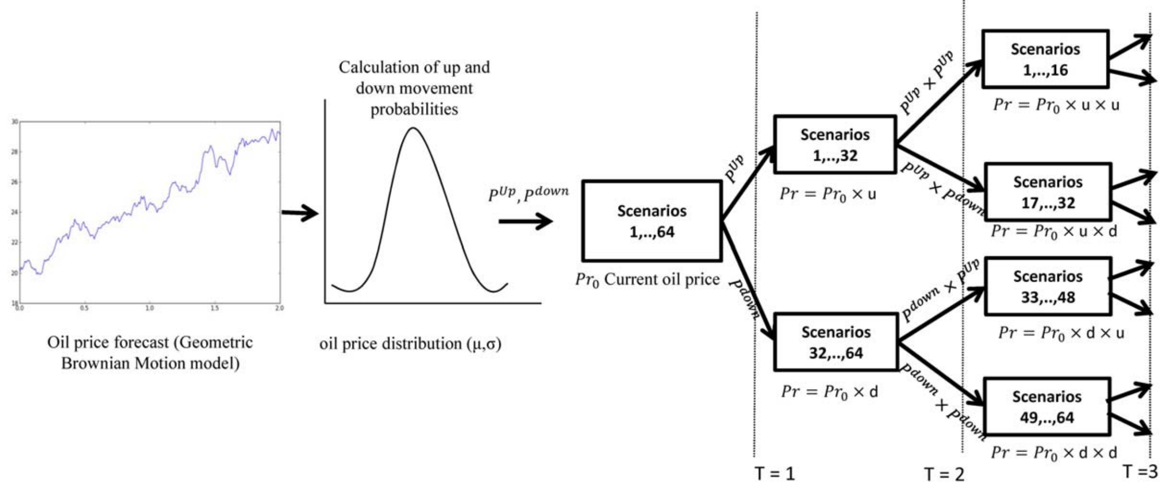

Figure 3. Oil price forecasting process and scenario generation.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

a 10-year treasury bond. The process for discretizing the stochastic variable is presented in Figure 3.

Calculation of the price and the demand of products (ethanol and succinic acid) is derived from the hypothetical market model proposed in the previously published journal article[49]; a simplified diagram of this model is presented in Figure 4 and its salient components are discussed here to give the readers a feel for the model structure.

Gross Domestic Product (GDP) growth and inflation rates are derived using stochastic oil price model as a proxy for the state of the economy in macroeconomic model. Liquid ethanol commodity market is determined by different market forces including oil price, Renewable Fuel Standard (RFS) mandates, and macroeconomic factors such as GDP growth, interest rates, and inflation rates.[50,51] For forecasting long-term trends in the proposed bio-based succinic acid market, certain qualitative assumptions are considered. It assumes that succinic acid will serve markets that are currently served by petroleum derivatives. Furthermore, marginal cost of production, environmental premium, and supply-demand balance are the other factors which have significant impact in determination of the dynamic market trend in the future. Since the focus of our strategic model has been on long-term decisions, the market model is formulated based on long intervals so that the development over one time step can be assumed to be a long-term change. Shorter term fluctuations in market such as seasonal variations in supply and demand of products are averaged out. It should be noted that the utilization of the hypothetical market model proposed by Sharma et al.[49] is purely with demonstrative motive to incorporate a fundamentally derived predictive model for value estimation of uncertain parameters in dynamic market to the development of our comprehensive optimization framework.

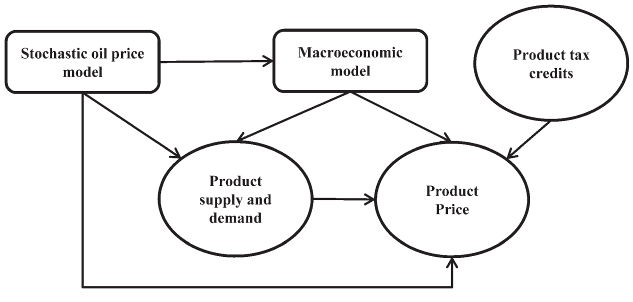

Figure 4. Simplified market model for evolution of price and demand in product.

Capital Cost, Operating Expenses, and Revenue Calculation. Capital cost (Capex) calculation during each time period for each scenario includes land establishment cost for biomass production, equipment cost for processing biomass, construction and engineering cost, contingency cost, legal and permitting cost, and working capital investment as shown in Eq. 14. The methodology for capital cost structure is adapted from Kazi et al.[5] that exemplifies NREL's *n*th plant cost analysis

$$\begin{aligned} \mathrm{Capex}_{t,s} = {} & \mathrm{Capex}^{\mathrm{land}}_{t,s} + \mathrm{Capex}^{\mathrm{toteqp}}_{t-1,s} + \mathrm{Capex}^{\mathrm{C\&E}}_{t-\mathrm{CD},s} \\ & + \mathrm{Capex}^{\mathrm{Cont}}_{t,s} + \mathrm{Capex}^{\mathrm{l\&p}}_{t,s} + \mathrm{Capex}^{\mathrm{wc}}_{t,s} \end{aligned} \tag{14}$$

Since NPV calculation (objective function) gives explicit consideration to the time value of money, charges considered in the capital cost calculation are distributed over the construction period (CD) instead of being charged all at once so as to minimize the present value of costs. Construction, engineering, contingency, and working capital costs are calculated as a percentage of total equipment and established land costs at each time period t. The equipment-specific investment ($\mathrm{Capex}^{\mathrm{eqp}}_{t,s}$) is calculated based on the linear method represented in Eq. 16. The linear approximation for equipment cost is based on the method presented by Sharma et al.[52] First, the base cost for each operating section is obtained from literature.[5,53] Then, capacity of each section is varied between ±%75 of the base capacity and the resultant costs for each capacity were calculated by scaling the cost using Eq. 15. The purpose of the exponent in this equation is to account for economies of scale. The costs are then plotted against the calculated capacities and a linear approximation is fitted to the cost curve to obtain the equation of a line (Eq. 16). This equation represents the equipment-specific investment during any period t and scenario s which is the summation of the fixed cost $\mathrm{FC}_{\mathrm{eqp}}$ (constant of the linear approximation) and variable cost $\mathrm{VC}_{\mathrm{eqp}}$ in terms of unit cost of capacity expansion (the slope of the linear approximation) associated with capacity expansion, $\mathrm{Capex}_{t,s}^{\mathrm{eqp}}$. It is worth mentioning that $\mathrm{Capex}_{t,s}^{\mathrm{eqp}}$ equals to zero if the binary variable for the capacity expansion of that equipment, $\mathrm{BVCI}_{\mathrm{eqp},t,s}$, is zero because of constraints 9 and 16 which means that capacity is not expanded at that specific time period. The total equipment cost is then calculated as the sum of all operating sections expenses during period t and scenario s (Eq. 17). It is important to model and value this decision-making flexibility (incremental capacity addition), especially for product markets such as biofuels and biochemicals that are in their nascent stages of development

$$\mathrm{NewCost} = \mathrm{Oldcost} \times \left(\frac{\mathrm{NewCapacity}}{\mathrm{OldCapacity}}\right)^{\partial} \tag{15}$$

$$\mathrm{Capex}_{t,s}^{\mathrm{eqp}} = \mathrm{BVCI}_{\mathrm{eqp},t,s} \times \mathrm{FC}_{\mathrm{eqp}} + \mathrm{CapExp}_{\mathrm{eqp},t,s} \times \mathrm{VC}_{\mathrm{eqp}} \tag{16}$$

$$\mathrm{Capex}_{t,s}^{\mathrm{toteqp}} = \sum_{\mathrm{eqp}} \mathrm{Capex}_{t,s}^{\mathrm{eqp}} \tag{17}$$

Operating cost (Opex) at time period t for scenario s is the summation of feedstock harvesting cost, process chemical costs, utility cost, other ancillary raw materials, labor costs, and selling, general and administrative costs. These costs are described by the following equation. It should be noted that to allow the large model development with short computational time and keeping the model tractable in strategic planning, nonlinear relations (such as feedstock transportation cost) are reformulated to maintain the model linear

$$\mathrm{Opex}_{t,s} = C_{t,s}^{\mathrm{HVST}} + C_{t,s}^{\mathrm{chemical}} + C_{t,s}^{\mathrm{utility}} + C_{t,s}^{\mathrm{other}} + C_{t,s}^{\mathrm{labor}} + C_{t,s}^{\mathrm{SGA}} \tag{18}$$

Revenues are generated from the sale of products at forecasted product prices as shown in Eq. 19

$$\mathrm{Revenue}_{t,s} = \sum_{p} (\mathrm{Sales}_{p,t,s} \times \mathrm{Price}_{p,t,s}) \tag{19}$$

Objective Function. Following the calculation of costs and revenues, free cash flow (FCF) of the enterprise which is a measure for financial performance is calculated as the difference between operating cash flows and capital expenditures. NPV of the enterprise is calculated as the sum of a time series of free cash flows that have been discounted back to the present for the whole planning horizon as shown in the following equations

$$\mathrm{NPV}_s = \sum_{t=1}^{t=T_L} \frac{\mathrm{FCF}_{t,s}}{(1+\mathrm{ir})^t} \tag{20}$$

Here, ir represents the discount rate (or annual rate of return), and T_L is the project lifetime. As we are dealing with uncertain future, the value of the process is not a fixed number but an expectation over a range of possible futures that follows a discrete probability function. We can think of it as an average value over a range of good and bad outcomes. The expected NPV (Eq. 21) is considered as the objective of our strategic optimization model to be maximized

$$E[\mathrm{NPV}] = \sum_{s} (P_s \times \mathrm{NPV}_s) \tag{21}$$

where, NPV_s is the net present value corresponding to the realization of each scenario s, and P_s is the probability of occurrence of such scenario.

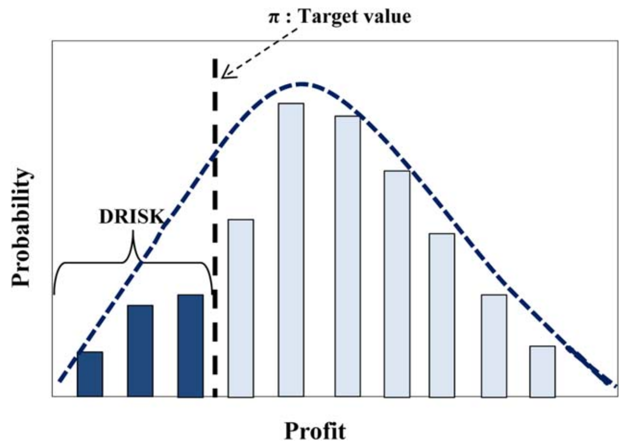

Figure 5. The concept of downside risk management.

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Risk management model

In the stochastic programming model, optimal solution is obtained by maximizing the total expected NPV which is optimal on average for all the scenarios. The expected value of NPV is a risk-neutral objective and does not reflect the variability of performances associated with each specific scenario. Therefore, there is no guarantee that the process will perform at a certain level over all the uncertain parameter space. The only guarantee is that the average value of objective function is optimized. However, in any decision under risk, expected profit is not the only objective. Management is also concerned about the risk involved in the model. The trade-off between financial risk and profitability of the plant should be incorporated to the stochastic programming formulation. Therefore, a two criteria approach is considered which profitability (NPV) and a specific risk metric are the objectives to be optimized. Different criteria for assessing the variability of performance (risk measures) have been proposed in the literature.[32,54,55] In this study, downside risk method proposed by Eppen et al.[55] is introduced to the model as the risk management strategy.

Downside Risk Management. In this approach, the risk associated with scenarios whose profits are not desirable is minimized. As shown in Figure 5, downside risk is calculated based on the area underneath the curve of probability function which has lower profitability than the defined threshold (π). To introduce the risk in the framework, a positive variable δ_s which is the deviation between the NPV of each scenario and the defined threshold is considered based on the following constraint

$$\delta_s \geq \pi - \mathrm{NPV}_s, \qquad \delta_s \geq 0 \tag{22}$$

These inequalities indicate that when the NPV of a scenario is higher than the target value π, δ_s equals to zero, and when NPV is lower than the target value, it equals to their difference. Therefore, downside risk is calculated as the expected value of positive deviations from the defined target π based on the following equation

$$\mathrm{DRISK}_{\pi} = \sum_{s} P_s \cdot \delta_s \tag{23}$$

Addition of downside risk management in the framework results in a multiobjective problem including two conflicting

Table 1. Lower and Upper Bounds for Optimization Variables

Optimization Variable	Lower Bound	Upper Bound
Hydrolysis temperature (°C)	30	50
Sugar allocation ratio (sugar to ethanol)	0.1	1
Enzyme load (g enzyme/kg cellulose)	5	50

objective functions (maximizing expected NPV and minimizing the financial risk). The ε-constraint method is utilized in our formulation for solving the multiobjective optimization model. This optimization method is based on formulating an auxiliary model by transferring one of the objectives of the original problem to the constraint.[56]

Operational Level Modeling and Optimization

After obtaining the capacity plan which is designed strategically by maximizing the expected NPV of the plant, this capacity is utilized in the operational level model for rigorous nonlinear process simulation and optimization. First, the process is simulated in the simulation software (Aspen Plus) and results from simulation are utilized in the optimization model implemented in MATLAB to maximize the profitability of the process. This strategy will be performed iteratively until the convergence criterion is met. Process simulator software (Aspen Plus) and a mathematical modeling software (MATLAB) communicate with one another to do the modeling and optimization tasks. Furthermore, by simulating entire model in Aspen Plus, the implicit correlations between upstream and downstream stages of the process are taken into consideration.

Process simulation

Simulation of the technological configuration was carried out using Aspen Plus with the optimal capacity plan obtained from strategic optimization. Main input data utilized for process simulation in bioethanol production are obtained from Humbird et al.,[57] Kazi et al.,[5] and Aden et al.,[58] and the process data for succinic acid fermentation and purification are based on the developed models of Vlysidis et al.[47] and Li et al.[46] Part of the physical property data of the components required for simulation were obtained from Wooley and Putsche.[59] One of the characteristics of our approach is the incorporation of the complex kinetics of bioreactions in our simulation model. An iterative dynamic data exchange between process simulation model in Aspen Plus and developed kinetic models in MATLAB is embedded as part of the process simulation based on the software architecture developed by Geraili et al.[60] The communication between Aspen Plus and MATLAB is based on Aspen Plus ActiveX Automation technology which enables the user to transfer data to and from other Windows applications. This method shows an efficient real-time data exchange model. Furthermore, it facilitates the integration of process simulation and operational level optimization.

Developed mathematical formulations for the kinetics are based on the experimentally validated models by Kadam et al.[61] for enzymatic hydrolysis, model by Morales-Rodriguez et al.[62] for simultaneous hydrolysis and cofermentation of ethanol, and the developed model by Song et al.[44] for succinic acid fermentation. It should be noted that for dilute acid pretreatment, suggested conversion rate values of the reactions in literature (NREL reports) are utilized. Implementation of a model for pretreatment in process simulation based on appropriate kinetics of reactions is an area of current research that is being pursued to enhance the practical application of our proposed framework.

Process optimization

Due to the complexities involved in biorefining processes including inherently nonlinear conversion mechanism, mathematical modeling of the process will comprise of nonconvex functions. Although deterministic methods are relatively fast, they might get trapped in local optima. Stochastic methods are more suitable for solving these types of problems, as a wide range of values for parameters would be searched. Furthermore, for solving large scale nonlinear optimization problems deterministically, constraints should be incorporated into the objective function. However, in many practical large-scale applications, models embedded in the simulation environments are used to mimic complex processes behavior.[63] In our case study, all the mass and energy balances are embedded in the simulation and constraints are satisfied when the simulation is converged. Stochastic approaches can overcome this problem as they do not require the manipulation of the mathematical structure of the objective function and constraints.[64]

There are numerous operating conditions which can affect the production cost and profitability of the biorefinery. The parameters which have significant effect on the plant's profitability were identified in our previously published paper,[60] which are related to the enzymatic hydrolysis of feedstock and fermentation of sugars. Enzyme loading, pretreated biomass allocation, and hydrolysis temperature have a complex set of impacts and can considerably affect the process yields as well as production costs and revenues of the plant. The lower bound and upper bound of the optimization variables are set as shown in Table 1.The optimization objective used here is to maximize the annual cash flow of the process (Eq. 24), which takes into account the revenues generated from the sale of products, the direct cost of raw materials, and the annual fixed costs

$$\mathrm{CF}=\mathrm{obj}(\vec{x}) = \sum_{p} P_p \times \mathrm{Price}_p - \sum_{r,p} \mathrm{RM}_{r,p} \times \mathrm{Cost}_r - \mathrm{FC} \tag{24}$$

Here, P_p represents the production of each product p including ethanol, succinic acid, and excess electricity, and $\mathrm{RM}_{r,p}$ is the amount of raw material type r utilized for the production of product p, and annual fixed costs, FC, includes the labor, maintenance, and transportation costs. Selected production capacity plan in strategic optimization is incorporated as constraints during process optimization to control the production rates, Eq. 25. These inequality constraints are handled by exploiting the penalty function approach. In this approach, modified objective function (penalized objective), $OBJ(\vec{x})$, is defined as sum of the original objective, $obj(\vec{x})$, and a penalty term, $g_j(\vec{x})$, which depends on the

Table 2. Differential Evolution Algorithm Parameters

Parameters/Operators	Value
Maximum number of function evaluation (MAXNFE)	1000
Population size (NP)	30
Weighing coefficient (F)	0.8
Crossover rate (CR)	0.9
Penalty coefficient (R_j)	100,000

Table 3. Comparison of the Base Case and the Stochastic Model

	Feedstock Capacity (1000 ton/year)	Sugar Allocation Ratio (for Ethanol Production)	Ethanol Production (MM gal)	Succinic Acid Production (1000 ton)	Net Present Value ($MM)
Base case	155.0	0.66	7.1	4.00	45.0
Stochastic case	218.0	0.62	11.1	6.00	62.8

constraint violation (Eq. 26). Here, R_j is the penalty coefficient of the jth inequality constraint to make it of the same order of magnitude as the original objective function

$$P_p^{\text{simulation}} \leq P_p^{\text{strategic planning}} \tag{25}$$

$$\text{OBJ}(\vec{x})=\text{obj}(\vec{x})+\sum_{j=1}^{j=p}(R_j \times g_j(\vec{x})) \tag{26}$$

To solve the operational level optimization problem, differential evolution (DE) algorithm, which is a stochastic optimization method, is selected and written in MATLAB. This algorithm is simple in concept and can be easily implemented. Table 2 provides the DE parameters utilized in this study. To facilitate the automation of process simulation and optimization, DE algorithm in MATLAB is linked with the simulation in Aspen Plus simulator.

Results and Discussion

In this section, the results for optimal strategic and operational level decisions of the multiproduct biorefinery are discussed based on the proposed decision making framework. The decision variables considered in the framework are composed of the optimal capacity plan for long-term production in biorefinery, optimal temperature for enzymatic hydrolysis, optimal enzyme amount utilized in hydrolysis reaction and optimal allocation of pretreated biomass for production of final products. To illustrate the effectiveness of the proposed strategy, different case studies are considered including: base case, stochastic model, and stochastic model coupled with risk management model.

Base case is considered as a deterministic model and all the economic parameters are fixed through the planning horizon. The economic parameters used for this case study are the same with those in Sharma et al.[52] and Geraili et al.[39] Stochastic model considers the variability in the market that is inherent in real world; thus, stochastic formulation based on scenario generation is developed for strategic optimization. Finally, the third case study is an extension of the stochastic model by incorporating financial risk through downside risk management. A multiobjective optimization model is implemented to establish the trade-offs between cost and risk. Plant life time considered for all the case studies is 14 years with an annual discount rate of 10%.

Based on the results of the MILP model for the strategic optimization which is implemented in the modeling system GAMS and solved with a CPLEX linear solver, optimal values of the decision variables are calculated. As the main focus of this work is to expand the scope of our proposed framework by incorporating uncertainty into the model, results for the deterministic model (base case) are presented in Table 3 for the comparison purposes, and detailed analysis of the results for stochastic programming model are presented as follows.

The expected NPV of the stochastic solution is 62.8 $MM which indicates that value is created through enterprise activities and it is a profitable project investment. Figure 6 illustrates a wide range of values for calculated NPVs of different scenarios considered in the model which represent the influence of market variability in the optimization of strategic model. Results in Table 3 show that a higher profitability (NPV) is obtained by the stochastic model which is 44% higher than deterministic solution. We can also see that feedstock processing capacity of the plant also increases 40% in comparison to the deterministic model and more sugar is allocated to succinic acid production. Currently, the market volume of succinic acid is relatively small due to the nascent stage of its market. However, with its high-value applications, product acceptance and diffusion, application market of bio-based succinic acid has the potential to improve fast over the planning horizon and this market growth is taken into account in the stochastic model.

Expected amount of biomass utilized in each time period is illustrated in Figure 7. As is shown in this figure, in the first time period there is no production due to the introduced growth delay functionality in the mathematical formulation (GD = 2 years) of biomass harvesting, and there is a growth

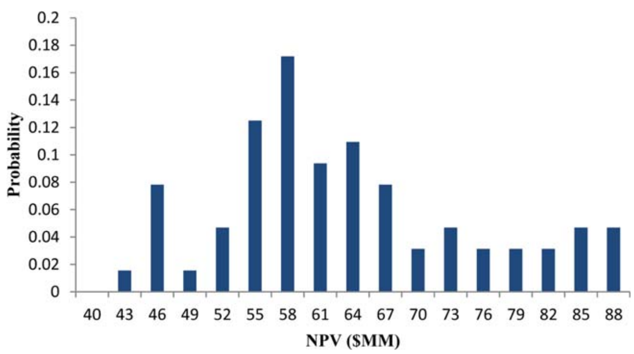

Figure 6. Histogram of the NPVs for the stochastic programming model.

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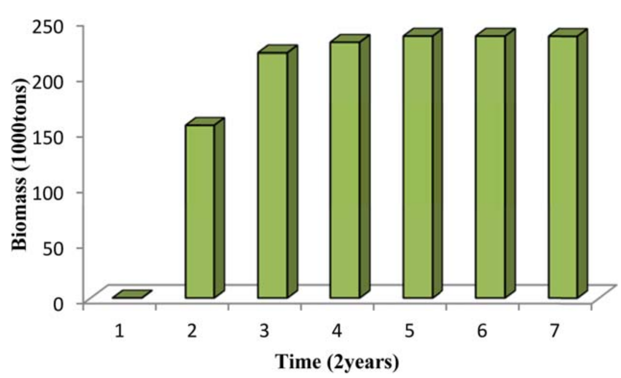

Figure 7. Biomass utilization.

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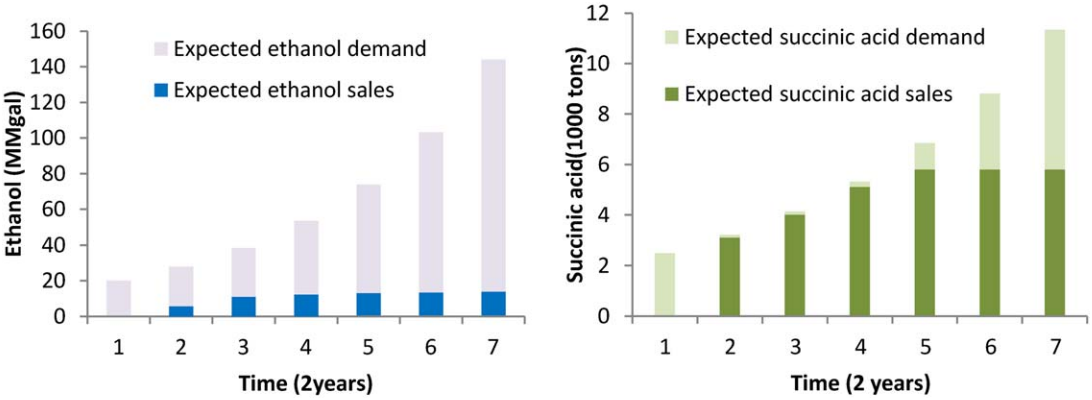

Figure 8. Ethanol and succinic acid production.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

in the expected amount of harvested biomass due to the additional capacities established in the plant and also the developments in the market parameters during the planning horizon which are explained in more detail as follows.

Figure 8 depicts the expected production trends of ethanol and succinic acid over the planning horizon. Demand and production rates are presented based on the expected values of all the considered scenarios in each time period.

Succinic acid sales follow the demand growth while ethanol market share decreases with increase in demand. It is apparent that succinic acid market provides the greatest opportunity for profitability and it can be enhanced if larger volumes of succinic acid can be sold into the market. In fact, ethanol is considered as the high-volume fuel that maintains healthy bottom-line while succinic acid is considered as a high margin chemical to improve overall margins. Furthermore, allocation of pretreated biomass to ethanol production increased over the planning horizon possibly because of additional capacity installed for ethanol production.

To illustrate the expansion in capacity of ethanol production, scenario 36 is taken as the reference scenario which has the closest NPV to the expected total NPV among all scenarios. Figure 9 shows that based on the strategic optimization model which utilizes binary variables for capacity expansion constraint in Eq. 9 to select a setup allowing the best compromise between cost and flexibility, additional capacity for ethanol production is installed during fourth and fifth periods in the planning period before the maximum capacity for ethanol production is reached.

Figure 10 represents the forecasted free cash flow (and its components) that are generated from the operation of the optimal design and the evolution of the cumulative expected NPV of the enterprise. The expected NPV is broken up into two major components: the discounted value of expected operating cash flow (ECFO) which is calculated based on the value of plant operation, and the discounted value of expected capital investment made in the plant (ECAPEX). We notice that the project payback period is 10 years which is not desirable for investment. One of the financial strategies that can be investigated to shorten the payback period for biorefinery project investments is to incorporate more profitable product portfolio comprising of higher margin, lower volume specialty products such as pharmaceuticals. Techno-economic modeling and analysis of different product portfolios is an area we are actively pursuing at the process systems engineering (PSE) group at Louisiana State University.

The major biomass capacity investments are made during the first period; however, as mentioned earlier, the charges are distributed over the planning horizon to mitigate the present value of the costs. Succinic acid production capacity is established at the beginning while two increments are made for ethanol recovery capacity in the fourth and fifth time periods and additional capital costs are incurred due to the capacity investments.

Iterative results of the hybrid optimization methodology are presented in Table 4 which shows that in two iterations the model is converged. Initial process yields are obtained from literature (step1); then these yields are utilized in strategic model to calculate the production capacity plan (step2);

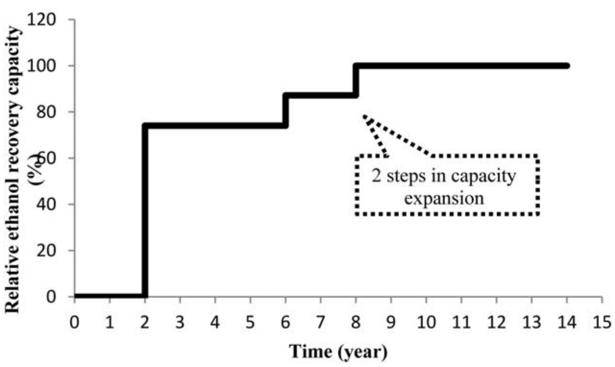

Figure 9. Capacity expansion in ethanol recovery section for scenario 36.

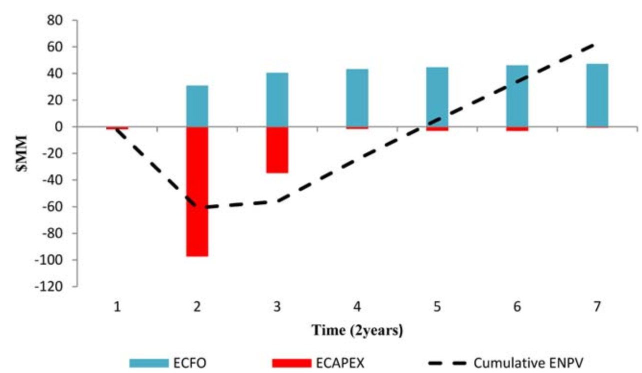

Figure 10. Free cash flow components and the evolution of the optimal expected NPV.

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Table 4. Iteration Results in the Hybrid Optimization Strategy

Parameters and Variables		Iteration1 Step1	Iteration1 Step2	Iteration1 Step3	Iteration2 Step1	Iteration2 Step2
Capacity constraints	Feedstock (1000 ton/year)	–	222.2	–	218.0	–
	Ethanol (MM gal/year)	–	15.3	–	11.4	–
	Succinic acid (1000 ton/year)	–	6.0	–	5.9	–
Yield parameters	Sugar (kg/kg)	0.87	–	0.65	–	0.65
	Ethanol fermentation	0.85	–	0.98	–	0.98
	Succinic acid fermentation	0.25	–	0.45	–	0.45
	Ethanol purification	0.99	–	0.98	–	0.98
	Succinic acid purification	0.78	–	0.78	–	0.78

Table 5. Optimal Values for Decision Variables and Objective Function

	DE
Temperature	33.55°C
Sugar allocation	0.62 (ethanol), 0.38 (succinic acid)
Enzyme loading ratio	34.8 (g enzyme/kg cellulose)
Cash flow	$71 million per year

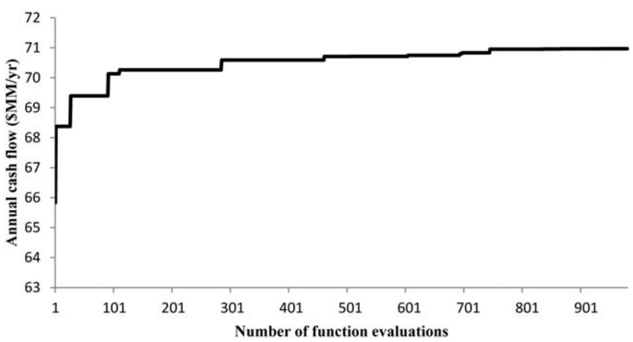

Figure 11. Convergence behavior of the operational level optimization.

the optimal values for the capacity are passed to the process level simulation and optimization to find the optimal process conditions and calculate the process yields based on the results of simulation (step3). These calculated yields are compared with the initial values used in the strategic model to check the convergence. Because the difference between calculated yields and initial yield values is greater than the threshold, this hybrid optimization needs to be carried out again based on the new yield values.

Values of the decision variables obtained from the hybrid optimization model are shown in Table 5. The convergence behavior of the proposed optimization algorithm is also plotted in Figure 11. It can be seen that the convergence is steady and stable.

Results for managing the downside risk

The impact of the proposed risk management procedure is presented in Figure 12 and Table 6. In the calculation of the downside risk, the target level π is set to $ 51 MM. We can see that how the risk management approach reconstructed the NPV distribution of the scenarios to reduce the risk of occurrence of unfavorable scenarios while maintaining an acceptable expected revenue. As expected, the results from multiobjective optimization model reveal that there is a conflict between the two objectives, economic performance and financial risk. As shown in Table 6, a reduction of the downside risk can be attained at the expense of a reduction in the expected NPV (economic objective) of the process.

Another interesting result as can be observed in Table 6 is that the minimization of the downside risk leads to allocation of more sugar to succinic acid production. Note that succinic acid is considered as a promising coproduct to improve the economics of industrial fermentation; consequently, allocation of more sugar to succinic acid production will make the optimal solution less sensitive to the fluctuations in the price and demand of the products. Additionally, reduction in the financial risk of the process leads to a reduction in the expected biomass processing capacity of the plant as shown in Table 6. Incorporation of the risk in the optimization framework will tend to give more conservative design which means although the capacity of the plant has decreased, NPV of scenarios have much higher chances to be between the desired target. This leads to a more robust behavior of the framework in the face of uncertainty.

Conclusion

The methodology proposed in this article provides a comprehensive and flexible framework within which different aspects of sustainability are considered to yield a full-fledged decision support and analysis system. This algorithm has the advantage of integrating long-term planning with operational level decisions. Furthermore, scenario analysis is conducted to incorporate uncertainty of market parameters in the framework and downside risk management is appended to the strategic model to control the variability of performance and incorporate the trade-off between risk and profitability of the plant within the decision making process. An integrated multiproduct lignocellulosic biorefinery producing value-added biofuels (ethanol) and bio-based chemicals (succinic acid)

Table 6. Comparison of Feedstock and Production Capacities Before and After Risk Management

Scenario	Expected NPV ($MM)	Downside Risk (%)	Feedstock Capacity (1000 tons/year)	Sugar Allocation Ratio (for Ethanol Production)
Stochastic case	62.8	10	218	0.62
Risk management case	60.0	3	152	0.59

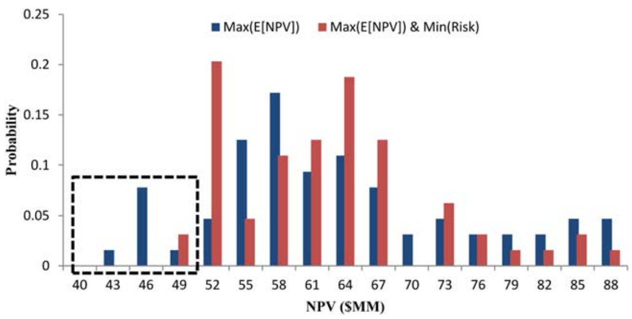

Figure 12. Comparison of cost distribution before and after risk management.

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has been presented to show the capabilities of the proposed approach.

The analysis of the results from stochastic formulation reveal that considering uncertainty will provide results that reflect the variation of market parameters and behave better than the deterministic model (yielding better expected NPV). Additionally, incorporating metrics for financial risk mitigation in the framework shows that there are two important factors that influence the performance of the model in the face of uncertainty including production capacity and allocation of pretreated biomass between ethanol and succinic acid production. The outcome of this work is a new distributed decision support framework which is intended to help economic development agencies, as well as policy makers in the renewable energy enterprises to carefully evaluate and plan investment and operating decisions before execution.

In the future study, inherent flexibility in operation of the plant will be included in the decision support framework by incorporating analysis of uncertainty in technical parameters in operational level optimization. Furthermore, seasonal variations and short-term fluctuations will be incorporated in the prediction of the long-run dynamics of biofuels and bio-based chemical markets by decreasing the time steps to impart greater fidelity in the proposed decision support framework. Moreover, the proposed framework is flexible enough that additional functionalities such as modeling environmental and social characteristics and implementation of mathematical models for pretreatment can be incorporated into the decision-making process.

Notation

Subscripts

t = time
s = scenario
p = type of product
r = type of raw material
eqp = type of equipment
GD = growth delay, 2 years
GC = growth cycle, 3 years
CD = construction delay, 2 years

Parameters

BYLD_t = expected biomass yield in time period t, 6 tons per acre at $t=1$
$\mathrm{Maxland}_t$ = maximum land available in time period t, 10,000 acres at $t=1$
$\mathrm{YLD}^{\mathrm{theoretical}}_{\mathrm{eqp},t}$ = theoretical amount of product expected from unit operation eqp at time period t, obtained from Kazi et al.[5] and Humbird et al.[57]
$\mathrm{YLD}^{\mathrm{actual}}_{\mathrm{eqp},t}$ = actual amount of product expected from unit operation eqp at time period t, obtained from process simulation results
$\mathrm{CSL}_{p,t}$ = customer service level in time period t for scenario p, obtained from Sharma et al.[52]
$\mathrm{CAP}^{\mathrm{UB}}_{\mathrm{eqp}}$ = upper bound to capacity expansion of unit operation eqp, obtained from Sharma et al.[52]
σ = standard deviation of average oil price, \$3 from Sharma et al.[52]
$\mathrm{FC}_{\mathrm{eqp}}$, $\mathrm{VC}_{\mathrm{eqp}}$ = fixed and variable cost for linear approximation of unit operation eqp investment, obtained from Sharma et al.[52]
ir = annual rate of return, 0.07
π = defined threshold in risk management model, \$ 51 MM

Variables

$\mathrm{BM}^{\mathrm{hvst}}_{t,s}$ = amount of biomass harvested in time period t for scenario s, ton
$\mathrm{land}^{\mathrm{hvst}}_{t,s}$ = harvested land in time period t for scenario s, acres
$\mathrm{land}^{\mathrm{new}}_{t,s}$ = new contracted land in time period t for scenario s, acres
$\mathrm{land}^{\mathrm{release}}_{t,s}$ = released land in time period t for scenario s, acres
$\mathrm{SystemInput}_{\mathrm{eqp},t,s}$ = amount of input to the unit operation eqp in time period t for scenario s
$\mathrm{SystemOutput}_{\mathrm{eqp},t,s}$ = amount of product from unit operation eqp in time period t for scenario s
$\mathrm{Sales}_{p,t,s}$ = amount of product p sold to the market in time period t for scenario s
$\mathrm{PI}_{p,t,s}$ = inventory of product p in time period t for scenario s
$\mathrm{Product}_{p,t,s}$ = amount of final product p produced in time period t for scenario s
$\mathrm{Demand}_{p,t,s}$ = demand of product p in time period t for scenario s
$\mathrm{CapExp}_{\mathrm{eqp},t,s}$ = capacity expansion of unit operation eqp in time period t for scenario s
$\mathrm{BVCI}_{\mathrm{eqp},t,s}$ = binary variable for capacity increment of unit operation eqp in time period t for scenario s, (1 if capacity is expanded, 0 otherwise)
$\mathrm{Cap}_{\mathrm{eqp},t,s}$ = capacity of unit operation eqp in time period t for scenario s
P^{up} and P^{down} = estimated probability of up and down movements in price based on market model
$\mathrm{Capex}_{t,s}$ = capital cost of the plant in time period t for scenario s
$\mathrm{Capex}^{\mathrm{land}}_{t,s}$ = land establishment cost in time period t for scenario s, based on the estimates derived from online sources (http://www.landandfarm.com)
$\mathrm{Capex}^{\mathrm{toteqp}}_{t,s}$ = total equipment cost in time period t for scenario s
$\mathrm{Capex}^{\mathrm{C\&E}}_{t,s}$ = construction and engineering cost in time period t for scenario s, 32% of total equipment cost
$\mathrm{Capex}^{\mathrm{Cont}}_{t,s}$ = contingency cost in time period t for scenario s, 20% of total direct and indirect capital cost
$\mathrm{Capex}^{\mathrm{l\&p}}_{t,s}$ = legal and permitting cost in time period t for scenario s, 25% of total equipment cost
$\mathrm{Capex}^{\mathrm{WC}}_{t,s}$ = working capital investment in time period t for scenario s, 15% of fixed capital investment
$\mathrm{Opex}_{t,s}$ = operating cost of the plant in time period t for scenario s
$C^{\mathrm{HVST}}_{t,s}$, $C^{\mathrm{chemical}}_{t,s}$, $C^{\mathrm{utility}}_{t,s}$ = feedstock cost, process chemical cost, utility cost based on the method derived from Sharma et al.[52]
$C^{\mathrm{other}}_{t,s}$, $C^{\mathrm{labor}}_{t,s}$, $C^{\mathrm{SGA}}_{t,s}$ = ancillary raw materials cost, labor cost, selling, general, and administrative cost based on the method derived from Sharma et al.[52]
$\mathrm{Revenue}_{t,s}$ = revenues generated from sale of products in time period t for scenario s
$\mathrm{Price}_{p,t,s}$ = forecasted price of product p in time period t for scenario s
$\mathrm{FCF}_{t,s}$ = free cash flow of the enterprise in time period t for scenario s
NPV_s = net present value of scenario s
$E[\mathrm{NPV}]$ = expected value of NPV

P_s = probability of occurrence of scenario s
δ_s = positive deviation between π and NPV of scenario s

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Manuscript received Dec. 23, 2014, and revision received Apr. 15, 2015.