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A Framework for Optimal Design of Integrated Biorefineries under Uncertainty

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Integrated biorefineries are processing facilities which convert biomass into value-added fuels and chemicals. From a commercial perspective, recent lignocellulosic biorefinerinig ventures have been fraught with technological and market uncertainties often leading to considerable financial losses for value chain actors. The objective of this work is to develop a comprehensive optimization framework for sustainable design of biorefineries. A structural approach is utilized for planning the production capacity, simulation of the process in detail, and optimizing the operating condition of the plant. A stochastic linear programming model is developed for strategic optimization under market uncertainty. Results from strategic model are sent to the lower level of optimization model in which operating conditions of the plant are optimized through an iterative process simulation and stochastic optimization. To demonstrate the effectiveness of the proposed approach, a hypothetical lignocellulosic biorefinery is considered as a case study. The results prove the efficiency of the proposed approach, and provide a quantitative analysis to determine the optimal design in the face of uncertainty.

1. Introduction

In recent years there has been a marked surge in the search for alternative sources of energy that wean the world off of dependence on fossil fuels and reduce the carbon foot-print. As the world has recognized the importance of diversifying its energy resource portfolio away from fossil resources and more towards renewable resources such as biomass, there arises a need for developing strategies which can design renewable sustainable value chains that can be scaled up efficiently and provide tangible net environmental benefits from energy utilization. After a boom in U.S. corn-based ethanol in the early part of the 21st century, the interest has gradually shifted towards more viable sources for production of biofuels and biochemicals. Second generation biofuels are examples of such fuels that are extremely attractive owing to the fact that the raw materials can be composed completely of “left-over” wastes of food crops and forest harvests that do not interfere with the human food chain and the natural ecosystem. It also can provide new income and employment opportunities in rural areas.
Several contributions have appeared over the last few years in order to manage the complexity of decision making process for designing profitable renewable energy production systems. Many of the proposed studies in the literature such as the work by Kazi et al. (2010) use deterministic modelling approaches which assume that all the parameters 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 (Sahinidis 2004).
In this study the development and implementation of a multi-layered decision support tool is presented that can be utilized by energy entrepreneurs, resource and technology investors, and value chain actors in the renewable energy industry to carefully design and optimize the business value of their energy endeavours in the face of uncertainty. A distributed, systematic approach is applied which is composed of different layers including strategic, tactical, and operational tasks. To demonstrate the effectiveness of the proposed methodology, a hypothetical case study of a multiproduct lignocellulosic biorefinery based on sugar conversion platform is utilized.

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2. Design of decision support framework

Linear programming (LP) models are suggested 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 simulation and process-level optimization. In the first stage (strategic model) different scenarios are developed based on stochastic forecasts for uncertain market parameters including price and demand of bioproducts. The process is formulated as a stochastic mixed integer linear programming (MILP) model which incorporates stepwise capacity expansion and financial risk minimization. The output of the model includes optimal design of production capacity of the plant for the planning horizon by maximizing the expected net present value (NPV). The results are then fed to the second stage of the optimization algorithm (operational level model). This stage, which optimizes the operating conditions of the plant, consists of three main steps including simulation of the process in the simulation software (nonlinear modelling), identification of critical sources of uncertainties through global sensitivity analysis affecting selected performance criteria, and employing stochastic optimization methodologies to maximize the annual cash flow of the plant. Figure1 shows a general schematic structure of the proposed iterative decision support strategy. The iterative process is used 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. Each component of the proposed algorithm is described in more detail in section 3.

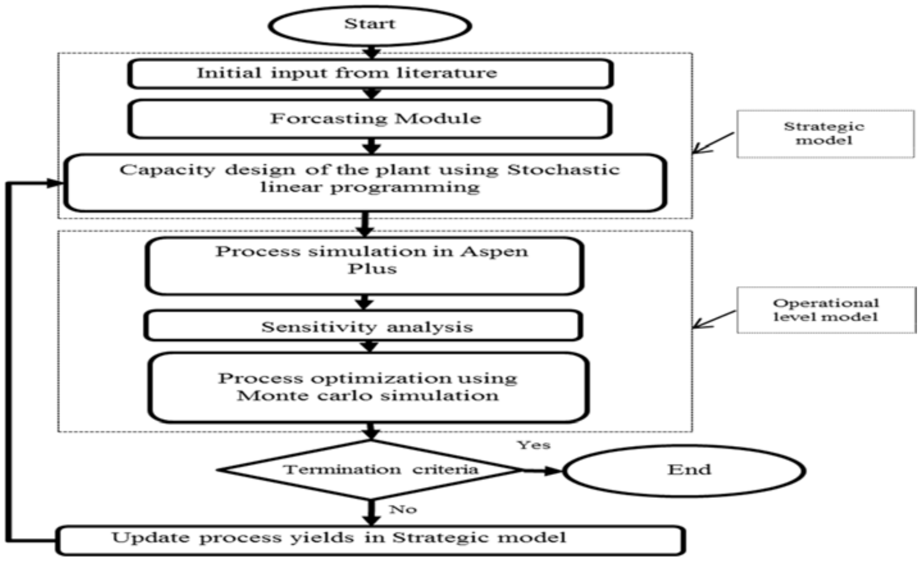

Figure 1: Framework for operational level optimization under uncertainty

3. Framework details

In this section each component of the proposed framework (Figure 1) is described in some detail. While the description of the framework is based on the design of the case study presented in Section 4, each component, and the framework, can readily be adapted to other energy value chains. Due to space limitations, all model equations used for optimization cannot be listed. A description of model constraints is provided for each layer of the proposed optimization model.

3.1 Strategic model

Strategic model is formulated as a mixed integer based linear program (MILP) with a 14-year planning horizon and bi-annual time steps. The mathematical formulation is broken into sub-models for ease of description which include a production model, financial model and risk management model. In the production model, all major process systems are represented as linear black boxes. Major equations include linearly approximated mass and energy balances for each node in the value chain. Production yields for each section of the plant are obtained from literature and used as inputs into the strategic planning model, and the expected net present value (objective function) of the biorefinery will be maximized by considering the optimization of production capacity (decision variable).

Financial model is broken into two salient aspects including market model and calculation of capital costs, operating expenses and revenues. In market model, price and demand evolution of bioproducts are described by considering that crude oil is represented as a stochastic input following Geometric Brownian Motion (GBM) and assuming that market of bioproducts are impacted primarily by the price of crude oil. Binomial lattice generation approach is utilized to discretize the continuous stochastic model of oil price yielding Markov chain decision tree. Each node in the decision tree is represented as a price scenario for crude oil (and consequently for bioproduct markets). Calculation of the price and the demand of products (ethanol and succinic acid) is derived from the hypothetical market model proposed by Sharma et al. (2013). Additionally, to reflect and control the variability of performances associated with each specific scenario, a risk metric based on the downside risk management approach is utilized.

3.2 Operational level model

Simulation of the technological configuration was carried out using Aspen Plus with the optimal capacity plan obtained from strategic optimization. By simulating the entire model in Aspen Plus, the implicit correlations between upstream and downstream stages of the process are taken into consideration. Additionally, complex kinetics of bio-reactions is incorporated in the simulation model based on the iterative dynamic data exchange between Aspen Plus and developed kinetic models in Matlab (Geraili et al., 2014b). Then, the Sobol global sensitivity method (Sobol, 2001), a variance–based Monte-Carlo technique, is used to test the sensitivity of the parameters. The global sensitivity analysis focuses on the pattern of change in model output due to change in model input parameters over a potential variation range of parameter value rather than a single parameter value. Once sensitivity measures have identified the significant sources of uncertainties in the process, a stochastic optimization algorithm based on Monte-Carlo simulation is used to find out the optimal operating conditions with the aim of maximizing the annual cash flow in the plant (objective function). Since the sampling is global rather than local thereby reducing the tendency to be entrapped in a local minimum and avoiding a dependency on an assumed set of initial conditions(Gallagher and Sambridge, 1994). The first step in the optimization is performed by sampling from operating conditions which is formed by a matrix of operating variables. Then a Monte-Carlo simulation is performed using sampling from the important uncertain parameters (identified in sensitivity analysis) space to estimate the uncertainty of model outputs used in the objective function calculation. The results from Monte-Carlo simulation are then evaluated based on statistical techniques (95% confidence interval) in order to identify the optimal operating scenario. Figure 2 represents the proposed strategy for the operational level optimization.

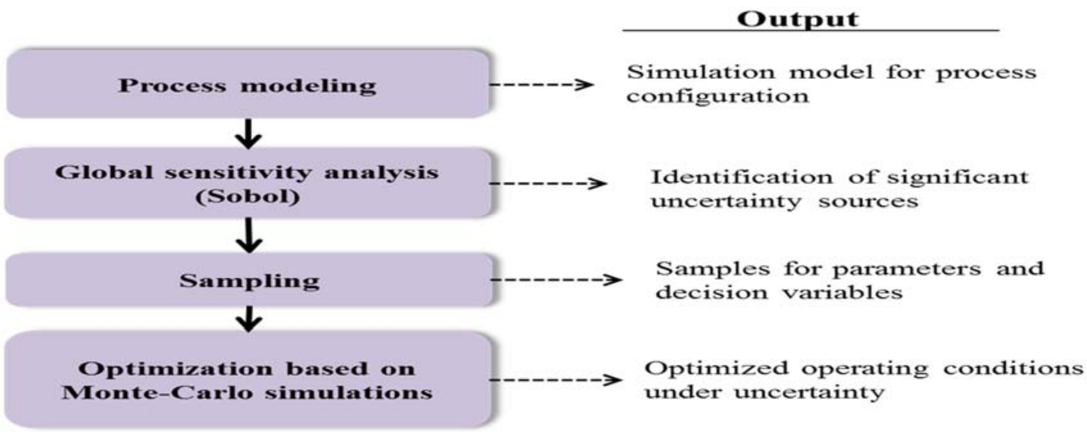

Figure 2: Operational level optimization strategy

4. Application case study: Lignocellulosic biorefinery

In order to demonstrate the utility of the proposed framework, the aforementioned decision support system is applied to a hypothetical biorefinery that utilizes lignocellulosic feedstock(s) to produce biobased fuels and chemicals. The lignocellulosic biorefinery used in this study is a multiproduct plant that uses a fermentation-based sugar conversion platform, with 3 products: cellulosic ethanol, biosuccinic acid, and bioelectricity. Switchgrass serves as the selected feedstock for the biorefining process. 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 Figure 3.

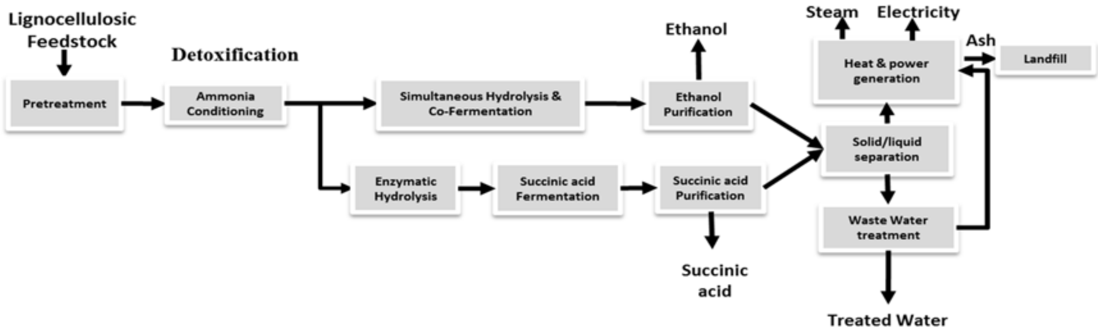

Figure 3. Block diagram for the multiproduct biorefinery plant

Technological configurations along with capital and operational cost, yield, and energy data for bioethanol production are obtained from Humbird et al. (2011) and Kazi et al. (2010). For succinic acid production, operational and economic data are obtained from Vlysidis et al. (2011); these are used as starting estimates to begin the iterative optimization process.

5. Results and discussion

In this section, the results for optimal strategic and operational level decisions of the multiproduct biorefinery are discussed. The decision variables considered in the framework are composed of the optimal capacity plan for long term production in biorefinery (strategic optimization), optimal temperature and enzyme amount for enzymatic hydrolysis (operational level optimization), and optimal allocation of pretreated biomass for production of final products (operational level optimization). The plant life time considered in this study is 14 y with an annual discount rate of 10%.
Results of the MILP model for the strategic optimization which is implemented in the modeling system GAMS and solved with a CPLEX linear solver are shown in Table 1. Two different cases are considered to illustrate the impact of the proposed risk management procedure. In stochastic case study, the variability in the market is taken into consideration by stochastic formulation based on scenario generation. The other case study (Risk managed case) is an extension of the stochastic model which incorporates financial risk through downside risk management strategy.As expected, the results from multi-objective optimization model reveal that there is a conflict between the two objectives, economic performance and financial risk. As shown in Table 1, a reduction of the downside risk can be attained in the expense of a reduction in the expected net present value (economic objective) of the process. Furthermore, results for these two cases show that minimization of downside risk leads to allocation of more sugar to succinic acid production and reduction in expected biomass processing capacity.

Table 1: Comparison of feedstock and production capacities before and after risk management

Scenario	Expected NPV ($MM)	Downside risk	Feedstock Capacity (1,000 t/y)	Sugar allocation ratio (for ethanol production)
Stochastic case	62.8	1 0%	218	0.62
Risk managed case	60.0	3 %	152	0.59

Kinetic parameters in simultaneous saccharification and co-fermentation of ethanol production, hydrolysis and fermentation of sugars for succinic acid production are considered as potential uncertainty sources in operational level model (technological risks) and Global sensitivity analysis is performed to assess the relative sensitivity of these model parameters. It is found that some parameters are rather insensitive. If the values of these insensitive parameters are fixed, a simplified model which reduces the complexity of the search space is obtained. Calculated sensitivity indices for model input parameters are shown in Figure 4. It is found that 20 of the kinetic parameters are significantly affecting the uncertainty on annual cash flow of the process. Due to space limitation, the description of the kinetic parameters is not provided here. A complete list of all the kinetic parameters and their description can be found in our previously published paper (Geraili et al., 2014a).

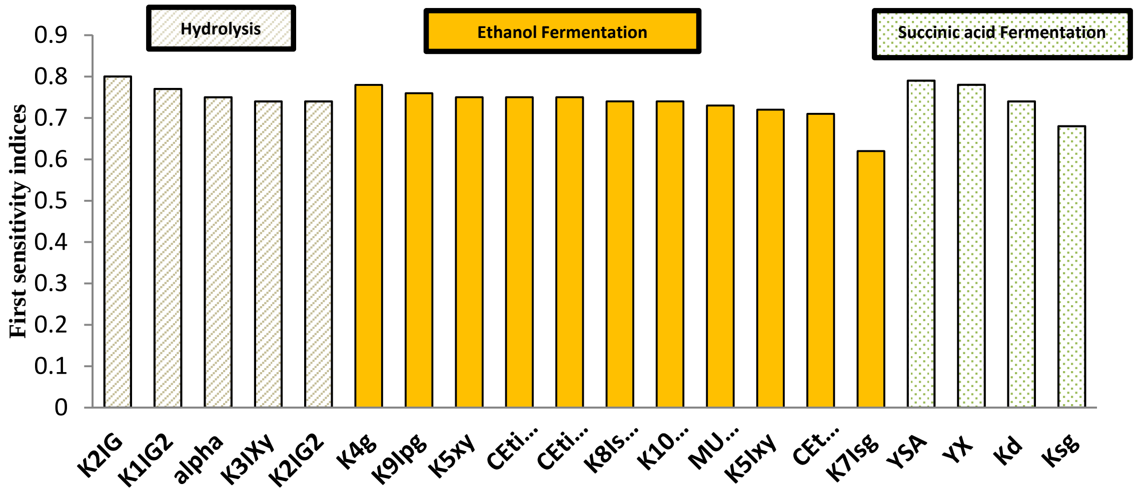

Figure 4. First order sensitivity indices of annual cash flow

Based on our previous studies, hydrolysis temperature, sugar allocation, and enzyme loading are selected as important operating variables to be optimized (Geraili et al., 2014b). Then a sample of selected operating variables and also a sample for the shortlist of uncertain parameters were created to perform a Monte Carlo stochastic optimization. Table 2 represents the results of scenarios from Monte Carlo simulation for the samples that had the best performance based on the mean value and 95% confidence interval of annual cash flow (objective function). Optimal values of the decision variables obtained from Monte Carlo stochastic optimization model are shown in Table 3.

Table 2. Monte Carlo simulation results for annual cash flow maximization

Scenario	Mean	95 % Confidence interval)	% saving (95% confidence interval)
Base case	8,700	120	--
Sample 14	9,570	83	30.8
Sample 47	9,153	104.3	13.1

Table 3. Base case and optimal operating conditions

Scenario	Hydrolysis Temperature (°C)	Sugar allocation (ethanol)	Enzyme loading ratio (g enzyme/ kg Cellulose)
Base case	33.45	0.44	25
Optimal	39.3	0.37	13.1

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 (for the scenario that includes financial risk management strategy) to calculate the production capacity plan (step 2); 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. Since 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.

Table 4: Iteration results in hybrid optimization strategy

Parameters and Variables		Iteration1			Iteration2	
		Step 1	Step 2	Step 3	Step 1	Step 2
Capacity Constraints	Feedstock (1,000 t/yr)	--	222.2	--	218.0	--
	Ethanol (MM gal/yr)	--	15.3	--	11.4	--
	Succinic Acid (1,000 t/y)	--	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

6. Conclusions

In this study a new hybrid optimization methodology to determine the optimal production capacity plan and operating conditions for an integrated multi-product biorefinery in the face of stochastic inputs and outputs was presented. The optimization problem was solved in a two-level approach, first stochastic linear model was developed to optimize production capacity for the desired planning horizon and then process simulation coupled with a stochastic optimization algorithm was employed to optimize the operating condition of the plant. Monte-Carlo based simulation and global sensitivity analysis were utilized to identify the most critical parameters and optimize the operating conditions of the plant. Incorporating metrics for mitigation of financial risk in the framework (strategic model) shows that there are two important factors that influence the performance of the model in the face of market uncertainty including production capacity and allocation of pretreated biomass between ethanol and succinic acid production. The global sensitivity analysis quantifies the uncertainty in the annual cash flow due to technological risks and the iterative results from hybrid optimization strategy reveal that there is a difference between calculated production yields and the ones which are suggested in literature. This is attributed to the nonlinear modeling and optimization strategies used in the optimization framework to impart a greater degree of realism to the actual representation of the biorefinery.

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