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Optimization of Renewable Energy Businesses under Operational Level Uncertainties through Extensive Sensitivity Analysis and Stochastic Global Optimization

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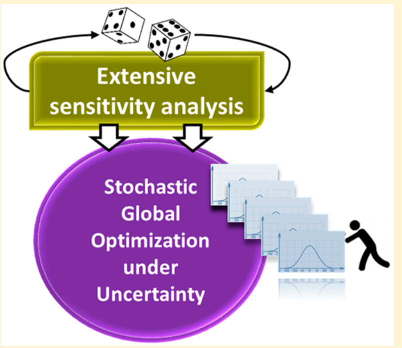
Supporting Information

ABSTRACT: This work presents a decision-making framework for stochastic optimization of renewable energy businesses considering technological uncertainties and risk management. With the help of a global sensitivity analysis based on Sobol's method, significant uncertain parameters from biochemical reactions are identified. Moreover, two options for selecting sensitive parameters are explored: (1) when all parameters are simultaneously evaluated, and (2) when parameters are separately evaluated based on their kinetic pathway. For both cases, the renewable energy facility is simulated considering uncertainty. To maximize the profitability of the business, a metaheuristic stochastic global optimization technique is incorporated to the framework. This method uses a radial basis function which approximates a computationally expensive objective function and permits intelligent selection of the best operating conditions. To evaluate the efficacy of this framework, a hypothetical multiproduct lignocellulosic biorefinery modeled under operational uncertainty is optimized.



1. INTRODUCTION

Propped by worldwide population and industry surge, it is estimated that global energy consumption will increase in the coming years. By 2040, the global energy consumption will grow in 56%, from 524 quadrillion of British thermal units (Btu) to 820 quadrillion Btu.[1] Around 85% of world's energy comes from fossil fuel sources. In the U.S., approximately 79% of energy comes from nonrenewables, making it the highest share of energy in the market.[2] Even though prices of fossil fuels have dropped to lower levels in the past two years, renewable energy sources still appear to be competitive and, in the long term, might have significant impact to global economy. Renewable energy costs are falling and show lower volatility than its competitors, making them attractive alternatives for decision-makers, investors, and governments.[3] The modern portfolio of available renewables includes second generation biofuels produced from biomass which is a sustainable solution for mobile energy services, giving also an innovative usage of organic waste. However, market volatility (e.g., in the second half of 2014 the price of WTI crude oil dropped from \$106/bbl to \$55/bbl in 6 months), technological uncertainty, and limited experience in renewable energy processes can prevent the development of this burgeoning industry.

By processing biomass in biochemical or thermochemical pathways, renewable energy facilities are able to produce fuels, value-added chemicals, heat, and bioelectricity. First and second generation biorefineries are already operating worldwide and are expected to stimulate economic growth while reducing mineral oil dependency.[4] Process systems engineering has contributed over the past few years in addressing the complexity of modeling and decision making in order to optimize and make cost-effective renewable energy projects. Usually, the optimization of renewable energy businesses considers a deterministic design approach[5−9] in which all model parameters are assumed to be known. However, during conceptual design there is lack of information and reliability especially in novel or recently developed processes.

Technical uncertainty is particularly high when a project is done for the first time. Biorefineries, in order to be competitive, require implementation of more efficient processes which can be relatively new due to the state of art of biorefining technology. Underestimating these limitations may lead into nonoptimal designs and generate extra expenses or difficulties during start-up and operation. Thus, for considering the unknown factors that exist in real life, to design and model including uncertainty is a powerful tool in optimization. Even though there are several parameters in renewable energy models that might introduce uncertainty, it is computationally expensive and unfeasible to include all of them when simulating uncertain conditions. Thus, a sensitivity analysis is required in order to reduce their quantity and select the significant ones to be incorporated. Global sensitivity analysis[10−12] is a widely used technique for selecting representative parameters from mathematical models. The identified sensitive parameters are later utilized for modeling the process under uncertainty.

A renewable energy business optimization problem can have several local optimal points because it is commonly of

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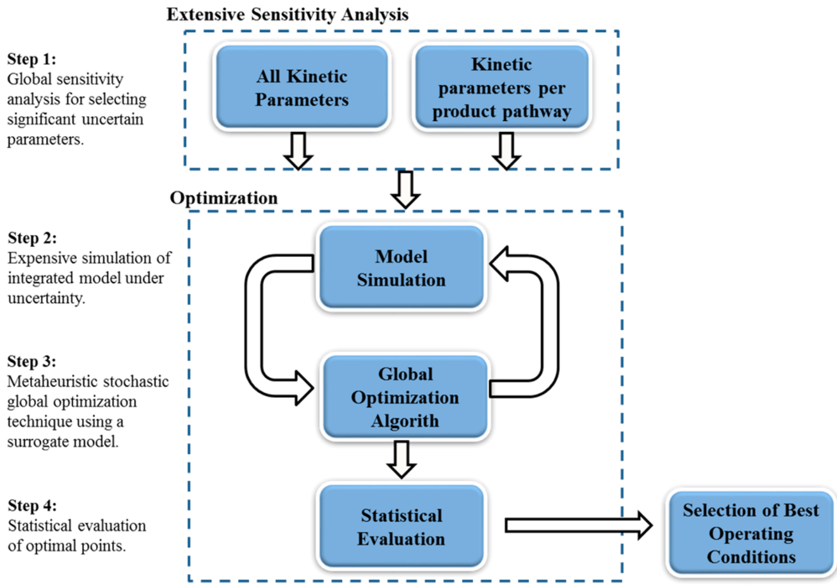

Figure 1. Framework for global optimization of a renewable energy businesses under uncertainty at operational level.

nonconvex nature. For optimization of renewable energy businesses, literature presents publications which studied optimization when uncertainties are introduced in price,[13] supply chain,[14] demand,[15] and at the operational level.[16,17] Usually, optimization strategies tend to reduce the complexity of the problem by simplifying it into a mixed integer linear programming (MILP) or using stochastic optimization strategies such as the Monte Carlo (MC) based optimization method. Even though these strategies can reach good solutions, they might leave better points unevaluated in the solution domain. Therefore, a more efficient and robust optimization method is required for improving results. Stochastic metaheuristic optimization strategies appear to be suitable for these types of optimization problems when its dimensionality is a few of tens. They treat the mathematical model as a black box which reduces computational effort while it is relatively easy to implement them. By using exploration and exploitation in the solution domain, better solutions, global optimum in some cases, are achievable.[18]

Surrogate models, also known as response surface or metamodels, can become approximations of detailed mechanistic models. They are incorporated into metaheuristic optimization strategies and are capable of simplifying highly nonlinear and computationally expensive problems. They are widely utilized in multiobjective optimization.[19] Surrogate modeling has applications in diverse fields of engineering.[20] Some relevant studies present their applicability in analysis and modeling of groundwater systems considering uncertainties,[21−24] optimization in groundwater bioremediation,[25−28] and uncertainty estimation in aviation environmental systems.[29] This type of metaheuristic optimization strategy has not been tested yet for renewable energy processes modeled under uncertain conditions. Therefore, this work aims to study their applicability, efficiency, and effectiveness in these processes.

In previous publications, a systematic optimization methodology for biorefining processes under both strategic and operational level uncertainties was developed.[16,30] The proposed framework is a continuation of this work and studies a new approach for selecting sensitive parameters to simulate uncertainty while implementing a stochastic global optimization algorithm that uses surrogate modeling to optimize operating conditions. By using this optimization strategy, we aim to overcome limitations found in MC based simulation because operating points are intelligently searched rather than randomly explored in the solution domain. For global sensitivity analysis, the previously implemented efficient computational method developed and tested by Wu et al.[12] is employed again with a variation. In this work, the sensitivity analysis is performed by considering two different approaches: to evaluate all parameters simultaneously and to evaluate them separately depending on their product pathway. The second approach intends to select sensitive parameters from each section of the integrated facility rather than evaluate them simultaneously. Once the two groups of sensitive parameters are identified, a metaheuristic stochastic global optimization technique[28] maximizes the profitability of a renewable energy business while considering uncertainty and risk management. The algorithm employs radial basis functions (RBFs) as the response surface or surrogate model. Finally, the optimal points obtained are contrasted with optimal values from other optimization methodologies, e.g., MC based optimization. To evaluate the efficiency of the proposed optimization framework, a hypothetical multiproduct lignocellulosic biorefinery is globally optimized at operational level.

2. MODEL-BASED FRAMEWORK FOR OPTIMIZATION UNDER UNCERTAINTY

2.1. Framework Design. The proposed framework in this paper considers the optimization of renewable energy businesses under uncertainty and it can be adapted to different production portfolios. One relevant characteristic achieved in this study are the two different approaches for selecting significant uncertain parameters while employing a metaheuristic optimization technique that uses a surrogate model. For optimizing the operating conditions of a renewable energy business under technological uncertainties four steps are required: (1) identification of significant uncertain parameters through global sensitivity analysis (simultaneously and separately per product pathway), (2) mechanistic simulation of the process introducing uncertainty, (3) optimization of relevant operating conditions of a renewable energy plant by seeking optimal points using a metaheuristic method which uses a surrogate model, and

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(4) statistical evaluation of results. Figure 1 shows a general schematic of the proposed framework.

2.2. Sensitivity Analysis. Uncertainties can be found in different sections of a renewable energy business, from volatility in the market to the process itself. The most common uncertainties that have been studied in renewable energy endeavors come from the strategic planning stage. At the operational level, uncertainties can be found in the process model, and a global sensitivity analysis is required for choosing the most significant parameters for simulating uncertain conditions. Operational level uncertainties may be introduced into the process mainly because of errors in experimental measurements, activity changes in microorganisms involved in chemical reactions, impurities in chemical species, and external factors such as weather or environmental conditions.

A sensitivity analysis is in general the study of how the uncertainty manifested in the output of a mathematical model can be distributed to different sources such as parameters or state variables.[31] A robust variance-based sensitivity analysis technique was developed by I. M. Sobol'.[10] The method considers on its standard form a function $Y = f(z_1, ..., z_q, ..., z_Q)$ whose input parameters are mutually independent, and it is defined as a *Q-dimensional* cube, K^Q, which deems the expansion of Y into terms of increasing dimensions such that all summands are mutually orthogonal. The function can be represented in the form of eq 1.

$$Y = f_0 + \sum_{Q}^{q=1} f_q(z_q) + \sum_{1\le q<b\le Q} f_{qb}(z_q, z_b) + \cdots + f_{1,2,\cdots,Q}(z_1, ..., z_Q) \quad (1)$$

The index q denotes an individual parameter of interest, b another parameter, and Q the total quantity of parameters evaluated. Each term in eq 1 is also square integrable over the domain of existence and are function of the values on their index; where f_0 is constant, $f_q = f_q(z_q)$, $f_{qb} = f_{qb}(z_q, z_b)$, and so on. Therefore, the variance of Y can be decomposed as presented in eq 2.

$$V(Y) = \sum_{Q}^{q=1} V_q + \sum_{1\le q<b\le Q} V_{qb} + ... + V_{1,...,q,...,Q} \quad (2)$$

where V_q, V_{qb}, $V_{1,...,q,...,Q}$ represent the individual variances of terms f_q, f_{qb}, $f_{1,...,q...,Q}$, respectively. The first-order sensitivity index, $\hat{S}_q$, permits selection and ranking of the most sensitive parameters depending on the individual importance of their contribution in changing the variance of the evaluated function. The main effect of varying parameter z_q on the output value Y is measured by $\hat{S}_q$ as presented in eq 3.

$$\hat{S}_q = \frac{\hat{V}_q}{\hat{V}} \quad (3)$$

The total sensitivity index, $\hat{S}_{Tq}$, incorporates the sum of all the effects that involve parameter z_q, where $\hat{V}_{-q}$ represents the sum of all variance terms which do not include z_q. The total sensitivity index for parameter z_q is computed as presented in eq 4.

$$\hat{S}_{Tq} = 1 - \frac{\hat{V}_{-q}}{\hat{V}} \quad (4)$$

An improvement of Sobol's standard method reduces the required computational effort by introducing sampling and resampling matrices.[11,32] Following this criteria further, Wu et al.[12] developed and tested an efficient computational method for global sensitivity analysis. This method reduces even more computational effort by averaging the results of the evaluated functions and using those results as data points. $\hat{S}_q$ and $\hat{S}_{Tq}$ can be compared to evaluate if the model is additive or not. For nonadditive models, $\hat{S}_q < \hat{S}_{Tq}$ and additive, $\hat{S}_q = \hat{S}_{Tq}$. A model is considered additive when there are no interactions present.[33]

When evaluating the sensitivity of parameters toward an output, literature presents that most of the time in renewable energy facilities[16,17] and other technical problems, e.g., heat exchanger design,[34,35] all parameters are evaluated simultaneously. Also, there are cases when parameters are evaluated in different process units, but the grouping criterion is driven by different outputs.[33] The current study has the characteristic of analyzing extensively the sensitivity of parameters by evaluating them in two different ways. The first approach evaluates the sensitivity of all uncertain parameters simultaneously. The second approach evaluates the sensitivity of parameters in separate groups which are conformed depending on their product pathway. This procedure aims to incorporate uncertainty by considering that process units are independent from each other.

This work follows the next steps in global sensitivity analysis:

(1) Define the dimension, N, for a sample of input parameters. For each parameter, define an uncertainty class. Class 1 corresponds to 5% of change, and class 2 corresponds to 20% of change with respect to the parameter default value.

(2) Build two random matrices, $\mathbf{M_1}$ and $\mathbf{M_2}$, of dimension $N \times Q$ based on the uncertainty class criterion previously defined. $\mathbf{M_1}$ is the sampling matrix, $\mathbf{M_2}$ resampling matrix, and Q the total quantity of parameters to be evaluated.

$$\mathbf{M_1} = \begin{bmatrix} z_{11}\cdots & z_{1q}\cdots & z_{1Q} \\ \vdots & \vdots & \vdots \\ z_{N1}\cdots & z_{Nq}\cdots & z_{NQ} \end{bmatrix} \quad \mathbf{M_2} = \begin{bmatrix} z'_{11}\cdots & z'_{1q}\cdots & z'_{1Q} \\ \vdots & \vdots & \vdots \\ z'_{N1}\cdots & z'_{Nq}\cdots & z'_{NQ} \end{bmatrix}$$

(3) Generate a matrix $\mathbf{N_q}$ formed by all columns of matrix $\mathbf{M_2}$, except the column of the z_q parameter, which is pulled from $\mathbf{M_1}$. Consecutively, generate another matrix $\mathbf{N_{Tq}}$ formed with all columns of $\mathbf{M_1}$ and with the column of the z'_q parameter, pulled from $\mathbf{M_2}$.

$$\mathbf{N_q} = \begin{bmatrix} z'_{11}\cdots & z_{1q}\cdots & z'_{1Q} \\ \vdots & \vdots & \vdots \\ z'_{N1}\cdots & z_{Nq}\cdots & z'_{NQ} \end{bmatrix} \quad \mathbf{N_{Tq}} = \begin{bmatrix} z_{11}\cdots & z'_{1q}\cdots & z_{1Q} \\ \vdots & \vdots & \vdots \\ z_{N1}\cdots & z'_{Nq}\cdots & z_{NQ} \end{bmatrix}$$

(4) Evaluate the row vectors of matrices $\mathbf{M_1}$, $\mathbf{M_2}$, $\mathbf{N_q}$, and $\mathbf{N_{Tq}}$ with function Y while decision variables are kept constant; $\mathbf{y}$ represents the output vector of the sampling matrix, $\mathbf{y_R}$ the output vector of the resampling matrix, $\mathbf{y'}_q$ the output vector of matrix $\mathbf{N_q}$, and $\mathbf{y'_{R_q}}$ the output vector of matrix $\mathbf{N_{Tq}}$. For the current study function, Y is later defined in eq 17. The values of the function are obtained in column vectors as illustrated:

$$\mathbf{y} = f(M_1),\ \ \mathbf{y_R} = f(M_2),\ \ \mathbf{y'}_\mathbf{q} = f(N_q),\ \ \mathbf{y'}_\mathbf{Rq} = f(N_{Tq})$$

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(5) By using MC methods, a given sample is capable to generate the following estimates, which are calculated based on scalar products of the vectors above.

$$\hat{f}_0 = \frac{1}{2N} \sum_{n=1}^{N} (\mathbf{y} + \mathbf{y_R}) \tag{5}$$

$$\gamma_q^{\ 2} = \frac{1}{2N} \sum_{n=1}^{N} (\mathbf{y} \cdot \mathbf{y_R} + \mathbf{y}'_q \cdot \mathbf{y}'_{Rq}) \tag{6}$$

$$\hat{V} = \frac{1}{2N} \sum_{n=1}^{N} (\mathbf{y}^2 + \mathbf{y_R}^2) - \hat{f}_0^{\ 2} \tag{7}$$

$$\hat{V}_q = \frac{1}{2N} \sum_{n=1}^{N} (\mathbf{y} \cdot \mathbf{y}'_{Rq} + \mathbf{y_R} \cdot \mathbf{y}'_q) - \gamma_q^{\ 2} \tag{8}$$

$$\hat{V}_{-q} = \frac{1}{2N} \sum_{n=1}^{N} (\mathbf{y} \cdot \mathbf{y}'_q + \mathbf{y_R} \cdot \mathbf{y}'_{Rq}) - \gamma_q^{\ 2} \tag{9}$$

where $\hat{f}_0$ represents the mean value of the outputs obtained with sampling and resampling matrices, and $\gamma_q^{\ 2}$ the squared mean value of the outputs for each parameter z_q. By averaging, the systematic error is compensated as explained by Homma and Saltelli.[32]

(6) The most sensitive parameters are selected based on first and total sensitivity indices. For calculating sensitivity indices from all parameters simultaneously, the method runs once. For calculating sensitivity indices separately depending on their product pathway, the method runs as many times as products of interest are produced by the renewable energy facility.

2.3. Objective Function under Uncertainty and Risk Management. The proposed framework requires a robust definition of the problem for minimizing technological risk while including uncertainty at operational level. Integrated risk management solves the task of maximizing the profitability while solving risk management together.[36] Following this approach, a generic mathematical expression of the optimization problem can be written as presented in eq 10.

$$\max Z(x) = c^T x + E[f(x, \Theta_{ih})] + z_c \cdot \sigma(x, \Theta_{ih}) \tag{10}$$

Constrained to

$$\gamma(x) = 0 \tag{11}$$

$$\eta(x) \le d_i \tag{12}$$

$$\Theta_i^{\mathrm{LB}} \le \Theta_i \le \Theta_i^{\mathrm{UB}} \tag{13}$$

$$x^{\mathrm{LB}} \le x \le x^{\mathrm{UB}} \tag{14}$$

Subscript i represents a sample generated of an h significant parameter considered as source of uncertainty in the mechanistic model. The objective function including uncertainty and risk management has a deterministic term $c^T x$, where c^T represents a constant vector and x a decision variables vector. Uncertainties are taken into account in the terms $E\ [f\ (x,\ \Theta_{ih})]$ and $z_c \cdot \sigma(x, \Theta_{ih})$. The first term represents the expected value that contributes uncertainty as a function of decision variables, x, and uncertain parameters' matrix, Θ_{ih}. The second term includes risk, in which z_c is the critical value with a corresponding level of significance, and $\sigma(x, \Theta_{ih})$ is the standard deviation which depends on decision variables, x, and uncertain parameters' matrix, Θ_{ih}. For limiting the objective function, vectors $\gamma(x)$ and $\eta(x)$ are written as the equality and inequality constraints, respectively. Finally, the decision variables vector x is constrained to a lower and upper bound.

For simplicity, the distribution of the results is assumed to be normal. Therefore, for minimizing the probability of attaining undesired results, the proposed framework considers a 5% of significance in a two-tail distribution. In other words, the 2.5th percentile is optimized, which means that z_c will be −1.96 for the case study. The best result is the one whose 2.5th percentile presents the highest value as illustrated in Figure 2. This definition permits the optimization algorithm to select the best scenario without requiring to compare variances or mean values because they are already included in the generic expression as presented in eq 10.

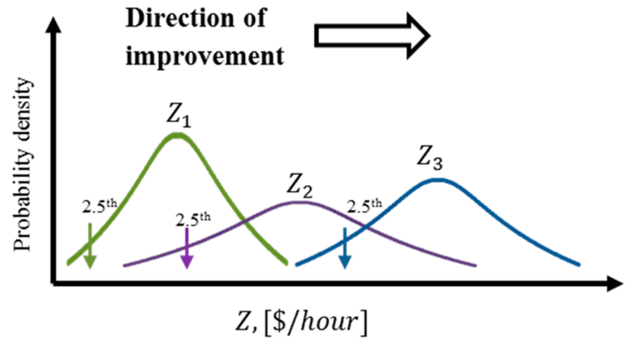

Figure 2. Technological risk management and level optimization criteria at operational level.

2.4. Metaheuristic Stochastic Global Optimization. The optimization strategies that take advantage of surrogate models are classified in three main groups. The first strategy, the traditional sequential approach, requires a relatively large number of sample points. The surrogate model is optimized once fitted. The second approach uses a validation or optimization loop which decides resampling or remodelling if determined conditions are not met or improvement is needed. The third strategy attains optimal point by generating guided adaptive sampling points or a smart search in the solution domain.[37] To optimize a renewable energy facility modeled under uncertainty, a strategy based on the third classification is selected.

The Parallel Local Metric Stochastic Radial Basis Function with Restart (*ParLMSRBF-R*) algorithm developed and tested by Regis and Shoemaker[26,28] seeks global maxima by guiding the search of optimal points in the solution domain until stop criterion is met. To avoid being trapped in local optima, the algorithm restarts from scratch when no improvement is attested, which permits a better exploration of the solution domain. Moreover, multiple points are generated for simultaneous evaluations, and a RBF interpolation is used as response surface or surrogate model. In each iteration, RBF's parameters are updated with the output of a point or group of points tested in the previous evaluation.

2.4.1. Radial Basis Function. From Powell's work,[38] fitting of the model starts with J different input points, $x_1, x_2, ..., x_j, ...,$ $x \in \mathbb{R}^d$, where their function values are known, $f(x_1), ..., f(x_j), ..., f(x_J)$. The interpolation can be written in the general form of eq 15.

$$s(x) = \sum_{=1J}^{j} \lambda_j \gamma(\| x - x_j \|) + p(x), \mathbb{R}^d \tag{15}$$

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where, $\|\cdot\|$ is the Euclidean norm, $\lambda_j \in \mathbb{R}$ for $j = 1, ..., J$. In this work, the RBF uses a linear polynomial tail, $p(x)$ and has cubic form, $\gamma(r) = r^3$. Other forms of tails and $\gamma(r)$ such as, linear, thin plate spline, Gaussian, multiquadric, and inverse multiquadric are available also. A matrix $\Gamma \in \mathbb{R}^{J\times J}$ by $\Gamma_{jk} := \gamma(\|x_j - x_k\|)$, $j, k = 1, ..., J$ is denoted. Simultaneously, a matrix $P \in \mathbb{R}^{J\times(d+1)}$ is defined, and its jth row is represented as $[1, x_j^T]$. eq 16 presents the system that needs to be solved for obtaining a fitted cubic RBF.

$$\begin{pmatrix} \Gamma & P \\ P^T & 0 \end{pmatrix}\begin{pmatrix} \lambda \\ c \end{pmatrix} = \begin{pmatrix} F \\ 0_{(d+1)} \end{pmatrix} \tag{16}$$

where $F = (f(x_1), ..., f(x_J))^T$, $\lambda = (\lambda_1, ..., \lambda_J) \in \mathbb{R}^J$, and $c = (c_1, ..., c_{d+1}) \in \mathbb{R}^{d+1}$ represent the coefficients of the linear polynomial tail, $p(x)$. Notice that the coefficient matrix is invertible only if rank$(P) = d + 1$.[26,38] Therefore, condition $n \geq d + 1$ is mandatory, where n is a set of evaluated points.

2.4.2. ParLMSRBF-R Algorithm. The algorithm runs following a master-worker criterion. It assumes that P processors are available and two function evaluations consume the same amount of time. The objective function is evaluated with a set of initial points that are generated from a space filling experimental design. These points are decision variables constrained as presented in eq 14. The RBF is fitted initially and updated in each iteration with every new output obtained. The expensive function is evaluated in P points which are obtained from a group of candidate points. Thus, P workers plus the master task ($P + 1$) are running. For starting the algorithm, the objective function is defined as a closed hypercube $\boldsymbol{D} = [a, b] \subseteq \mathbb{R}^d$; a number of processors, P, fixed; a set of initial evaluation points, $\boldsymbol{J} = \{x_1, x_2, ..., x_{n_o}\}$, generated ($n_o = k \cdot P$, where k is a positive integer); a number of candidate points per iteration, t, set ($t \gg P$), and a maximum number of objective function evaluations, N_{max}, defined. When N_{max} simulations are completed, the algorithm stops. From a set of n points, the outputs, $\boldsymbol{A}_n = \{x_1, x_2, ..., x_n\}$, are the values that the algorithm maximize.[28] Figure 3 represents how *ParLMSRBF-R* algorithm works.

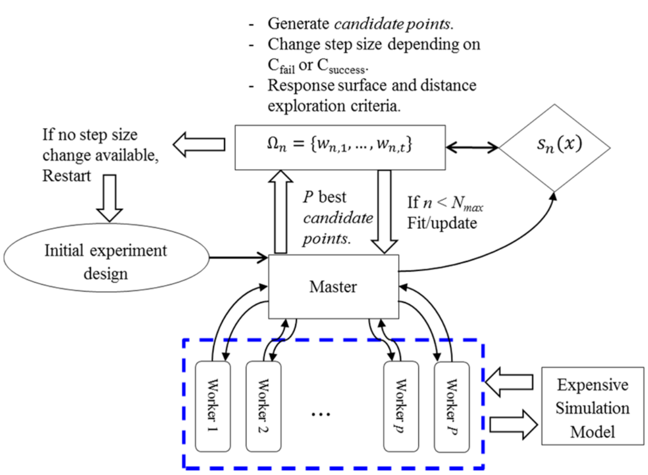

Figure 3. *ParLMSRBF-R* algorithm scheme.

ParLMSRBF-R achieves exploitation by keeping track of the consecutive failed and successful iterations. It is denoted as C_{fail} and $C_{success}$, respectively. Whenever $\boldsymbol{C}_{fail}$ or $\boldsymbol{C}_{success}$ exceed a predefined tolerance value, $\boldsymbol{T}_{fail}$ or $\boldsymbol{T}_{success}$, the step size is reduced by half or doubled, respectively. Then, the recorded values of $\boldsymbol{C}_{fail}$ and $\boldsymbol{C}_{success}$ are reset to zero. When the algorithm exceeds a maximum imposed limit of failed synchronous parallel iterations, $\boldsymbol{M}_{fail}$, local minima is inferred and it restarts from scratch. In other words, the algorithm restarts for avoiding the bias from previously evaluated points. Global optima is searched in the current best decision variable's neighborhood. The next point(s) to be evaluated are selected following two scored criteria: (1) the estimated value generated by the response surface model (response surface criterion), and (2) the minimum distance from the previously evaluated points (distance criterion). A good candidate point should be far from the previously evaluated point, and its estimated function value, obtained from the fitted RBF, should be as close as possible to the actual value.[26,28] Table 1 presents the parameters employed in stochastic optimization.

Table 1. Parameter Values for *ParLMSRBF-R*

parameter	value
Ω_n, number of candidate points for each parallel iteration	500 d
$\boldsymbol{Y}$, weight pattern	$\langle 0.3, 0.5, 0.8, 0.95\rangle$
κ, number of weights in $\boldsymbol{Y}$	4
σ_n, initial step size	$0.2l(\boldsymbol{D})$
σ_{min}, minimum step size	$(0.1)\left(\frac{1}{2}\right)^6 l(\boldsymbol{D})$
δ_{tol}, radius tolerance	$0.001l(\boldsymbol{D})$
$\boldsymbol{T}_{success}$, threshold parameter for deciding when to increase the step size	3
$\boldsymbol{T}_{fail}$, tolerance parameter for deciding when to reduce the step size	$\max\left(\left\lceil \frac{d}{P}\right\rceil, \left\lceil \frac{|\kappa|}{P}\right\rceil\right)$
$\boldsymbol{M}_{fail}$, maximum failure tolerance parameter	$5\boldsymbol{T}_{faiul}$

3. APPLICATION CASE STUDY OF RENEWABLE ENERGY BUSINESS: MULTIPRODUCT LIGNOCELLULOSIC BIOREFINERY

The proposed framework is tested with a hypothetical multiproduct biorefinery that considers uncertainty at operational level. A lignocellulosic biorefinery is integrally modeled in the simulation software Aspen Plus in order to guarantee rigorousness in the process simulation while representing complex nonlinear processes and unit operations. The biorefinery model is linked with a complex kinetic model of bioreactions previously implemented in Matlab. Biokinetic parameters vary between a lower and upper bound[16] for simulating uncertainty as presented in the Supporting Information, Table S2.

3.1. Process and Profitability Calculation Description.

The main desired products are biofuels and value-added chemicals. Even though other feedstocks can be used as lignocellulosic material, the simulation assumes a sample feedstock whose composition is similar to switchgrass. The conversion pathway used is sugar platform with two main products: bioethanol and succinic acid. Secondary products such as, heat, bioelectricity and treated water are obtained as well.

The selected scheme is composed of six major treating units; including, raw material pretreatment, sugar hydrolysis, sugar fermentation, product purification, heat and power generation, and wastewater treatment. The optimal configuration utilized in the current work comes from a previous work (Geraili et al., 2014) that tested different process arrangements, and selected the optimum. Figure 4 shows the process flow diagram of the

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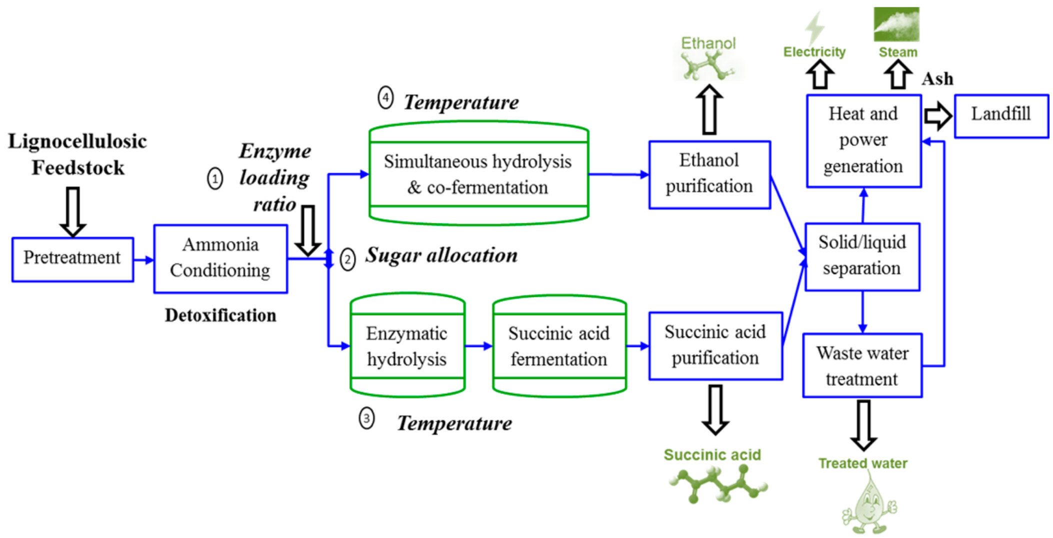

Figure 4. Multiproduct biorefinery flow diagram plant and process variables to be optimized under uncertainty.

integrated multiproduct biorefinery. The subprocesses are as written:

(1) Low concentration acid pretreatment for breaking the structures of the feedstock material into smaller pieces of hemicellulose, lignin, and cellulose while increasing the fragmentation of cellulose;
(2) Ammonia conditioning for detoxification and pH stabilization of pretreated biomass;
(3) Simultaneous enzymatic hydrolysis and cofermentation for bioethanol production (EHCF);
(4) Separate hydrolysis (SAEH) and cofermentation (SACF) for succinic acid production;
(5) Bioethanol purification with distillation columns and molecular filtration;
(6) Solid separation for extracting residual solids;
(7) Succinic acid recovery using a configuration based on cell filtration followed by crystallization;
(8) Anaerobic and aerobic digestion of organic materials contained in the produced wastewater from biorefining processes, and
(9) Combined system of combustion, boiler, and turbo-generator for steam and electricity production.

The operational variables that have significant impact in the profitability of the biorefinery were identified in a previous publication.[5] These operational and decision variables are (1) enzyme loading ratio, (2) sugar allocation, and (3) temperature of enzymatic hydrolysis in succinic acid production. Because temperature turns out to be an important operational variable (4) temperature of simultaneous enzymatic hydrolysis and cofermentation for bioethanol production is included as a new decision making variable to be optimized in this work.

Information related to succinic acid production, including operational and economic data, was obtained from Vlysidis et al.[39] Operational expenditures, product yields, and energy information for bioethanol production was obtained from a publication about technical and economic studies for production of cellulosic bioethanol.[40,41] Finally, the biochemical reactions' models implemented in Matlab for rigorous simulation of bioethanol and succinic acid production were obtained from literature.[17,42,43] These data from literature are utilized as starting points and reference estimates during sensitivity analysis and stochastic optimization.

The function which is used in global sensitivity analysis as presented in eq 1 and in the optimization problem propound in eq 10 is the cash flow of the multiproduct biorefinery as presented in eq 17. The cash flow is written similarly as defined by Geraili et al.[5] It considers sale of products, cost of raw materials, and fixed costs.

$$Y = f(x) = \mathrm{CF} = \sum_{p} P_p \times \mathrm{price}_p - \sum_{r,p} \mathrm{RM}_{r,p} \times \mathrm{cost}_r - \mathrm{FC} \tag{17}$$

The cash flow, CF, considers P_p production of products including bioethanol, succinic acid, and excess bioelectricity. $\mathrm{RM}_{r,p}$ is the quantity of raw material type r employed in producing p, and FC fixed costs. For the current study, CF is set in $\left[\frac{\mathrm{USD}}{h}\right]$.

3.2. Process Modeling. The process is modeled and simulated with high resolution of the mechanistic model under uncertainty. The overall renewable energy facility is simulated in the software Aspen Plus, and it is linked with the numerical computing software Matlab where biokinetic reactions for obtaining biofuels and value-added chemicals are modeled. ActiveX Automation technology permits Aspen Plus to transfer data from and to other Windows applications. In this particular case, it links Aspen Plus with Matlab. Figure 5 shows a representation of the input data required, output generated, and interaction between the two software packages.

The simulation model generates an uncertain parameter' matrix, $\mathbf{\Theta}_{ih}$. This matrix contains h sensitive uncertain parameters in each row. With the help of a sampling technique, e.g., Latin hypercube sampling, i parameter groups are generated between a lower and upper bound. The dimensions of the resulting matrix are $D \times H$, where D is the sampling size and H is the quantity of selected sensitive parameters. For a certain set of F decision variables, D stochastic evaluations of the objective function are performed. The obtained results are assumed to have normal distribution.

4. RESULTS AND DISCUSSION

4.1. Sensitivity Analysis: Simultaneous Evaluation of Parameters. When all 86 kinetic parameters are evaluated simultaneously through global sensitivity analysis, sensitivity

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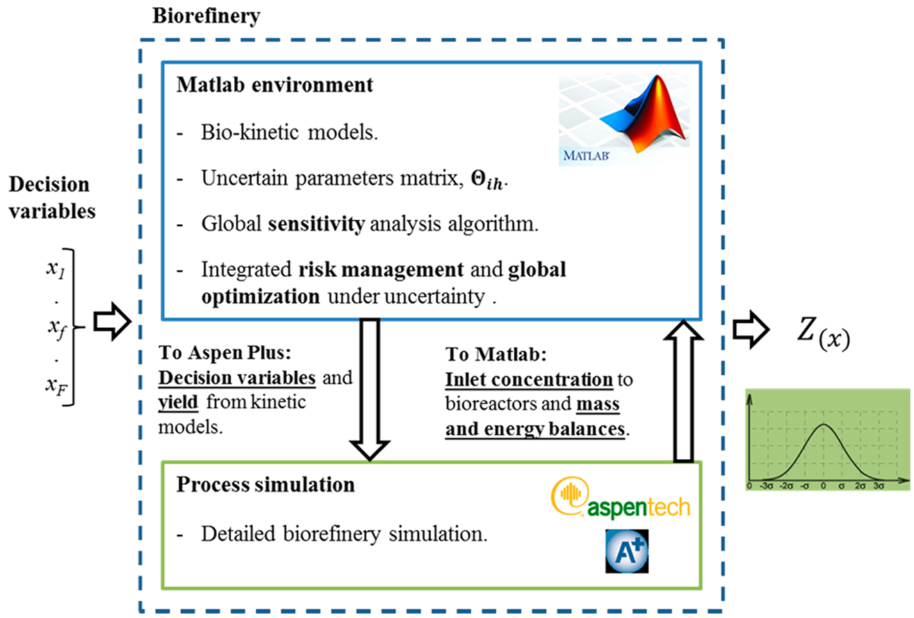

Figure 5. Matlab and Aspen Plus interaction for modeling renewable energy business under uncertainty.

indices show that 18 parameters are sensitive for the biorefinery' cash flow after tax. Results show that most of the sensitive parameters are involved in succinic acid production. This result is expected when all parameters are evaluated simultaneously because succinic acid has a higher price in the market and its separation cost is more expensive than bioethanol separation cost. Global sensitivity analysis illustrates that succinic acid production has a dominant role in the optimization problem because succinic acid's kinetic parameters appear to be more important in the profitability of the biorefinery. Moreover, comparing $\hat{S}_q$ and $\hat{S}_{Tq}$ reveal that the model presents nonadditive properties and has high interactions between parameters because $\hat{S}_q < \hat{S}_{Tq}$. First-order and total sensitivity indices of relevant parameters are presented in Figures 6 and 7, respectively.

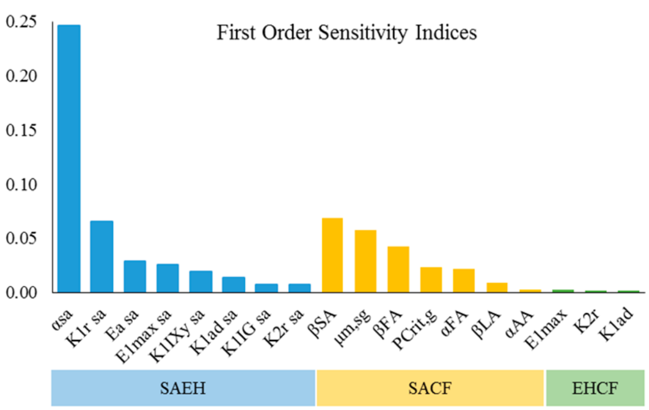

Figure 6. First-order sensitivity indices for cash flow (simultaneously evaluated).

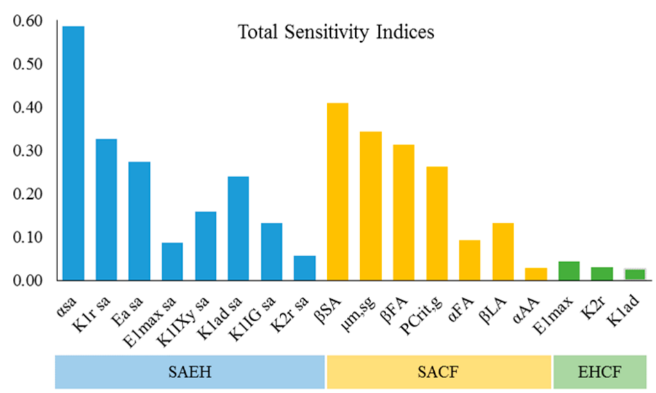

Figure 7. Total sensitivity indices for cash flow (simultaneously evaluated).

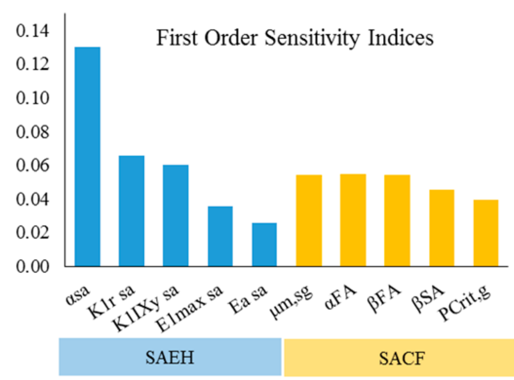

Figure 8. First-order sensitivity indices for cash flow after tax (succinic acid).

Sensitive parameters show that in the enzymatic hydrolysis of sugars for succinic acid production (SAEH), the conversion rate of cellulose to cellobiose is an important step in the reaction mechanism and a bottleneck in the pathway of reaction. Also, high sensitivity in α_{sa}, $K_{1\mathrm{r\ sa}}$, $E_{\mathrm{a\ sa}}$, and $E_{1\ \mathrm{max\ sa}}$ evidence the competition in glucose consumption between formic acid and succinic acid generation. Thus, proper operating conditions should minimize glucose conversion to formic acid while increasing succinic acid production. In simultaneous hydrolysis and cofermentation for bioethanol production (EHCF), only three parameters from enzymatic hydrolysis appear to be sensitive.

4.2. Sensitivity Analysis: Evaluation Per Product Pathway. Parameters evaluated separately per product pathway consider that each section of the biorefinery is autonomous

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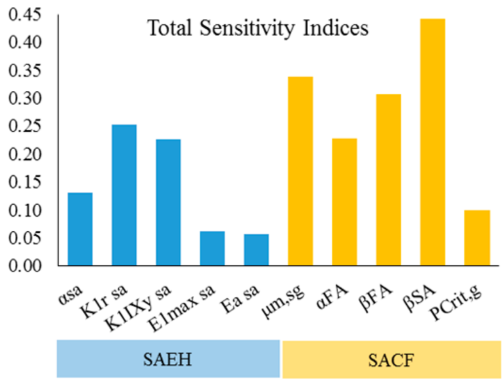

Figure 9. Total sensitivity indices for cash flow after tax (succinic acid).

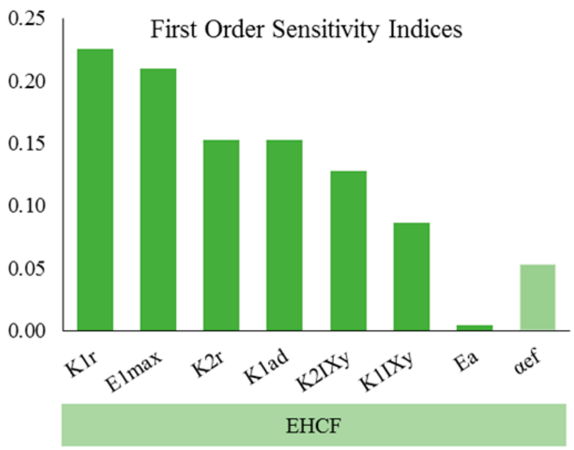

Figure 10. First-order sensitivity indices for cash flow after tax (bioethanol).

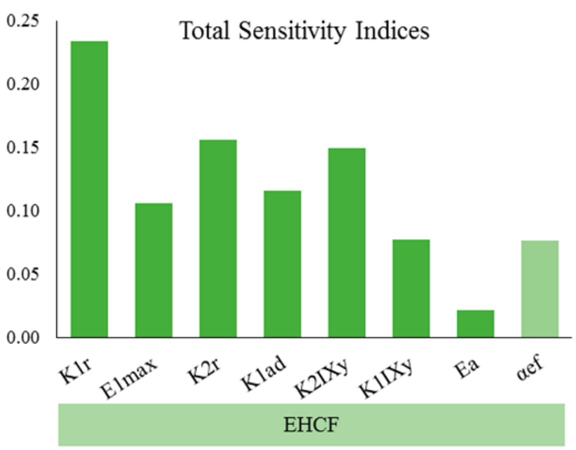

Figure 11. Total sensitivity indices for cash flow after tax (bioethanol).

Table 2. Inputs Definition for Stochastic Global Optimization with *ParLMSRBF-R*

evaluation	new samples, P
eval 1	1
eval 2	2
eval 3	4

and its uncertainty requires to be evaluated independently. This novel approach allows to perform sensitivity analyses in facilities that process two or more types of biofuels or value-added chemicals without requiring to modify the model

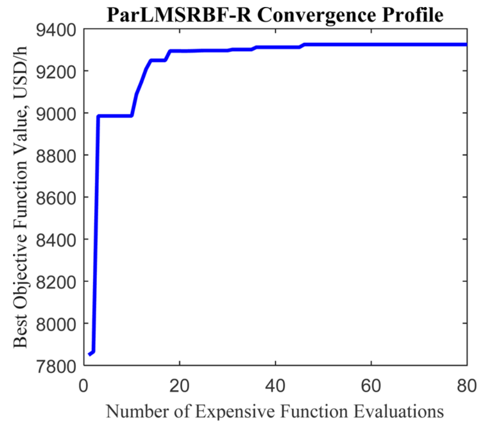

Figure 12. Convergence profile UC1 eval 1, *ParLMSRBF-R*. Uncertainty simultaneously calculated.

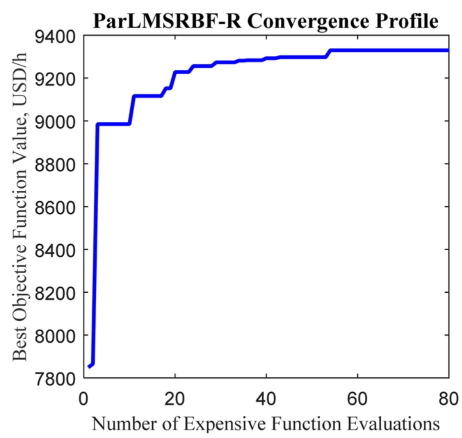

Figure 13. Convergence profile UC1 eval 2, *ParLMSRBF-R*. Uncertainty simultaneously calculated.

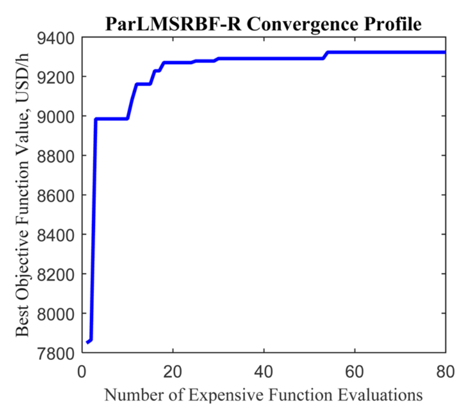

Figure 14. Convergence profile UC1 eval 3, *ParLMSRBF-R*. Uncertainty simultaneously calculated.

simulation or include additional objective functions. In the following sensitivity analyses, 37 parameters from the kinetic model for succinic acid production are evaluated first. Later, 49 parameters for bioethanol production are evaluated.

4.2.1. Succinic Acid. From 37 parameters conforming the kinetic model for succinic acid production, 10 parameters are selected as significant sources of uncertainty. $\hat{S}_q$ and $\hat{S}_{Tq}$ reveal that for succinic acid production the model presents non-additive properties and has interactions between parameters because $\hat{S}_q < \hat{S}_{Tq}$. Figures 8 and 9 show first-order and total

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Table 3. Best Operating Conditions (Uncertainty Simultaneously Calculated): Evaluations Using *ParLMSRBF-R* and Point 38 from MC Based Optimization (Best Point)

	best operating points			
scenario	T, hydrolysis for succinic acid [°C]	enzyme loading ratio [g enzyme/kg cellulose]	sugar allocation (sugar to bioethanol)	T, hydrolysis and cofermentation for bioethanol [°C]
UC1 eval 1	30.66	16.41	0.200	51.57
UC1 eval 2	34.30	15.47	0.200	50.96
UC1 eval 3	37.68	14.36	0.200	52.12
UC1MC (38)	30.77	14.62	0.223	46.35

sensitivity indices for sensitive parameters, respectively. This result is consistent with the previous evaluation because the selected parameters were chosen as well. Parameters α_{sa}, $K_{1r\ sa}$, $K_{1IXy\ sa}$, $E_{1\ max\ sa}$, and $E_{a\ sa}$, from SAEH, show the importance of cellobiose generation in the enzymatic hydrolysis. The conversion of cellulose to cellobiose shows an important role in the reaction mechanism. In SACF, parameters $\mu_{m,sg}$, α_{FA}, β_{FA}, and β_{SA} present again sensitivity and indicate that succinic acid production and formic acid production compete in glucose consumption. Proper operating conditions will reduce formic acid and increase succinic acid production which increases the profitability of the biorefinery.

4.2.2. Bioethanol. From 49 kinetic parameters for bioethanol production, eight parameters are selected as significant sources of uncertainty. $\hat{S}_q$ and $\hat{S}_{Tq}$ reveal that for bioethanol production the model presents additive properties, and it has low interactions between parameters because $\hat{S}_q \approx \hat{S}_{Tq}$. Figures 10 and 11 illustrate first-order and total sensitivity indices of sensitive parameters, respectively. Sobol' indices from parameters K_{1r}, $E_{1\ max}$, K_{1IXy}, and K_{1ad} denote that the production of cellobiose from cellulose is important during the simultaneous hydrolysis and cofermentation (EHCF). Cellulose to cellobiose reaction can be considered as a bottleneck in the reaction pathway. The weighing factor for glucose consumption, α_{ef}, shows that for cell growth, consumption of glucose is a key factor in bioethanol production and under adequate operating conditions the biorefinery will be profitable.

4.3. Global Optimization under Uncertainty. For maximizing eq 10, the *ParLMSRBF-R* algorithm previously described is employed. For each uncertain scenario, the algorithm

Table 4. Results (Uncertainty Simultaneously Calculated) and *ParLMSRBF-R* Improvement Respect MC Best Operating Conditions (Point 38)

	cash flow, USD			improvement			
evaluation	2.5th	mean	97.5th	2.5th [%]	mean [%]	97.5th [%]	convergence
UC1 eval 1	9283.6	9704.0	10124.4	1.67	1.38	1.09	sim 46
UC1 eval 2	9291.1	9712.7	10134.4	1.75	1.48	1.20	sim 54
UC1 eval 3	9291.6	9718.0	10144.4	1.76	1.53	1.31	sim 54
UC1MC (38)	9130.9	9577.8	10024.8				after 80 sim

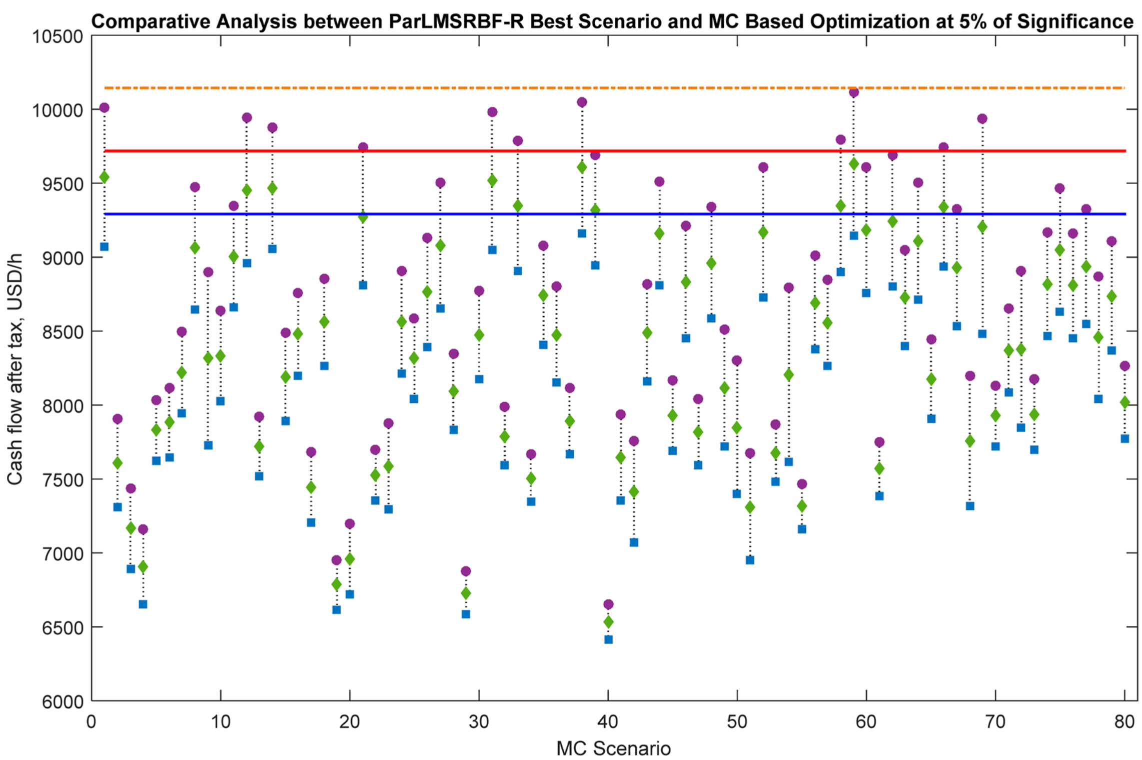

Figure 15. Comparative analysis *ParLMSRBF-R* best scenario and MC based optimization for uncertainty simultaneously calculated, where (blue squares) 2.5th percentile MC; (green diamonds) mean value MC; (purple circles) 97.5th percentile MC; (solid blue line) 2.5th percentile best scenario; (solid red line) mean value best scenario; (broken orange line) 97.5th percentile best scenario.

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runs three times using different number of P new samples and the stop criteria selected is N_{max} = 80. Input values are as presented in Table 2.

4.3.1. Optimization for Simultaneous Evaluation of Uncertain Parameters. For the first type of uncertain conditions (UC1), evaluation 1, presented in Figure 12, shows convergence in the 46 evaluated function. In this evaluation, the algorithm restarts after simulation 56 once local optima is noticed. Evaluations 2 and 3, Figures 13 and 14, respectively, show convergence in simulation 54 in both cases.

The best operating points reported by *ParLMSRBF-R* are compared with results obtained from a MC based optimization where 80 random points are tested following the procedure presented by Geraili et al.[16] Table 3 presents the best operating conditions obtained in each method. In SAEH, optimal temperature values when compared with enzyme loading ratio illustrate a trend. Lower temperature will be required if there is higher enzyme loading ratio. Also, when using *ParLMSRBF-R* method, optimal temperature values in EHCF show that temperature has to increase from its previously set value (48 °C).[16,17]

To evaluate the efficacy of the method employed, optimal points are tested under the same uncertain conditions, in other words, with the same uncertain parameters' matrix for comparing their results. Table 4 presents the 2.5th percentile, mean value, and 97.5th percentile of cash flow after tax for each point. Evaluation 3 using *ParLMSRBF-R* achieves the best 2.5th percentile for the hypothetical multiproduct lignocellulose biorefinery. Results show that the proposed framework presents an improvement of 1.76% in the profitability of a renewable energy business in contrast to MC based optimization. Figure 15 presents a comparison between the best overall result and all the points generated by MC based optimization.

4.3.2. Optimization for Separate Analysis of Uncertainty Per Product Pathway. For the second type of uncertain conditions (UC2), the optimization algorithm runs three times with the same inputs as presented in Table 2. The convergence profiles obtained are illustrated in Figures 16, 17, and 18.

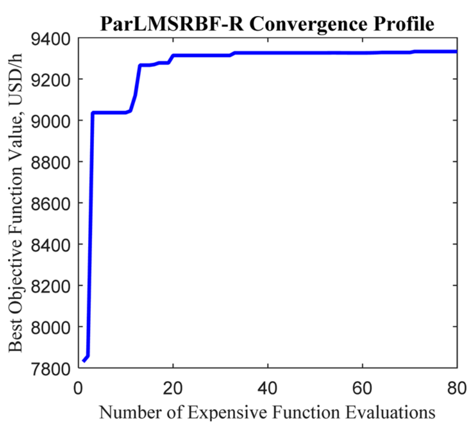

Figure 16. Convergence profile first evaluation, *ParLMSRBF-R*. Uncertainty per product pathway.

Evaluation 1, presented in Figure 16, converges at simulation 71. In this case, *ParLMSRBF-R* restarts after simulation 48. Evaluation 2 and 3, Figures 17 and 18, converge at simulations 65 and 45, respectively. Optimal points obtained with *ParLMSRBF-R* algorithm are compared with the best value obtained with MC based optimization when 80 random points are generated as explained before. Table 5 presents the best four operating conditions.

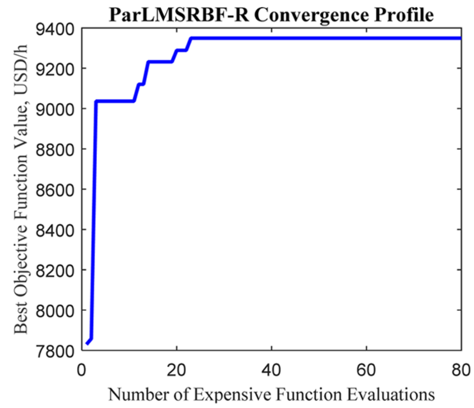

Figure 17. Convergence profile second evaluation, *ParLMSRBF-R*. Uncertainty per product pathway.

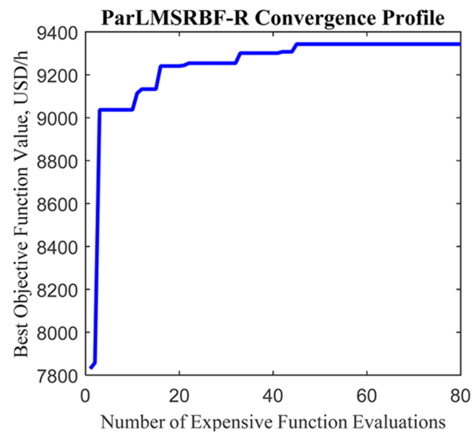

Figure 18. Convergence profile third evaluation, *ParLMSRBF-R* with uncertainty per product pathway.

Table 5. Best Operating Conditions (Uncertainty Calculated Per Product Pathway): Evaluations Using *ParLMSRBF-R* and Point 38 from MC Based Optimization

	best operating points			
scenario	T, hydrolysis for succinic acid [°C]	enzyme loading ratio [g enzyme/kg cellulose]	sugar allocation (sugar to bioethanol)	T, hydrolysis and cofermentation for bioethanol [°C]
UC2 eval 1	31.19	17.49	0.200	53.00
UC2 eval 2	30.26	17.61	0.200	53.00
UC2 eval 3	30.60	16.30	0.200	53.00
MC (38)	33.83	16.57	0.237	46.21

Likewise, optimal points are tested under the same uncertain conditions. Table 6 presents the 2.5th percentile, mean value, and 97.5th percentile of cash flow after tax for each point. Evaluation 3 using *ParLMSRBF-R* achieves the best 2.5th percentile of cash flow after tax. Results indicate that the proposed framework has an improvement of 1.69% in the profitability of the biorefinery in contrast to MC based optimization. Figure 19 presents a comparison between the best overall result and all the points generated by MC based optimization.

4.4. Extensive Sensitivity Analysis Evaluation. In this work, sensitive parameters are selected following two different approaches, when all are simultaneously evaluated, and when they are evaluated in groups depending on product pathways. Once the two groups of parameters are obtained, simulations of

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Table 6. Results (Uncertainty Calculated Per Product Pathway) and *ParLMSRBF-R* Improvement with Respect to MC Best Operating Conditions (Point 38)

	cash flow (USD)			improvement			
scenario	2.5th	mean	97.5th	2.5th [%]	mean [%]	97.5th [%]	convergence
UC2 eval 1	9252.90	9729.31	10205.73	1.42	1.46	1.50	sim 71
UC2 eval 2	9260.91	9731.22	10201.54	1.51	1.48	1.46	sim 65
UC2 eval 3	9276.87	9729.33	10181.78	1.69	1.46	1.26	sim 45
UC2MC (38)	9123.10	9588.86	10054.63				after 80 sim

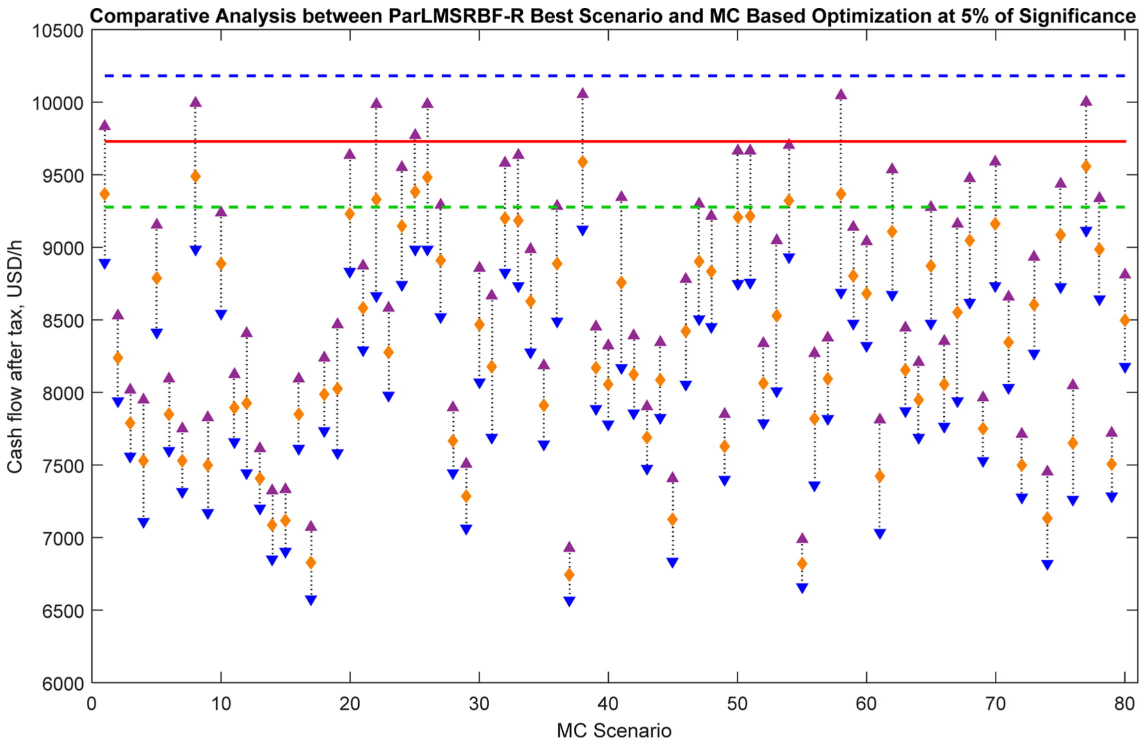

Figure 19. Comparative analysis between *ParLMSRBF-R* best scenario and MC based optimization method considering uncertainty per product pathway, where (blue inverted triangles) 2.5th percentile MC; (orange tilted squares) mean value MC; (purple upward triangles) 97.5th percentile MC; (green broken line) 2.5th percentile best scenario; (red solid line) mean value best scenario; (blue broken line) 97.5th percentile best scenario.

Table 7. Number of Uncertain Parameters Selected in Each Process Section Depending on the Type of Uncertainty Considered

type of uncertainty	EHCF	SAEH	SACF
UC1	3	8	7
UC2	8	5	5

the mechanistic model run for both uncertain conditions. Table 7 presents a comparison of the quantity of kinetic parameters selected in each section of the multiproduct biorefinery. The quantity of sensitive parameters obtained in EHCF for UC2 is higher than UC1 and lower in the two processes related to succinic acid production (SAEH and SACF). These results illustrate that because UC2 is performed considering autonomy of the processes, less importance is given to parameters from SAEH and SACF while permitting evaluation of the individual importance of parameters in EHCF.

Table 8 presents optimal operating conditions for both types of uncertainties. Differences are found in SAEH for enzyme loading ratio and EHCF temperature for bioethanol production. Because UC1 includes more uncertain parameters from succinic acid production, to overcome it, temperature in SAEH increases while maintaining a low enzyme loading ratio. On the other hand, when there are fewer uncertain parameters from succinic acid production, a lower temperature is suggested in SAEH while more enzyme considered. In the case of EHCF, both uncertain scenarios increase temperature from the previous set value (48 °C), but UC2 suggests a higher temperature. Final values of profitability are slightly different between UC1 and UC2. What can be inferred in general is that the greater the uncertainty is (more uncertain parameters),

Table 8. Best Operating Conditions and 2.5th Percentile of Cash Flow after Tax for Both Uncertain Conditions

	best operating conditions				
scenario	*T*, hydrolysis for succinic acid [°C]	enzyme loading ratio, [g enzyme/kg cellulose]	sugar allocation (sugar to bioethanol)	*T*, hydrolysis and cofermentation for bioethanol [°C]	$Z(x)$, 2.5th percentile [USD/h]
UC1 eval 3	37.68	14.36	0.20	52.12	9291.60
UC2 eval 3	30.60	16.30	0.20	53.00	9276.87

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the more temperature is recommended by the optimization algorithm.

5. CONCLUSIONS AND FUTURE WORK

To model uncertain conditions at operational level, global sensitivity analysis of uncertain parameters is carried out in two different ways, evaluating all simultaneously and evaluating them in groups based on product pathways. UC1 considers less sensitive parameters than UC2 in EHCF and more sensitive parameters than UC2 in SAEH and SACF. Also, comparing $\hat{S}_q$ and $\hat{S}_{Tq}$ reveals that in UC1 the model presents nonadditive properties and has high interactions. In UC2, the succinic acid model shows nonadditive while for bioethanol production the model presents additive properties and low interactions. The novel approach for selecting sensitive parameters based on their product pathway has the advantage that by using a single objective function a wider portfolio of biorefinery products can be tested while it considers a larger variety of uncertainties in the output result. Also, it gives the opportunity of visualizing additive or nonadditive properties of production processes separately.

The optimization method implemented in the proposed framework appears to be competitive with conventional procedures, e.g., MC based optimization. The algorithm searches optimal operating points using RBFs to select candidate points to be evaluated in the expensive function which is considered as a black box. When optimizing for UC1, *ParLMSRBF-R* converges after 54 simulations, and for UC2, it converges after 45 simulations of the mechanistic model. The improvement registered in contrast to the best value attained using MC based optimization is 1.76% for UC1 and 1.69% for UC2.

Future work includes renewable energy facilities with a wider portfolio of biofuels and value added chemicals and the integration of biorefining operations with fossil fuel power plants. Through integration an optimal operation scheme and energy portfolio can be propound while minimizing greenhouse gases emissions. The mentioned super structure shall consider strategic and operational optimal conditions.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.iecr.6b04395.

Nomenclature and Input uncertainty of biokinetic parameters (PDF)

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Notes

The authors declare no competing financial interest.

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