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Optimal management of bio-based energy supply chains under parametric uncertainty through a data-driven decision-support framework

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ABSTRACT

This paper addresses the optimal management of a multi-objective bio-based energy supply chain network subjected to multiple sources of uncertainty. The complexity to obtain an optimal solution using traditional uncertainty management methods dramatically increases with the number of uncertain factors considered. Such a complexity produces that, if tractable, the problem is solved after a large computational effort. Therefore, in this work a data-driven decision-making framework is proposed to address this issue. Such a framework exploits machine learning techniques to efficiently approximate the optimal management decisions considering a set of uncertain parameters that continuously influence the process behavior as an input. A design of computer experiments technique is used in order to combine these parameters and produce a matrix of representative information. These data are used to optimize the deterministic multi-objective bio-based energy network problem through conventional optimization methods, leading to a detailed (but elementary) map of the optimal management decisions based on the uncertain parameters. Afterwards, the detailed data-driven relations are described/identified using an Ordinary Kriging meta-model. The result exhibits a very high accuracy of the parametric meta-models for predicting the optimal decision variables in comparison with the traditional stochastic approach. Besides, and more importantly, a dramatic reduction of the computational effort required to obtain these optimal values in response to the change of the uncertain parameters is achieved. Thus the use of the proposed data-driven decision tool promotes a time-effective optimal decision making, which represents a step forward to use data-driven strategy in large-scale/complex industrial problems.

1. Introduction

The limited availability of fossil fuels, together with the dependence on these non-renewable resources and the hard environmental regulations have exposed the need for alternative energy generation technologies (mainly oriented to promote the green engineering). However, it was after the apparition of large government subsidies to eco-friendly processes when the development and application of green energy generation technologies were trully promoted. One of the most significant initiatives is the use of agro-industrial wastes (e.g., biomass) as a fuel for power generation systems. The proper and systematic management of a bio-based energy production supply chain (SC) presents two major challenges that need to be faced simultaneously, in addition to the usual design and planning optimization issues (Silvente et al., 2013). Firstly, since the bio-based process is essentially focused on solving a sustainability problem, a multi-objective (MO) approach is needed to address the economic performance while reducing the associated environmental impact (Ehrgott, 2005). Secondly, an enhanced strategy capable of providing a reliable/quick response to those unpredictable situations inherent to the system such as variability in demands, prices and raw material availability/quality is necessary (Guillén-Gosálbez & Grossmann, 2009).

A wide variety of approaches are available in the literature to address MO problems, generally leading to a set of feasible/optimal solutions known as Pareto space. Nowadays, the most important challenge is the identification of the best solution within the Pareto sets rather than the Pareto space itself. Historically, many decision-making techniques have been used to address such an issue. One of the first tools used is the well-known Goal-programming (Guillén, Mele, Bagajewicz, Espuña, & Puigjaner, 2005) which is based on defining a set

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Nomenclature

Abbreviations

AHP	Analytical Hierarchical Processes
ELECTRE	ELimination and Choice Expressing REality
LCIA	Life Cycle Impact Analysis
LP	Linear Programming
M-MP	Meta-Multiparametric Programming
MCDM	Multi-Criteria Decision Making
MILP	Mixed Integer Linear Programming
MO	Multi-Objective
MP	Multiparametric Programming
MPC	Model Predictive Control
MP-MPC	Multiparametric Model Predictive Control
NRMSE	Normalized Root Mean Square Error
PSE	Process Systems Engineering
RO	Robust Optimization
SC	Supply Chain
WS	Weighted Sum

Indices

c	Scenario/sampling point
e	Supplier site
f	Potential sites
i	Treatment/distribution tasks
j	Equipment's
k	Input dimensionality
l	Input dimension counter
m	Market site
p	Production site
s	Material states
t	Time period

Set/Subset

FP	Biomass states associated with final products
Mkt	Market sites
n	Sampling plan size
RM	Biomass states for raw material
RSS	Raw set of solutions
Sup	Supplier sites
Tr_c	Training samples plan subset
u	Number of output variables
Va_c	Validation samples plan subset
Φ	Space of uncertain parameters

Parameters

A_{sftc}	Maximum availability of raw material s in period t in location f and for scenario c
Dem_{sft}	Demand for product s at market f in period t
err	Rolerance value for the *NRMSE*
HV_{sc}	Lower heating value for material s at scenario c
$NormF_g$	Normalizing factor of damage category g
p_l	Smoothness parameter
$WeightEnv_c$	Economic equivalence for environmental objective
$WeightSoc_c$	Economic equivalence for social objective
ω	Input variables for scenario c
$\widehat{yy}_{max}$	Boundary for the maximum output value
$\widehat{yy}_{min}$	Boundary for the minimum output value
$Z(\omega)$	Residual term
α_{sij}	Mass fraction of material s produced by task i in equipment j
$\bar{\alpha}_{sij}$	Mass fraction of material s consumed by task i in equipment j
β_{jf}	Minimum utilization rate of technology j capacity that is allowed at location f
Υ_l	Degree of correlation along the l^{th} input
μ	Constant term for meta-modeling
$\hat{\mu}$	Constant value that leads to the "optimal" values
ζ_{ag}	g endpoint damage characterization factor for environmental intervention a

Variables

F_{jftc}	Total capacity of technology j during period t at location f and scenario c
$FCost_t$	Fixed cost in facility f for period t and scenario c
IC_{aftc}	Mid-point a environmental impact associated to site f which rises from activities in period t and scenario c
$Impact^{2002}_{overall_c}$	Total environmental impact for the whole SC
NPV	Net Present Value
OF	Global objective function
$P_{ijf'ftc}$	Production level of task i in equipment j in location f' and delivered (if required) in location f at time t and scenario c
$Profit_{tc}$	Profit achieved in period for each facility f at time period t and scenario c
$Purch_{etc}$	Economic value of sales executed in period t during scenario c
Pv_{sijftc}	Input/output of material s for i with variable input/output, by using technology j during period t in location f and scenario c
r	Vector of correlation
S_{sftc}	Storage level of material s at location f in time t and scenario c
$Sales_{sf'ft}$	Amount of product s sold from location f in market f' in period t and scenario c
SoC_c	Social performance at scenario c
x	First stage decision variables
ω_c	Input variables for scenario c
ω_{new}	Point to be predicted at a particular time
$\bar{x}^*$	Optimal set of solutions for scenario c
y_c	Second stage decision variables
$\hat{y}(\omega)$	Kriging prediction for specific input values
σ^2	Process variance
$\hat{\sigma}^2$	Process variance that leads to the optimal values
$[X]_{c\cdot k}$	Sampling plan
$[Y]_{c\cdot u}$	Outputs of the sampling plan

Binary variables

V_{jftc}	Technology installed at location f in period t and scenario c

of target values as constraints in the optimization model. Later, the Analytical Hierarchical Processes (AHP) and the Weighted Sum (WS) were used to scalarize the objectives into a common function (Chen, Wang, & Lee, 2003), although in this case representativeness of the defined parameters appear as the main challenge to overcome. Fractional approaches (Gao & You, 2015; Yue, Guillén-Gosálbez, & You, 2013) and Fuzzy based optimization formulations (Govindan, Paam, & Abtahi, 2016; Medina-González, Rojas-Torres, Ponce-Ortega, Espuña, & Guillen-Gosalbez, 2018; Moreno & Blanco, 2018) were also used as a way to stablish a clear and reliable objective hierarchy, but also to avoid the subjectivity sources during the decision-making process. Even if these approaches consider the performance and hierarchies of at least two conflicting objectives, there is a complete lack of control/measurement of the decision maker desirability over the final solution. Therefore, integrated frameworks that combine MO approaches and Multi-Criteria-Decision-Making (MCDM) methods have been recently applied to optimize the design and planning of sustainable SC's. These frameworks include Pareto filters (Antipova et al., 2015; Medina-González, Pozo, Corsano, Guillén-Gosálbez, & Espuña, 2017) and derivations of the ELECTRE method (ELimination and Choice Expressing REality for its acronym in French) (Greco, Ehrgott, & Figueira, 2016; Medina-González, Graells, Guillén-Gosálbez, Espuña, & Puigjaner, 2017) used as post-optimization strategies. For these frameworks, a set of parameter values has to be defined as well for each decision criteria, but this time they are used to identify the most dominant solution for a set of them by creating membership functions for each combination. It is important to highlight that the defined parameters represent the decision-maker preference and the variability in such a definition highly affects the strategy performance. From all the above strategies, two main limitations can be identified regarding decision-making: (i) The reliance on the quality of the pool of solutions (options) and; (ii) the large computational effort required to produce such a set of solutions by running the optimization procedures. These limitations increase in complexity when the problem is subject to multiple types/sources of uncertainty (Kopanos & Pistikopoulos, 2014). Therefore, the application of currently available decision-support systems for the systematic identification of the optimal solution as a function of the decision-maker preferences for real/complex problems under uncertain conditions is still an open issue and represents a step forward (Felfel, Ayadi, & Masmoudi, 2016; Greco et al., 2016).

So far, different methods and tools have been proposed to manage the system uncertainties while addressing the optimization of industrial problems (such as multi-hierarchical SC's). Uncertainty approaches are classified into reactive and proactive being the second ones the most widely used. Studies for proactive approaches are vast in the Process Systems Engineering (PSE) literature describing mainly robust optimization (RO) (Jalilvand-Nejad, Shafaei, & Shahriari, 2016; Li, Ding, & Floudas, 2011; Ning & You, 2017) and scenario-based formulations (such as stochastic optimization). In general, these approaches produce a conservative solution at the expense of assuming a financial/performance risk against uncertain conditions, nevertheless, two main limitations can be highlighted. First, the computational effort required to produce a solution highly depends on the number of scenarios and uncertainty sources. Secondly, a complete knowledge of the uncertainty parameter values is required. On the contrary, a risk-averse attitude against uncertainties promotes the use of reactive approaches. Nowadays reactive approaches are gaining interest over proactive ones since the right management of the first ones guarantees a better overall performance even under uncertainty conditions. Within reactive approaches, the well-known model predictive control (MPC) (Liu, Lei, Wu, & Zhang, 2018; Perea-López, Ydstie, & Grossmann, 2003), rolling horizon (Kopanos & Pistikopoulos, 2014; Silvente, Aguirre, et al., 2015, Silvente, Kopanos, Pistikopoulos, & Espuña, 2015) and multiparametric programming (MP) (Pistikopoulos, Galindo, & Dua, 2011) can be highlighted. Even if most of the above methods are able to handle multiple uncertainty sources, MP surpass the others as the most feasible alternative to solve problems in which the uncertainty affects both, the process conditions and the optimization parameters (such as decision-maker preferences or objectives hierarchy).

Basically, MP aims to obtain a set of equations that reproduce the optimal solution as a function of multiple uncertain/varying parameters (Charitopoulos, Papageorgiou, & Dua, 2017). In addition, the specific feasible regions for these equations within the solution space are obtained (Sakizils, Kouramas, & Pistikopoulous, 2007). One of the most interesting advantages of MP is the significant reduction in computational effort obtained by avoiding the repetitive optimization procedure when the uncertainty is unveiled (Pistikopoulos, Dua, Bozinisa, Bemporad, & Morari, 2002). Even if it is hard to define the first record of MP, its use has been exponentially increased after being combined with MPC (Bemporad, Borrelli, & Morari, 2002; Kouramas, Faísca, Panos, & Pistikopoulos, 2011). In such a framework (MP-MPC) a model is used to control the process in a finite time horizon, but in particular, two major conditions are required to be successfully applied. First, a complex mathematical knowledge associated to the development of the MP framework (Shokry & Espuña, 2015a, 2015b) and second, the availability of a clear discrete-time linear state space model of the process (Bemporad et al., 2002, Pistikopoulos et al., 2002; Kouramas et al., 2011). These requirements hinder the application of the MP analysis to problems in which a highly nonlinear, high dimensional, complex structure (sequential simulation models), and/or non-transparent mathematical model are considered.

To address the MP limitations, the use of data-driven optimization techniques has been proposed, including data-driven robust optimization (Ning & You, 2017) and meta-multiparametric analysis (M-MP) (Medina-González, Shokry, Silvente, & Espuña, 2015; Shokry & Espuña, 2015a, 2015b). In the recent past, M-MP has been successfully applied to several industrial cases including the optimal management of a utility plant (Shokry & Espuña, 2015b) and energy production process (Medina-González et al., 2015). Additionally, M-MP has been used for the control of batch processes (Shokry, Dombayci, & Espuña, 2016), emission control in scheduling systems (Lupera Calahorrano, Shokry, Campanya, & Espuña, 2016) and the dynamic optimization of batch processes (Shokry & Espuña, 2017). However, all these applications address continuous variables and the use of this framework to Mixed-Integer optimization problems is dramatically compromised. Even if in the works of Shokry, Medina-González, and Espuña (2017) and Lupera Calahorrano, Shokry, Kopanos, and Espuña (2017) a combination of M-MP with classification techniques has been successfully applied to simple small-scale problems (i.e. managing continuous plus discrete variables), the applicability of M-MP approaches to manage large scale problems still requires a systematic definition of the most significant decision variables.

The use of the M-MP methodology to address SCM problems is particularly challenging due to the high dimensionality and complexity of these problems and the existence of different sources of uncertainty that often interrupt the supply chain dynamics. For the best knowledge of the authors, there is only one contribution in the PSE literature that uses the M-MP for the management of a supply chain (Medina-González et al., 2015), so this study focuses on stressing the decision-making capabilities of the M-MP framework presented there through the evaluation of the data-driven strategy capabilities and its impact over the decision-making process. This analysis is aimed to highlight the practical advantages of the M-MP as an optimization approach and to evaluate the time effectiveness and reliability of the obtained solution.

2. Problem statement

This paper tackles the planning of a centralized multi-objective multi-echelon bio-based energy production SC affected by raw material uncertainties as described in Fig. 1. The biomass availability is the primary source of variability in bio-based energy generation systems and it is addressed through a tailor-made approach (see Section 4). The capabilities of the proposed strategy were illustrated using a modified version of a case study proposed by Pérez-Fortes, Laínez, Arranz-Piera, Velo, and Puigjaner (2012). In addition to the original process data (i.e., potential sites (*f*), material states (*s*), treatment/distribution tasks (*i*) and equipment's (*j*)), a given expected raw material availability profile was defined for each period and supplier site. The main objective considered in this work is the global sustainability of the system, quantified through its net present value (NPV), the environmental impact of the entire SC and the creation of job opportunities (social performance). The associated mathematical model that describes the bio-

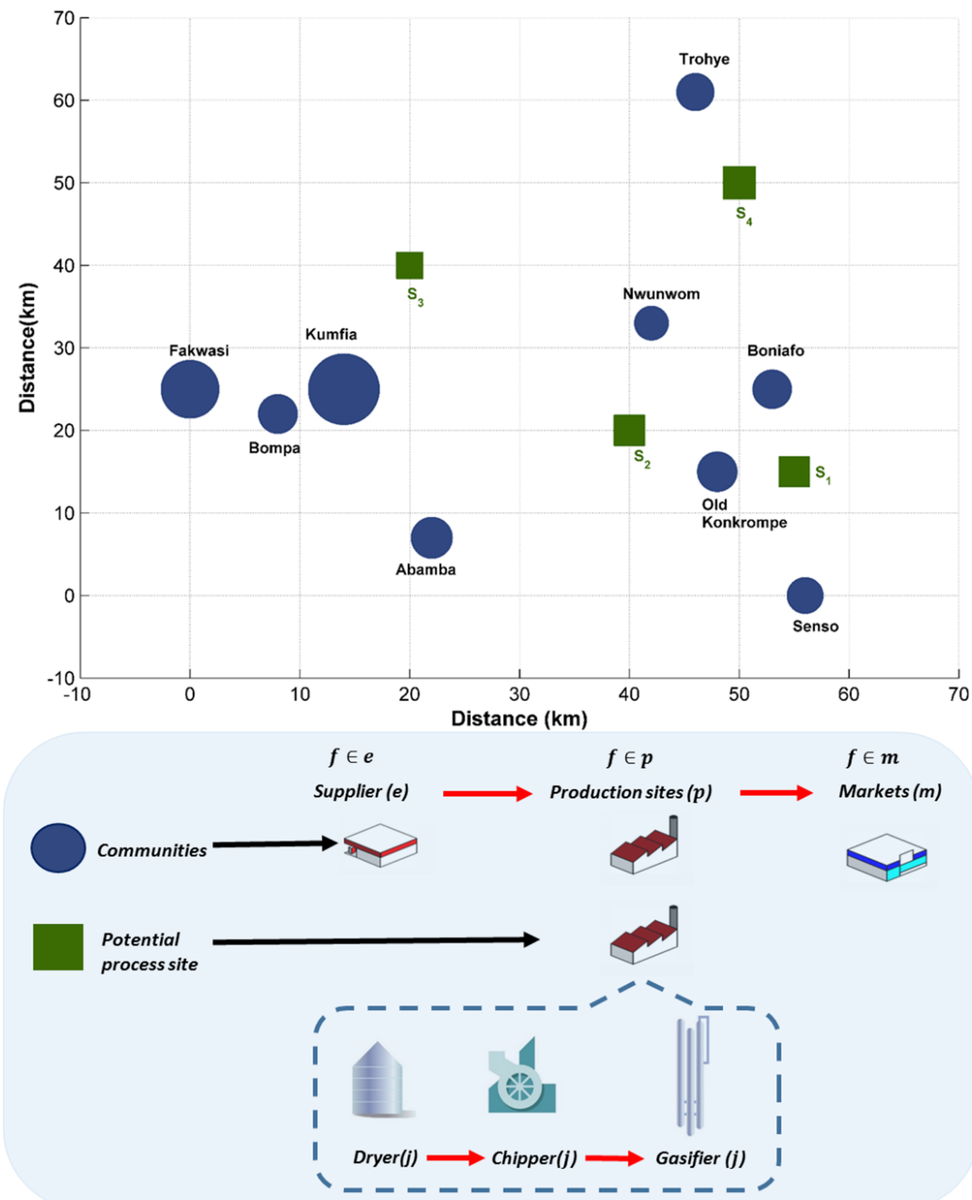

Fig. 1. The general scheme for bio-based energy supply chain.

based energy generation problem includes not only the mass and energy balances but also constraints associated to the considered technologies. The resulting MO problem will be assessed using the WS approach, and consequently, a set of weighting factors should be defined for the environmental and social performances to scalarize them into a single economic result.

The following data allows describing the particular problem under study:

- The set of materials $s \in S$, which includes raw, intermediates and final products.
- The set of tasks $i \in I$, which include on-site treatments, pre-treatments, and transportation.
- The set of economic weights allowing normalize the environmental and social objectives ($WeightSoc_c$ and $WeghtEnv_c$ respectively).
- The set of locations $f \in F$, fixed in the initialization step.
- A time horizon $t \in T$, which represents the months of the year.
- A given expected energy demand profile for each short-term period and market, considering different (uncertain) target values.
- Product and consumable prices.
- Environmental impacts of raw material production, process, and transportation systems.
- The social impact as a function of the size of the different installed processes, although again, the importance of this assessment on the decision-making procedure is uncertain.

Furthermore, the goal is to maximize the economic vector by modifying the following decisions concerning the strategic and tactical management of the resulting SC:

- All the amounts of materials processed by task i using equipment j during period t, at site f.
- Storage levels at each site and time.
- Type and capacities of the installed equipment, at each site and time.

In the next section, a brief description of the mathematical constraints that model the case study is presented. Further details about the process data, equipment description, and nominal capacities, can be found in Pérez-Fortes et al. (2012).

3. Mathematical formulation of the deterministic problem

The capabilities of our methodological framework are demonstrated by solving the MILP model formulated by Pérez-Fortes et al. (2012). Notice that, since the novelty of the contribution does not lie in the model formulation, here, only the main elements in the mathematical formulation are briefly described for continuity of the work; however, interested readers are referred to Pérez-Fortes et al. (2012) or Medina-González, Graells, et al. (2017), where a detailed description of the model can be found. The material balance is represented in Eq. (1), in which the raw material that it is not consumed as fuel ($P_{ijf'ft}$) with a defined efficiency (α_{sij}) can be stored (S_{sft}) at any time.

$$S_{sft} = S_{sft-1} + \sum_{f'} \sum_{i \in T_s} \sum_{j \in (j_i \cap \bar{j}_{f'})} \alpha_{sij} P_{ijf'ft} - \sum_{f'} \sum_{i \in \bar{T}_s} \sum_{j \in (j_i \cap \bar{j}_f)} \bar{\alpha}_{sij} P_{ijff't} \qquad \forall\ s, f, t \tag{1}$$

Similarly, Eq. (2) represents the energy balance of the system, in which the latent heat value (HV_s) of the material (Pv_{sijft}) is considered at the input and output ($s \in T_s$ and $s \in \bar{T}_s$, respectively) of all the tasks across the entire system.

$$\sum_{s \in T_s} HV_s \cdot Pv_{sijft} = \sum_{s \in \bar{T}_s} HV_s \cdot Pv_{sijft} \qquad \forall\ i \in \bar{I}, f, t \tag{2}$$

A minimum energy and treated/pretreated material production level is guaranteed using β_{jf}, which represents the minimal proportion of the total available capacity used in technology j at site f and it is defined by the decision maker. Similarly, Eq. (3) limits the production to the respective equipment capacities.

$$\beta_{jf} \cdot F_{jft-1} \le \sum_{f'} \sum_{i \in I_j} P_{ijff't} \le F_{jft} \qquad \forall\ j \in j_f, f, t \tag{3}$$

In a similar way, Eq. (4) ensures that the raw material s purchased at site f delivered to location f' at time t satisfies the physical availability, while Eq. (5) limits the sales to a specified demand. The above represents the assumption that the energy produced using biomass never exceeds the forecasted demand.

$$\sum_{f'} \sum_{i \in \bar{T}_s} \sum_{j \in \bar{j}_i} P_{ijff't} \le A_{sft} \qquad \forall\ s \in RM, f \in Sup, t \tag{4}$$

$$\sum_{f' \in M} Sales_{sf'ft} \le Dem_{sft} \qquad \forall\ s \in FP, f \in Mkt, t \tag{5}$$

The economic performance (NPV) is represented by the net present value of the entire SC. Without loss of generality, the NPV is obtained considering the traditional incomes ($Sales_t$) and costs functions, annualized using a defined interest rate ($rate$) as stated in Eq. (6). Note that process costs include fixed/investment costs ($FCost_t$) and variable ones, including transportation, acquisition and production costs ($Purch_{et}$).

$$NPV = \sum_{t} \left(\frac{Sales_{tc} - (FCost_t + \sum_e Purch_{etc})}{(1 + rate)^t} \right) \qquad \forall\ t \tag{6}$$

As well as in the base case study, a Life Cycle Impact Analysis (LCIA) is performed using the well-known Impact 2002+ methodology. Thereby, a useful assessment of the process environmental impact may be obtained by combining midpoint/damage approaches (Jolliet et al., 2003). Impact 2002+ needs a database to assess the system impact, which for this case is the Ecoinvent database (Ecoinvent Centre, 2008). Thus, the environmental impact quantification considers the traditional 14 mid-point categories associated with biomass production (e.g., cassava waste), transportation, pre-treatment (chipping and drying) and generation of electricity through biomass gasification. Eq. (7) displays the resulting equation. For more details about the life cycle analysis and the implementation of Impact 2002+ methodology readers are referred to Jolliet et al. (2003). Notice that it is possible to use alternative databases and methodologies; however, the analysis of the effect of these elements over the strategy performance is out of the scope of this work.

$$Impact_{overall}^{2002} = \sum_{f} \sum_{g} \sum_{t} \sum_{a \in A_g} NormF_g \zeta_{ag} IC_{aft} \tag{7}$$

Finally, Eq. (8) calculates the social impact and represents the number of treatment/pre-treatment sites installed/used. Here, the binary variable V_{jft} represents the use or not of a particular unit.

$$SoC = \sum_{j} \sum_{f} \sum_{t} V_{jft} \tag{8}$$

For comparison purposes, the proposed formulation assumes a fixed superstructure thus; the number of units installed will be the same for further comparisons. The original formulation models a MO problem considering the profit, environmental and social impact as objectives. In the presented work the objective function is reformulated by scalarizing the non-economic criteria into an economic one by applying a defined factor ($WeightSoc$ and $WeghtEnv$, respectively) as described in Eq. (9).

$$OF = \sum_{t} Profit_t - (WeightEnv * Impact_{overall}^{2002}) + (WeightSoc * SoC) \tag{9}$$

The value of these factors directly affects the OF value, compromising the solution reliability. Therefore, the creation of a meta-model facilitates future optimization for different economic factors.

3.1. Methodology: Meta-multiparametric framework

The general idea of the M-MP is to replace complex functions with simpler approximations that require less computational effort. These approximations are created by the training of a set of meta-models (in this work, based on Ordinary Kriging as machine learning technique) using input-output information (Lupera Calahorrano et al., 2016; Medina-González et al., 2015; Shokry & Espuña, 2015a, 2015b). In particular, the uncertain parameters are considered input information while the corresponding optimal decision variables and objectives of the SC are the outputs obtained through a multiparametric approach. The resulting meta-models represent the multiparametric black box relations that describe the behavior of the decision variables and objectives over the entire uncertainty space. Thus, for any further change in the uncertain parameters, these meta-models will be used to perform simple interpolations in order to predict the new optimal values of the decision variables and objectives. The M-MP method comprises three main tasks (5 steps) as shown in Fig. 2. A detailed description of each step (including the specific methods/algorithms used) is provided in the following subsections.

3.1.1. Initialization

During initialization step, the original MILP problem is solved under deterministic conditions (i.e., for a specific set of pre-defined values of the uncertain information). Using the results from the MILP problem, all discrete variables are fixed. Thus, the original MILP is transformed into a Linear Programming (LP) problem. There are two reasons for fixing the binary variables. Firstly, a planning/operation problem is addressed since the impact of the uncertain parameters over the management decisions is more significant, and the time effective response to face those changes is of essential importance. And secondly, the fixed design ensures a comparable environment/situation. Also in this initialization step, the uncertain parameters that are expected to influence the supply chain operations are defined, as well as their upper and lower bounds (i.e. their domain of variation).

Design of computer experiments and data generation. To obtain accurate meta-model predictions, the training step requires as much information as possible about the output behavior over the inputs domain (uncertainty space). Thus, the main issue to be addressed to ensure the reliability and feasibility of such a data is the identification of a reasonable number of input combinations (i.e., sample points or sampling plan) well-distributed through the input domain

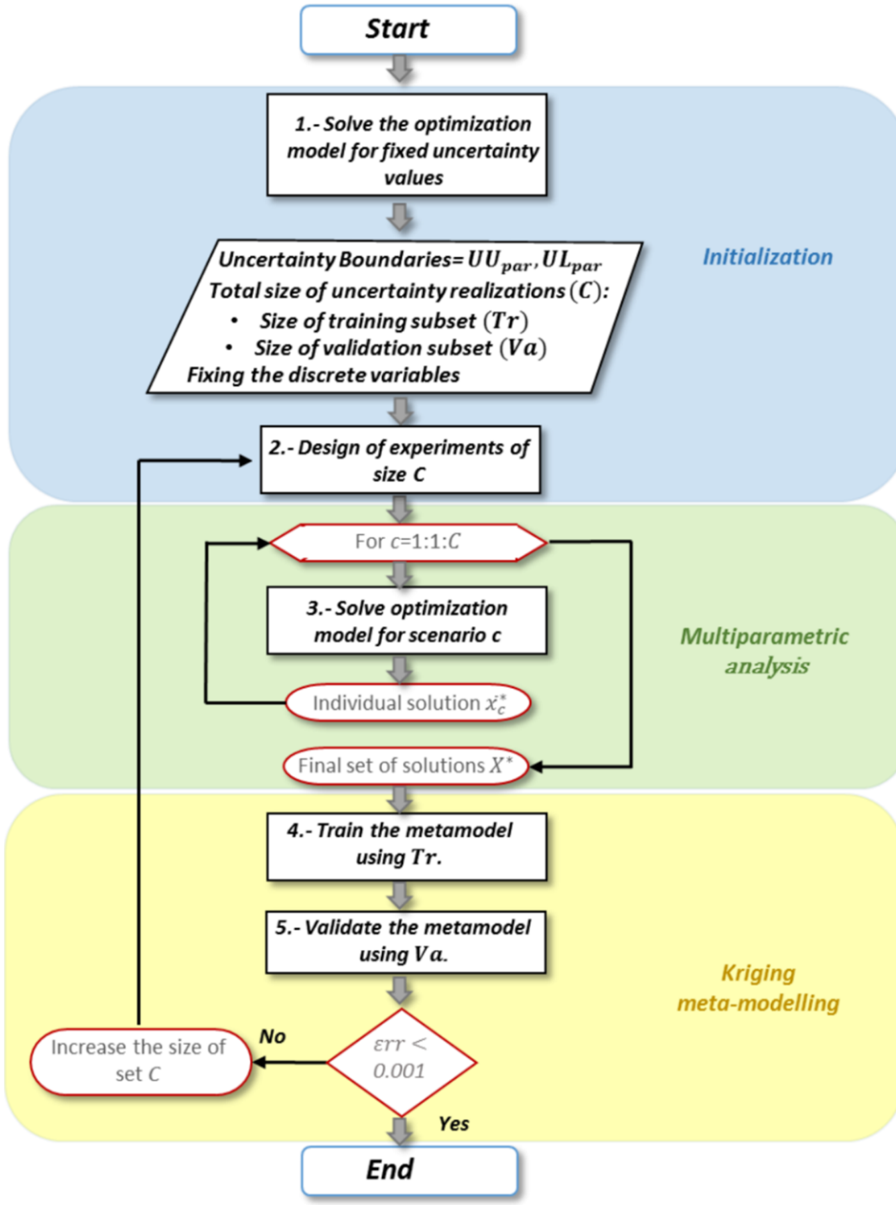

Fig. 2. The detailed description of the solution strategy proposed.

(uniformity) (Shokry & Espuña, 2014).

From the different existing techniques for the design of computer experiments that generate well-distributed sampling plans at the low computational effort, in this work the Hammersley sampling technique is used. The analysis of the effect of the sampling technique over the final solution is out of the scope of this paper. Therefore, interested readers are referred to Forrester and Keane (2009) and Fang, Li, and Sudjianto (2006) for more details.

The resulting sampling plan has the form of $[X]_{c'\cdot k}$, where c' is the size of the training data set, and k represents the number of uncertain parameters affecting the system (i.e. input dimensionality). After designing the sampling plan, the optimization problem has to be solved for each sample point (i.e. n times) to obtain the associated outputs $[Y]_{c'\cdot u}$ (see Section 3.1). Where, u is the number of output variables including the main objective function and the decision variables under control ($u - 1$). In addition to the training set, a different validation set must be generated in the same way, in order to assess the prediction accuracy of the meta-models. The size of the uncertainty set is increased until a minimum accuracy level is achieved by the meta-model.

3.1.2. Multiparametric analysis step

As commented before, a fixed superstructure is used to reduce the computational effort and enable the proper comparison required by the subsequent steps in the M-MP strategy. Particularly such a fixed data defines the different production sites, treatment, pre-treatment units as well as distribution links. Thus, once the superstructure is defined, the mathematical formulation has the following general form (*Model P*).

$$\textit{Model } P \quad \max_{x \;\; y_c} \left\{ \sum_c NPV_c - (WeightEnv_c * Impact^{2002}_{overall_c}) + (WeightSoc_c * SoC_c) \right\}$$
$$s.t.$$
$$Eq.\ (1) - (9)$$
$$x \in X,\ y_c \in Y$$

Following a traditional two-stage stochastic formulation, x represents the first stage decision variables while y_c are the second stage ones, which are directly affected by the uncertain parameters c, belonging to the uncertain space ϕ. In addition to Eqs. (1)–(9) this model uses constraints associated to materials availability, production levels, equipment and storage capacities, which has not been described here to avoid repetitive information and can be found in Medina-González, Graells, et al. (2017). According to the proposed solution strategy (see Fig. 2), at this stage *Model P* has to be solved iteratively for each sampling point within the design of experiments. Therefore, first the LP model is solved optimizing the single-objective economic function. Then, the values obtained are collected (e.g. production, storage and flow levels across the supply chain). This process is repeated recursively by replacing the parameters values used in the solution of the deterministic model by those associated with another sampling point in order to obtain the optimal supply chain plan for each of the remaining $|C| - 1$ scenarios so that, at the end, $|C|$ different solutions are generated.

The results of all the scenarios represents a poorly approximation of the global problem, however, the meta-model is built using the whole set of solution for all the sub-problems which represents a better approximation. The following subsection describes such a meta-model construction.

3.1.3. Meta-model training and validation

In many engineering applications, the well-known Kriging modeling (Cressi, 1993; Krige, 1951) has exhibited two main outperforming features: (i) a high prediction accuracy using a relatively small number of training data points, and (ii) the simple tunning of its adjustable parameters function, which can be easily optimized to obtain the best fit. Thus, Kriging models offer high flexibility for parameters tuning while measuring the effect of each input variable over the output. The Kriging is particularly useful for the approximation of nonlinear computer models (Caballero & Grossmann, 2008; Shokry & Espuña, 2014). Moreover, the Ordinary Kriging meta-model is generally used as the machine learning technique (Fang et al., 2006; Forrester & Keane, 2009).

For this strategy, the result from steps one and two (Fig. 2) leads to a set of uncertain parameters combinations $[X]_{c^{'}\cdot k}$ and their corresponding optimal solutions $[Y]_{c^{'}\cdot u}$. Thus, a set of k Kriging meta-models are constructed, each of them representing a data-driven multiparametric relation that identifies the underlying mapping between the uncertain parameters and the optimal behavior of each output. Notice that the Kriging meta-model assumes a stochastic process, where the error in the predicted value is also a function of the input variables ω. The Kriging predictor $\hat{y}(\omega)$ is composed by two main parts: a constant term μ, and a residual $Z(\omega)$ form that constant, leading to the following equation (Forrester & Keane, 2009).

$$\hat{y}(\omega) = \mu + Z(\omega) \tag{10}$$

The residual $Z(\omega)$ is considered as a stochastic Gaussian process with expected value zero $E(Z(\omega)) = 0$, and a covariance between two points (in this case scenarios) ω_c, ω_{c*} calculated as: $cov(Z(\omega), Z(\omega_{c*})) = \sigma^2 R(\omega_c, \omega_{c*})$, where σ^2 is the process variance, and $R(\omega_c, \omega_{c*})$ is a spatial correlation function which is usually selected exponential, see Eq. (11). The parameter Υ_l represents a measure of the degree of correlation among the data along the l^{th} input dimension, and p_l is a smoothness parameter that is usually fired at the value of 2.0 (Forrester & Keane, 2009).

$$R(\omega_c, \omega_{c*}) = exp\left(-\sum_{l=1}^{k} \Upsilon_l\ |\omega_c - \omega_{c*,l}|^{p_l}\right) \quad l = 1, 2, \cdots, k \tag{11}$$

Maximizing the likelihood function (Eq. (12)) of the observed data $[Y]_{c^{'}\cdot l}$ yields the optimal expressions of the parameters μ, σ^2 that depend on l. This task is accomplished through differentiating the natural logarithm of the likelihood function concerning μ and σ^2, and after some mathematical derivations, their optimal formulas are obtained and displayed in Eq. (13), and Eq. (14) (Jones, Schonlau, & Wel, 1998). Being **1** in Eqs. (12) and (13), the column vector of ones with length c. Substituting by the optimal values of $\hat{\mu}$ and $\hat{\sigma}^2$ in the likelihood function leads to obtaining a concentrated log-likelihood function (Eq. (15)) (Jones et al., 1998).

$$Lik = \frac{1}{(2\pi\sigma^2)^{c/2}|R|^{1/2}} exp\left(\frac{-(Y - 1\mu)^T R^{-1}(Y - 1\mu)}{2\sigma^2}\right) \tag{12}$$

$$\hat{\mu} = \frac{1^T R^{-1} Y}{1^T R^{-1} 1} \tag{13}$$

$$\hat{\sigma}^2 = \frac{(Y - 1\mu)^T R^{-1}(Y - 1\mu)}{n} \tag{14}$$

$$Max_{(\Upsilon_l, p_l)}\left[-\frac{n}{2}\ln(\hat{\sigma}^2) - \frac{1}{2}\ln(|R|)\right] \tag{15}$$

The Kriging final predictor in Eq. (16) is obtained through deriving the augmented likelihood function of the original training data set and a new interpolating point (ω_{new}, yy_{new}). Where: r is the $c \times 1$ vector of correlations between the predicted xx_{new} and the sample design points (i.e., $R(\omega_{new}, \omega_c)$). Detailed information about the required mathematical development can be found in (Caballero & Grossmann, 2008).

$$\hat{y}(x\omega_{new}) = \mu + r^T R^{-1}(Y - 1\mu)^T \tag{16}$$

The optimal parameters of the Kriging meta-model [Υ_l, p_l, $\hat{\mu}$,$\hat{\sigma}^2$] were obtained by the optimization of the concentrated log-likelihood function. In this work, the Matlab "*fmincon*" algorithm is used to solve this nonlinear optimization problem, while Cholesky factorization is used to find the inverse of to avoid the ill-conditioning. After fitting, the Kriging meta-models should be assessed to verify that they show a range of accuracy for the intended application as recently used in (Shokry & Espuña, 2014). Hence, the Kriging meta-model is used to estimate the outputs of the previously generated validation set; then, an accuracy measure can be calculated by comparing the outputs with their corresponding real values. The Normalized Root Mean Square Error (NRMSE%) is used in the work as an accuracy measure, see Eq. (17). where y_c, and $\hat{y}_c$ are the real and the estimated outputs, and c_v is the number of validation data points.

$$NRMSE = 100 \times \frac{\left[\frac{1}{c}\cdot \sum_{c=1}^{c}(\hat{y}_c - y_c)^2\right]^{0.5}}{(yy_{max} - yy_{min})} \tag{17}$$

As commented before, if the accuracy measure is not satisfactory enough (NRMSE $<$ err), the training set size should be extended. Even if Fig. 2 proposes an automatic sequential modeling framework in which the size of the training set is automatically updated to achieve a defined satisfaction level, a manual validation was performed. Nevertheless, the automatic algorithm was presented for illustrative purposes, since the algorithm automation can be simply coded.

4. Case study

This work uses a real case study firstly introduced by Pérez-Fortes et al. (2012) to illustrate the application of the proposed procedures. The problem was modeled as MILP problem and later relaxed into an LP to address the optimal management of a biomass-based energy SC system. The model considers nine communities, and all of them can be simultaneously biomass suppliers, potential energy generation as well as market sites. This case study contemplates 40 different biomass states (s), six available technologies (j) (including four transformation treatment/pretreatment and two transportation forms) and 79 activities(i). Each task implies either biomass processing or biomass transportation. These tasks may be developed in one or more of the 31 defined sites (f) (i.e., nine suppliers, nine potential pre-treatment and treatment sites, nine markets and four additional sites). Planning problems are typically formulated to cover a medium-term horizon (months) thus, in this case, a three months planning horizon was assumed. An annual interest rate of 15% (monthly discretized) is used (Seider, Seader, Lewin, & Widagdo, 2009).

The scope of the paper is limited to provide an effective management strategy to support the decision-making processes under multiple types of uncertainties. In particular, this work evaluates the effect of the changes in the electricity demand and weighting criteria over the planning decisions. Thus, Table 1 shows the considered variable parameters range.

In this case study 36 output variables were considered (the detailed energy production and economic benefit of the nine plants at each period ((9 * 3) + (9 * 1))). Even if the study considers the energy demand as one of the principal uncertainty sources, technical electricity supply challenges are out of the scope of this paper. As commented before, there are studies addressing those issues, including, switching on/off the transfer grid or availability of power supply in certain hours of a day (Silvente & Papageorgiou, 2017). Nevertheless, additional studies, extending this formulation and addressing electricity supply challenges, are also required to explore the differences in the solution in terms of economic, environmental and social performances.

4.1. SC superstructure

The proposed M-MP method is limited to continuous variables. Thus, the SC superstructure to be considered has been identified by optimizing the deterministic MILP problem assuming values of 50 €/Unit, 1,000 €/Unit and 50,000 kWh/month for the three uncertainty parameters ($\theta_1 = Demand$, $\theta_2 = WeightEnv_c$ and $\theta_3 = WeightSoC$, respectively) as displayed in Fig. 3. The mathematical model has been written in GAMS 23.8.2 and solved using CPLEX 11.0 on a PC Intel Core i7-2600 M CPU 2.70 GHz and 16.00 GB of RAM. The model contains 27,015 equations, 830,554 continuous and 1,106 binary variables and it entails a CPU time of approximately 300 s.

Fig. 3 shows that those communities with the highest population and biomass availability (Kumfia and Fakwasi) use all the pre-treatment/treatment equipment. The above is logical considering that it is cheaper to treat the raw material onsite rather than distribute it to communities with better geographical allocation. Similarly, for the case of Old Konkrompe all the pre-treatment/treatment equipment were installed, in order it can work as a central plant that treats the biomass for the closest communities. The above results match with the design found in the original paper for the economic optimization (Pérez-Fortes et al., 2012) which justifies the use of such a fixed structure for the following planning decisions.

The planning decisions are not displayed here, since these decisions change for further values in the uncertainty parameters. At this point, all the binary variables are fixed (i.e. the design decisions), thus, the model changes from MILP into an LP which reduced the computational effort required. Remarkably, the decisions to be made in the following sections includes raw material flows, production levels, and equipment/storage capacities, among others.

4.2. Meta-modeling training and evaluation

For this part of the method, a set of 150 sampling points was considered. Later, 50 points were used for validation while for the rest of the data four different sizes sets have been defined as training points as described during design of experiments (being 25, 50, 75 and 100 sampling points). The above avoids the use of common points between the training and validation data. On the other hand, in this particular case, the use of an increasingly size in the sampling points allows exploring its effect on the performance accuracy. Fig. 4, shows how the sampling points for the four sets provide uniform representations of the complete uncertainty space. Logically, the bigger the number of sampling points, the better the representation of the uncertainty space.

The LP optimization problem is deterministically solved for each one of those points. In this case, the mathematical model contains 27,015 equations and 830,554 continuous variables. For each iteration, the optimization process entails a CPU time of approximately 33 s.

The optimization procedure obtains sets of 25, 50, 75 and 100 solutions that, individually describe poor approximation for the global stochastic problem but can be used to evaluate the obtained meta-model. To demonstrate the uneven behavior of the economic performance as a function of uncertainty parameters a 3D plot that relates the *ENPV*, total demand and total *WeightEnv* was build (Fig. 5). It is important to comment that the missing parameter under evaluation (*WeightSoC*) is not represented in Fig. 5; however, the response surface is clearly irregular, confirming that the parametric function may be nonlinear although the basic problem formulation is linear.

From Fig. 5 it is clear that there is a messy behavior associated with the meta-model space, which compromises the reliable prediction of system performance. Thus, the relation between the values obtained by both, the surrogate model (estimation) and the traditional optimization values (real values), displays the accuracy of the resulting Kriging meta-model (for ENPV and global energy production) for all the training sets as shown in Fig. 6.

Fig. 6 clearly shows the obtained high accuracy. In particular, Fig. 6 (left) shows a line of 45 degrees for both outputs suggesting a highly accurate prediction of the optimization results. Nevertheless, additional analysis was made regarding the quality of the meta-model as a function of the size of the training set to stress the strategy benefits. In this line, Fig. 6 (right) demonstrates that the accuracy of the obtained solution increases as a function of the size of training sets. However, even if a better accuracy is obtained at large training size sets, Fig. 6 proves and justifies the use of the surrogate model even for small training sets (NRMSE < 0.01).

In summary, we can conclude that, for this case, a design of experiments of 75 sampling points is large enough to produce an accurate prediction of the objective function performance. Notice that the methodology allows finding the minimum number of sampling points to obtain representative results. The above has a significant impact on the computational effort, which represents a significant step forward for the current state of the art in decision-making literature for PSE.

4.3. Computational effort analysis

Until now, the meta-models analysis has been focused to the objective function (*ENPV*) and the global energy production function, however, the detailed analysis of the rest of the decision variables can be found in the Appendix A (including the energy production performances at each community). This subsection describes the strategy performance in terms of the computational effort, stressing the advantages achieved using the meta-model strategy. Table 2 shows the computational effort required at each step of the solution strategy using both the traditional optimization formulation and the ones based on Kriging meta-modeling. It is important to notice that a set of solutions from a deterministic problem is required as input for the Kriging meta-modeling. The stochastic MILP model that includes 100 scenarios and maximizes the ENPV as unique criterion cannot be solved in less than 48 h (172,800 s) due to CPU limitations (i.e., after this CPU time, CPLEX is unable to close the optimality gap below 5%). The above justifies

Table 1
The range of the input data.

Data	Type	Ranges	
		Lower	Upper
Environmental cost (€/unit)	Input	10	100
Social benefit (€/unit)	Input	100	10,000
Electricity demand 1 (kWh/month)	Input	49,916	61,009
Electricity demand 2 (kWh/month)	Input	50,536	61,767
Electricity demand 3 (kWh/month)	Input	51,156	62,524
Profit (€/year)	Output		
Energy production level at each facility (kWh/month)	Output		

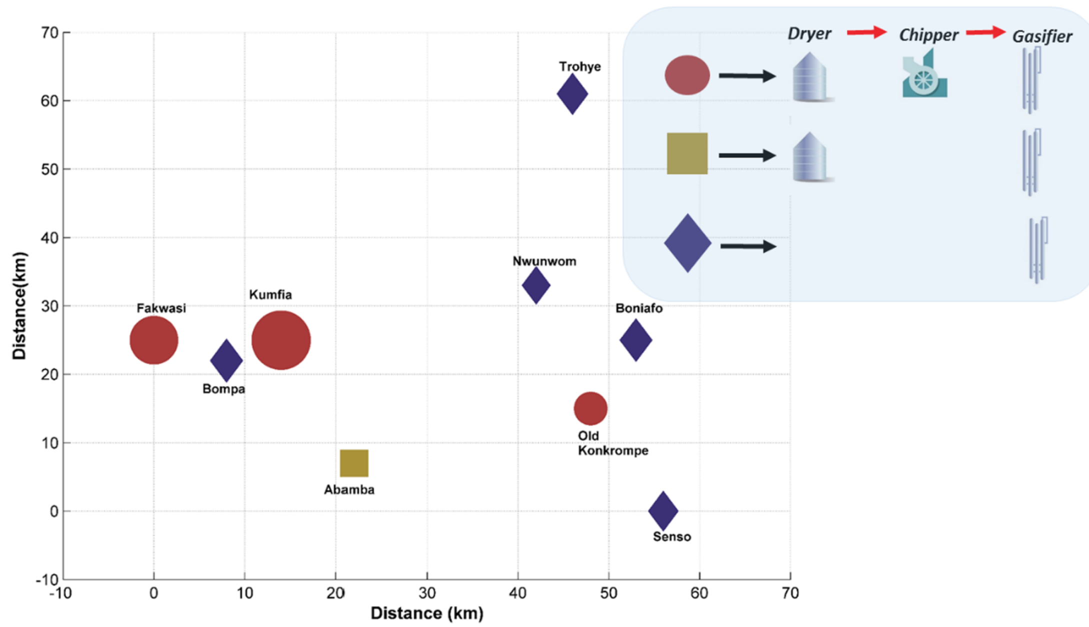

Fig. 3. Optimal deterministic bio-based energy production superstructure.

solving the LP problem deterministically and using such information to compare the computational effort obtained with the proposed Kriging modeling strategy. Remarkably, the values associated with different problem formulations and/or optimization issues are out of the scope of this analysis. In order to provide a better understanding of the computational efforts, it is important to mention that the model contains 24,515 equations and 820,350 continuous variables.

Table 2 shows the time consumed for each solution approach at five different categories. Each solution strategy presents its highest computational effort at a defined step. For the traditional mathematical programming, the optimization step requires the largest effort, while for the Kriging meta-modeling this is associated to the training/building step. For this case (150 sampling points) the difference in the computational effort is relatively low. However, a bigger difference is foreseeable for a complex model. From Table 2 it is clear that the time required for the training part shows the highest CPU time in the proposed strategy.

Additionally, the last evaluated category (re-optimization) in Table 2 emphasizes the most important quality of the meta-multi-parametric strategy presented here. Although the solution of the 150

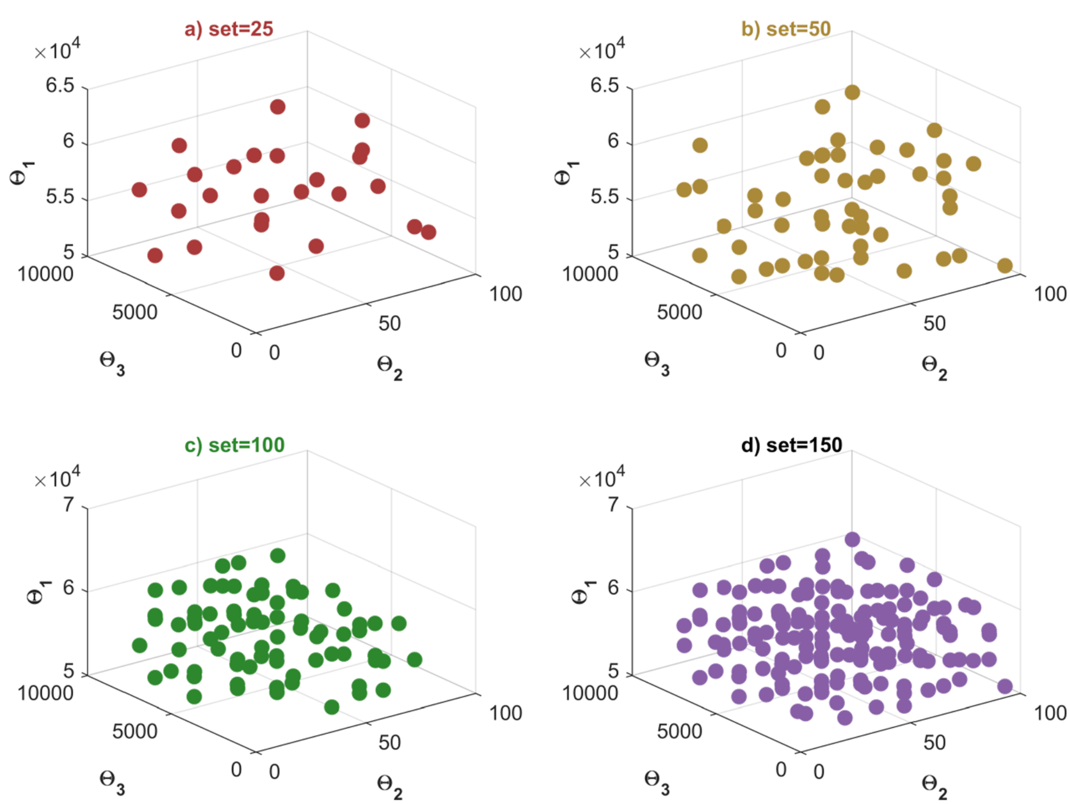

Fig. 4. Representation of the uncertainty space for different set size. (a) 25 sample points; (b) 50 sample points; (c) 100 sample points and (d) 150 sample points.

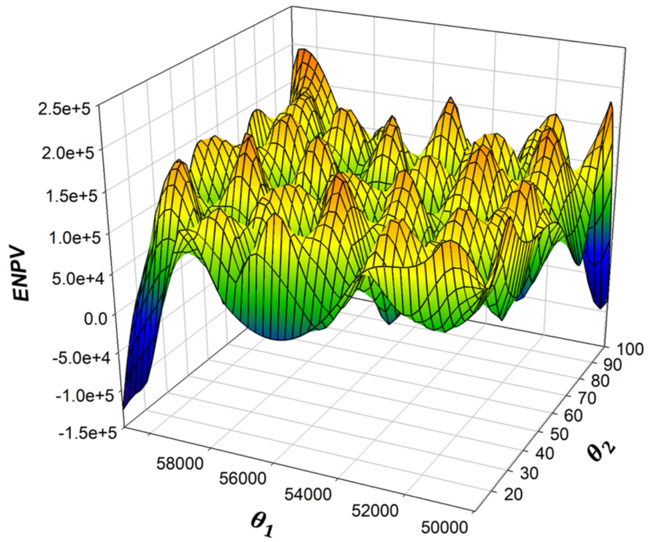

Fig. 5. The behavior of the optimal objective function for different values in *WeightEnv* (θ_2) and total demand (θ_1) parameters.

problems used for the training and validation requires a relatively high computational effort (this problem may become very important for models that are more complicated) after the definition of the surrogate model the optimization time drops dramatically. For this example, the time to obtain the solution is more than three orders of magnitude lower (1/7,085) and, of course, larger reductions are expected for more complex optimization problems.

Table 2
Computational effort required.

	Computational effort (CPU seconds/scenario)	
	Math. programming	Kriging meta-model
Model building	Variable	Variable
Solve optimization model (MILP)*	3,300	N/A
Training*	N/A	3,300
Validation*	N/A	70
Re-optimization (LP)*	33**	0.00466**
Total	4,322	4,370

* (CPU s).
** This value is for a single sample point.

Table 3
Input data for the two considered case studies.

Case study	θ_2 (€/unit)	θ_3 (€/unit)	θ_1 (t/month)		
			t1	*t2*	*t3*
1	27.4	7215.63	57448.71	59610.78	53708.64
2	67.6	332.03	52838.21	54849.14	60701.91

4.4. Optimal planning strategies

At this point, the high accuracy and low computational effort of the meta-models have been both discussed. Moreover, this section describes the importance of the meta-models results in the supply chain operation and production management. For this purpose, two particular sampling points were considered as case studies (Table 3).

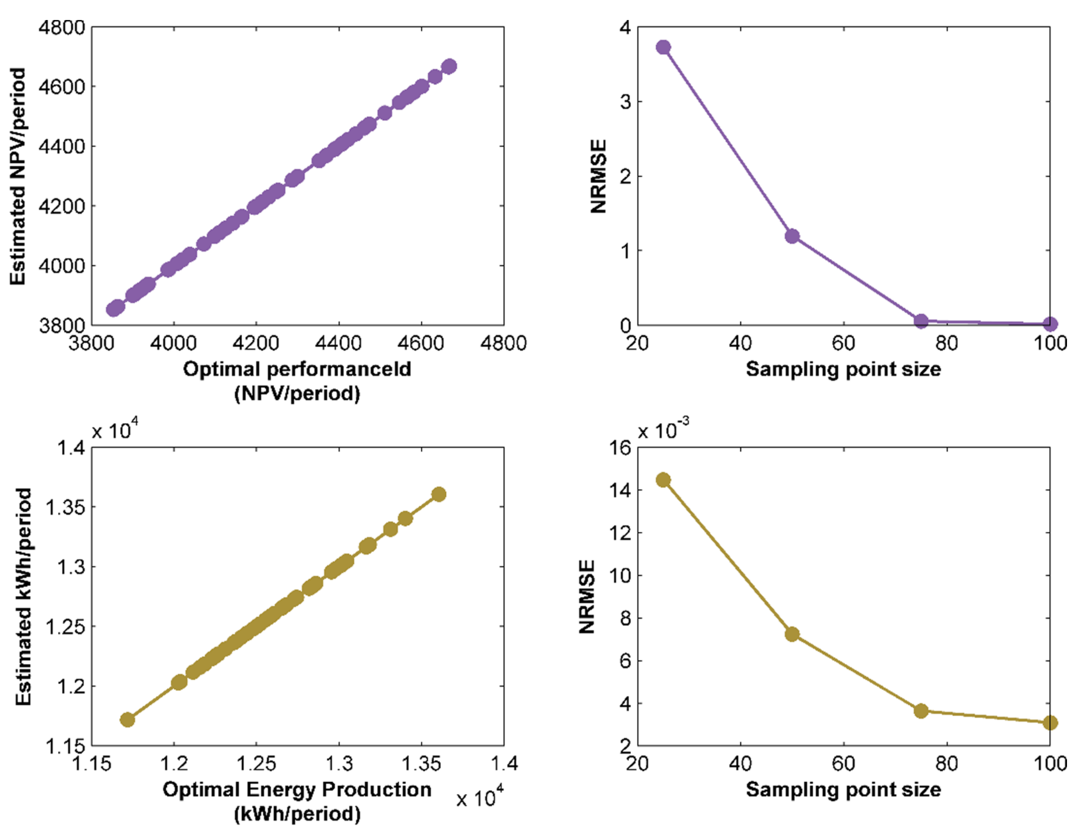

Fig. 6. Direct meta-model validation (Left) and Meta-model performance assessment as a function of the training set size (Right). In the top, the ENPV is considered while the bottom plots represent the global energy production.

Table 4
Output data for the two considered case studies.

Case study	Plant	Traditional optimization					Meta-model deviation***				
		Production (kWh/month)				OF	Production deviation				OF deviation
		t1	*t2*	*t3*	Total		*t1*	*t2*	*t3*	Total	
1	1	2,011	2,087	1,880	5,978	170,768	−1.3	−1.1	+0.2	−2.1	+8.2
	2	4,201	4,358	3,927	12,486		−2.0	−1.8	+0.6	−3.2	
	3	15,796	16,391	14,768	46,955		+10.8	−7.5	+2.1	+5.4	
	4	20,056	20,811	18,751	59,618		+14.3	−9.5	+2.2	+6.9	
	5	2,780	2,885	2,599	8,264		−0.9	−1.2	+0.8	−1.3	
	6	3,313	3,437	3,097	9,847		+2.1	−1.6	+0.5	+1.1	
	7	0,946	0,982	0,885	2,813		+0.2	−0.8	+0.6	+0.1	
	8	4,023	4,174	3,761	11,958		−1.3	−1.4	+0.9	−1.7	
	9	4,319	4,481	4,037	12,837		−1.5	−2.1	+0.2	−3.4	
2	1	1,850	1,920	2,125	5,896	14,908	+1.2	−1.1	+3.1	+3.2	−5.2
	2	3,863	4,010	4,438	12,312		+1.6	−2.1	+5.5	+5.0	
	3	14,529	15,082	16,691	46,302		−4.4	−7.4	+12.5	+0.6	
	4	18,447	19,149	21,192	58,788		−5.7	+10.0	+15.2	+19.5	
	5	2,557	2,654	2,938	8,150		+0.5	−1.8	+4. 1	+2.7	
	6	3,047	3,163	3,500	9,711		−0.8	−1.5	+4.2	+1.9	
	7	0,870	0,903	1,000	2,774		−1.0	−0.9	0.0	−1.9	
	8	3,700	3,841	4,251	11,792		+1.1	−2.4	+4.6	+3.2	
	9	3,972	4,123	4,563	12,659		+0.7	−2.4	+5.0	+3.3	

*** (10ˆ−3).

Table 4 shows the associated production levels of each plant/location and period obtained for the traditional optimization. Plants from one to nine represent Senso, Old Konkrompe, Fakwasi, Kumfia, Trohye, Bompa, Nwunwom, Boniafo, and Abamba respectively. Table 4 also shows the deviation of the results obtained through meta-model in comparison with the traditional optimization results.

Results shows that there is a very small difference in the quality of the solutions obtained, being the largest difference of 0.03%. Notice that planning decisions (such as production levels) are different for each case study. It is important to emphasize that disregarding the different total production at each plant, ultimately the demand is satisfied through different paths. For instance, plants two and three (Old Konkrompe and Fakwasi, respectively) have the largest energy productions at time periods one and two for the first case, while for the second case the period with the largest production is achieved at time three. Similar behaviors may be found for different sampling points. These results show that M-MP strategy is significantly sensitive and thus, small changes in the uncertain values can be properly managed. In addition to the sensitiveness of the strategy, it is important to illustrate that the M-MP allows also to completely emulate the system behavior across the entire uncertainty space. For example Fig. 7 shows the energy production at locations 2, 4 and 7 (Old Konkrompe, Kumfia, and Nwunwom respectively) for the whole uncertainty solution space. It is important to mention that the obtained meta-models in this work were generated using five different uncertainty sources (inputs in Table 1), however, in order to graphically illustrate the process behavior, only two out of these five series of uncertain values were plotted against the output variable (energy production).

From Fig. 7 it can be seen that the three different displayed locations show different energy production performances (first row). The above suggests that using this strategy a particular process control may be obtained. Particularly, for Kumfia and Nwunwom, θ_2 and θ_3 have a significant impact on the energy production while for Old Konkrompe the effect of θ_3 can be neglected. Similarly, for the second row, it is clear that for Old Konkrompe and Kumfia both uncertain parameters ($\theta_{1,(t1)}$ and θ_2) affect the energy production performance in completely different ways. Finally, the third row represents the energy demand at two different time periods, showing that there is not a significant effect in that combination of parameters at any energy production site. Remarkably, disregarding the application, the detailed process behavior (i.e. the effect of each variation over the system performance) can be extracted. In this particular case, it is important to highlight that the system behaviors shown in Fig. 7 represent only few outputs for few locations, although similar conclusions may be obtained from different output variables. Traditional stochastic optimization produces a single robust solution (i.e. one main plan works for any uncertainty realization) while for the M-MP the plan changes as a function of the uncertainty realizations. Even if the implementation of the M-MP optimization results may be challenging due to the highly dynamic process obtained (i.e. challenging logistic problem), the detailed knowledge of system behavior will be useful for the accurate assessment of the effects of the uncertain parameters, even if they are evolving along the time. Additionally, using such a detailed information data-driven decision-making strategy may significantly enhance addressing issues such as (i) the systematic estimation of the effects of the uncertain parameters over the objective function and (ii) the optimal solution identification for multi-criteria problems (i.e. selecting the alternative solution that performs better from the overall perspective, which may be sub-optimal for the traditional stochastic formulation).

It is important to comment that this work focuses on the M-MP strategy capabilities evaluation to assess SC planning. The production levels were the only outputs under analysis, proving the usefulness of M-MP. Notice that to implement the detailed the SC plan, additional meta-models have to be built in order to identify all the required outputs (such as material flows, etc.).

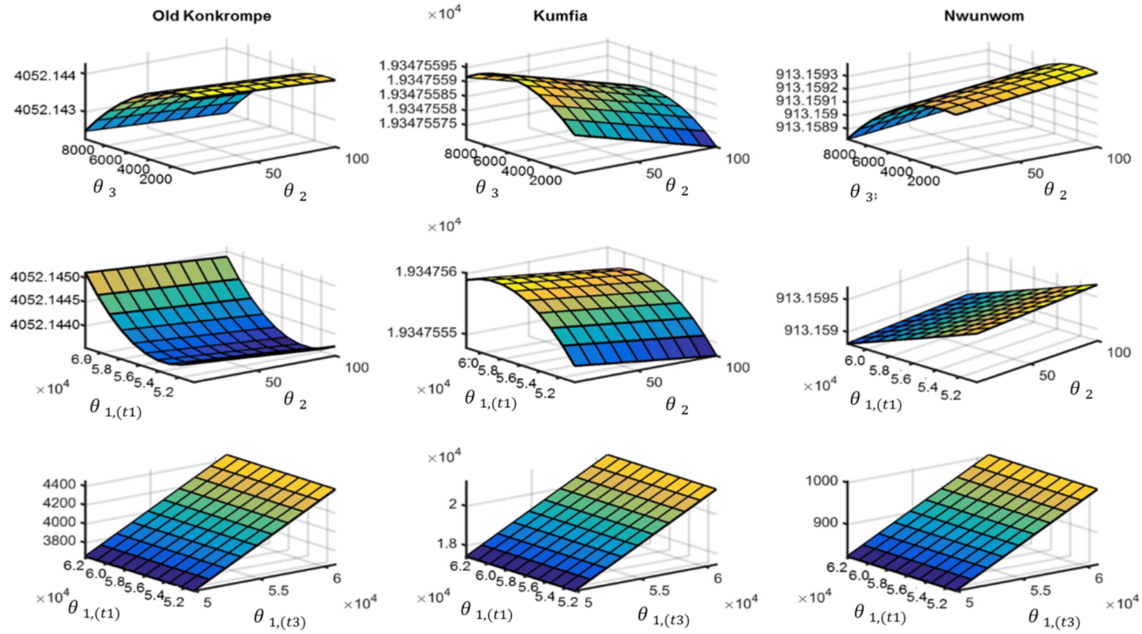

Fig. 7. Energy production behavior for Old Konkrompe, Kumfia and Nwunwom and uncertainty parameters variations in θ_1, θ_2 and θ_3.

5. Concluding remarks

In this contribution, a sophisticated strategy that integrates explicit optimization techniques and data-driven (surrogate) modeling has been presented. The strategy has been used to successfully address the tactical decision-making in a bio-based energy supply chain affected by different and independent uncertainty sources.

Numerical results show that the resulting data-driven model predicts the optimal decisions with high accuracy and time efficiency proving that the M-MP technique successfully addresses complex real-world problems. More importantly, this strategy is flexible enough to handle simultaneously several uncertainty sources disregarding their distributions, which represents the main strength of this method. Additionally, it has been proved that the proposed strategy provides information about the importance of each uncertainty source over the expected performance, which settles the basis for building a strategy able to identify those uncertain parameters having the most significant effect over the process.

In all these senses, the proposed M-MP strategy represents a step forward for the management of sustainable issues, becoming a feasible alternative to multiparametric programming since a single meta-model can cover the entire uncertainty space. Even if compared with traditional optimization approaches (such as two-stage stochastic programming), M-MP may be considered as a more challenging strategy since the detailed information on the system behavior provides additional advantages to be potentially combined with sophisticated decision-making strategies. For example, the whole set of solutions produced with M-MP may be evaluated through a multi-criteria decision-making strategy (ELECTRE-IV) to produce a systematic solution selection considering the decision-maker preferences.

Despite the simplicity of the presented case study, the results show that the methodology is robust and flexible enough to handle problems with a large amount of optimization variables as well as high model complexity, including highly non-linear models and mixed integer formulations.

To wrap-up, the two main advantages of applying the proposed data-driven decision-making strategy are:

I. The capacity to produce a very accurate prediction about the best way to operate a Supply Chain from very scarce information.
II. The individual identification of the effects of the different uncertainty sources over the process performance, further than the global accumulated result, settling the basis to combine this approach with other approaches (e.g.: scenario reduction strategies) to ensure a more robust solution.

Finally, it must be noted that the adjustment of a single continuous function to each decision variable hinders the applicability of the proposed approach to synthesis problems, since in these cases it is often required to use non-smooth functions to represent the decisions on the system structure. In order to overcome this limitation, future research may consider the application of clustering techniques (such as K-Means or DBSCAN) to manage the use of multiple functions that emulate the behavior of each decision variable, extending in this way the capabilities of the proposed approach.

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Appendix A. Detailed meta-model analysis/results

In this section, a detailed analysis of the results for each meta-model is performed. In particular, the effort (time) required to validate and train/fit the meta-model (See Fig. A1) is of significant interest.

From Fig. A1, notice that even if the time required for both, fitting and validation of a meta-model highly depends on the number of points used for such training, such a time can be negligible since the difference is of 1.5 s and 0.03 s for training and validation respectively. Also, it is important to notice that for the energy production meta-models (< 27) a significantly fitting time is required if compared with the Profit (> 27). The above can be explained since the majority of the considered uncertainty sources directly affect the objective function (*WeightEnv* and *WeightSoc*). This result is particularly interesting when discussing the selection of the most "important" uncertainty source(s) from a decision maker point of view. Logically, such a difference is not observed in the validation step since for this part the meta-model has been already produced. The validation of these meta-models guarantees the quality of the results obtained through the meta-model. Fig. A2 shows the relation of the results obtained by both, the traditional optimization ("Real values") against the M-MP optimization ("Estimated").

Currently, several studies of data-driven strategies suggest that the variables (meta-models) may be jointed in clusters to improve the estimation of traditional optimization behaviors (Shokry et al., 2017). Such a clustering strategy is particularly interesting when dealing with MI problems (due to the presence of binary variables). Nevertheless, such a strategy may be applied to problems involving exclusively continuous variables (which is the case under study), too. Thus, Fig. A3 shows the performance of the resulting meta-models using different clusters (from two to ten). Such a figure proves that for this particular case the use of clustering strategies may be omitted.

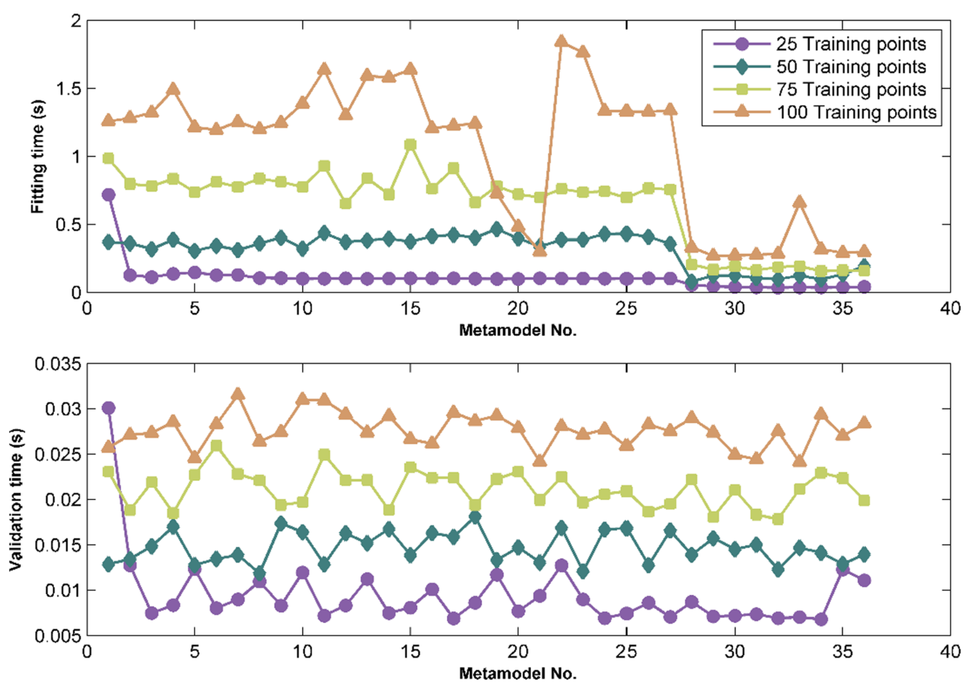

Fig. A1. The computational behavior of meta-model training and validation.

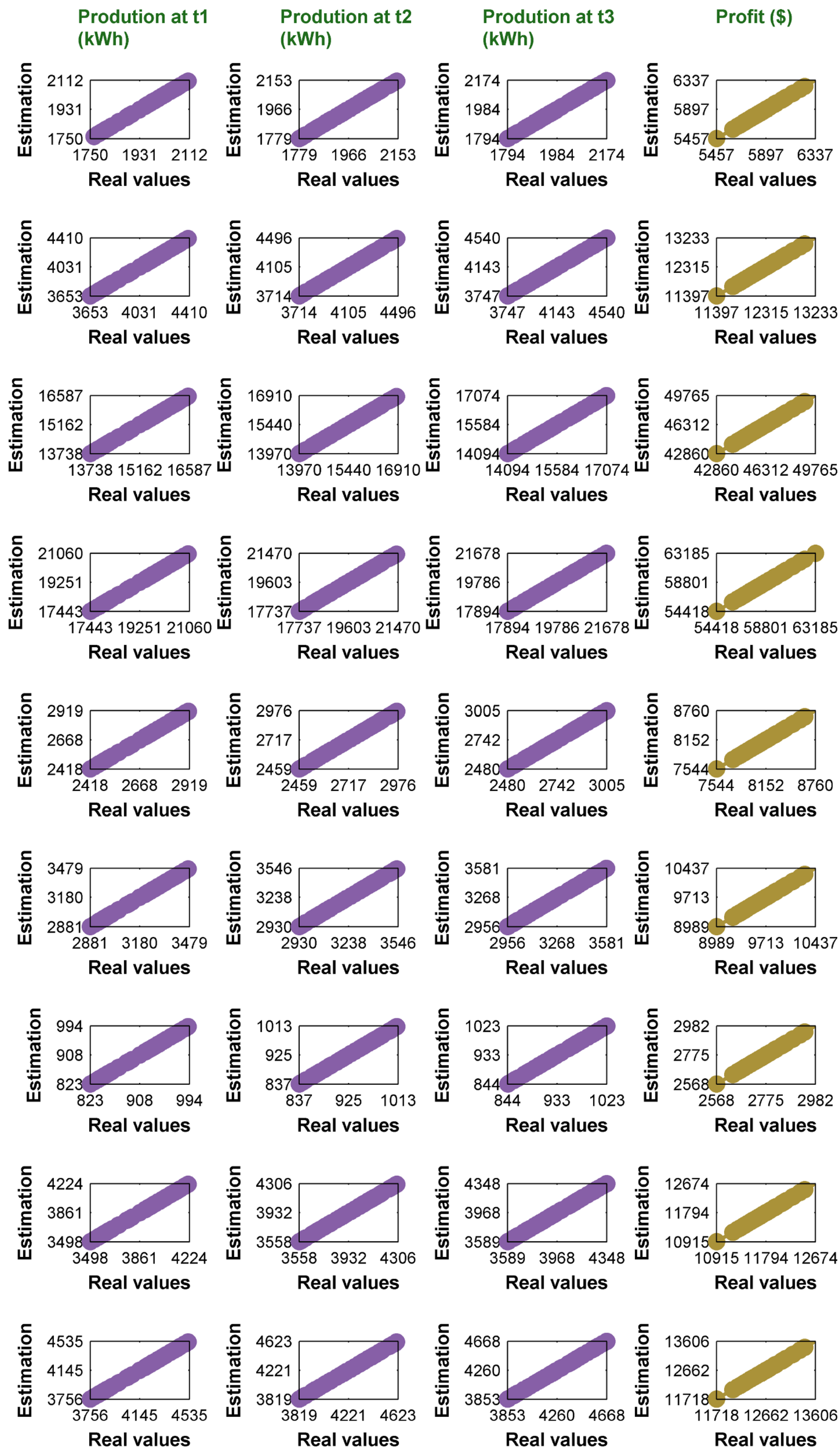

Fig. A2. The validation of the meta-models for each variable.

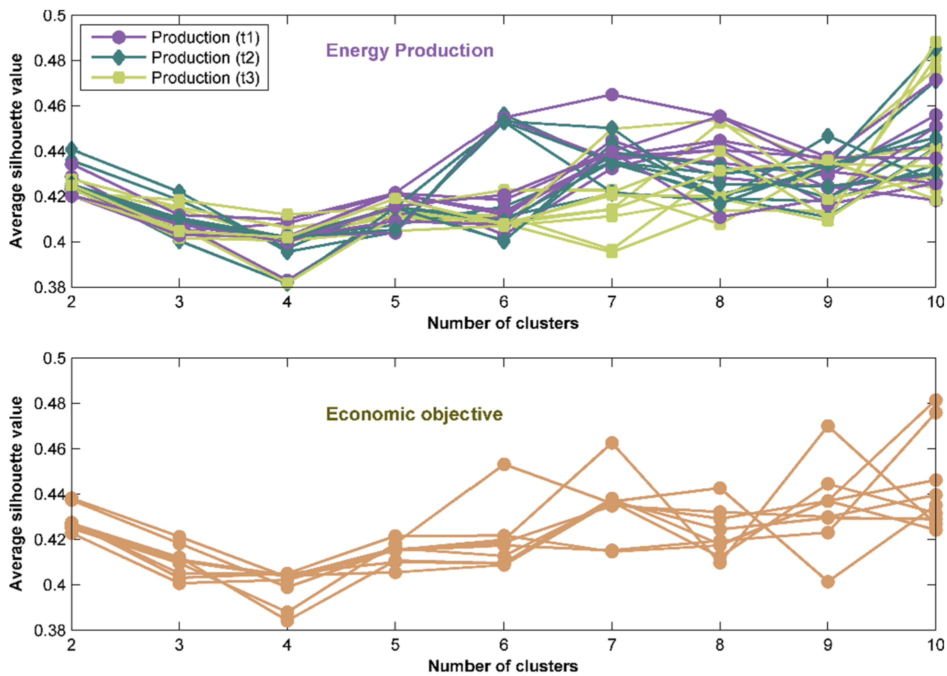

Fig. A3. Parallel coordinated plot for different defined clusters.

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