A robust sustainable optimization & control strategy (RSOCS) for (fed-)batch processes towards the low-cost reduction of utilities consumption

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1. Introduction

Recently, the social claim for the reduction in the pollution/environmental impact, originating from industrial activities, has paved the way to new research studies in the area of sustainable process design, optimization and real-time operation along with sustainable corporate-scale management. The primary aims of these new research areas consist of:

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- the development of new process configurations and the revamping of the existing ones towards improved sustainability;
- the online or offline search for sustainable operating conditions, limited to the single plant or extended to the whole corporate scale.

Many authors have been testing problems belonging to these research fields. Their efforts have produced a huge number of contributions concerning sustainable process design, offline optimization and corporate-scale management. For instance, studies concerning the optimization of supply-chain networks subject to additional sustainability constraints can be found in several papers. In detail, Giarola et al. (2014) and Ng and Lam (2013) study the problem limited to the field of bio-refineries while Vance et al.

(2013) focus on a specific problem implementation based on graph theory. Also, a strategy for the sustainable scheduling of batch productions is described in Yue and You (2013). Moreover, sustainable process design methods for batch units are reported in papers like (Halim and Srinivasan, 2009, 2008) and the application of a sustainability metric to the selection of the best reactive path for the succinic acid production is described in Pinazo et al. (2015). On the contrary, methodologies aimed at achieving sustainable real-time process operation are still at an early stage, thus being more suitable to be investigated. In fact, only limited work has already been carried out in this area: Rossi et al. (2014b) address the sustainable deterministic dynamic optimization and optimal con-trol of a batch reactor while Luo et al. (2014) and Zhu et al. (2014) report on the application of deterministic optimal control strate-gies to reduce energy costs in manufacturing processes.

In parallel to this sustainability-oriented research, the last two decades have widely demonstrated the effectiveness of non-linear model predictive control (NMPC) and dynamic real-time optimization (DRTO) techniques for optimal online process management. Many authors have confirmed that NMPC can be used to effectively and safely control even strongly non-linear systems, typical of chemical plants. In detail, Balasubramhanya and Doyle (1997), Joly and Pinto (2004), Mahadevan et al. (2001) and Viganò et al. (2010) clearly prove what is stated above limited to a distillation column, a nylon 6,6 production process, a fed-batch bio-reactor and a CVD reactor, respectively. In addition, also robust NMPC strategies, which can be applied to uncertain controlled systems, have been successfully developed for many types of manufacturing systems like bio-processes (Logist et al., 2011), special micro-organisms cultures (Santos et al., 2012) and polysilicon rods production (Vallerio et al., 2014). Similarly, DRTO algorithms have shown to be an appealing solution for the real-time optimal management of hard-to-operate process units: batch distillation columns (Greaves et al., 2003) and reactors (Arpornwichanop et al., 2005), fed-batch reactors (Pahija et al., 2013), polymerization autoclaves (Zavala et al., 2005), and so on. Limited to batch productions, detailed studies have also been performed on which type of control systems can be conveniently coupled with DRTO schemes (Pahija et al., 2014). However, despite a huge number of NMPC/DRTO-like schemes is now available, almost none of them is configured to allow for process sustainability in addition to process performance.

Therefore, it appears that the target of sustainable real-time process operation could be achieved through the development and application of sustainable NMPC/DRTO-like methodologies or alike strategies. This work addresses the theoretical and practical description of a framework that falls into this category. In detail, a robust sustainability-oriented model-based integrated optimization & control framework for (fed-)batch processes is proposed, which aims at simultaneously providing its controlled system with profitable and clean management policies in real-time. The clean nature of this methodology shows up in its target of ensuring low-cost reduction in utilities usage while its robustness is revealed in the capability of handling also uncertain controlled systems. Moreover, since it works in real-time, also the effect of any incoming external perturbation is considered, analysed and optimally handled. To the best of the knowledge of the authors of this paper, no simultaneously sustainability-oriented and robust frameworks of this type can be found in the literature, thus the strategy proposed in this paper appears to be relevantly novel. Moreover, it also seems appealing for future real industrial applications towards a cleaner and more energy-efficient future.

In the rest of the paper, at first the aforementioned robust sustainable model-based integrated optimization & control framework will be described with underlying theoretical concepts. Then a validation case study, based on a fed-batch version of the well-known Williams–Otto process, will be employed to demonstrate its tangible benefits. Finally, some conclusions will be drawn.

2. The robust sustainable optimization & control strategy (RSOCS)

The robust sustainable DRTO/NMPC-like strategy, proposed in this work, can be classified as a multi-scenario online optimization and control framework coupled with a suitable set of utilities-usage-related penalty terms that are added to its objective function. The usage of the multi-scenario logic (see section [2.2] for further details) ensures the robustness required to manage uncertain controlled systems while the employment of the set of penalty terms (see section [2.3] for further details) allows to balance the need for process performance and that for low utilities consumption, i.e. low environmental impact. By ensuring the best trade-off between performance and environmental impact, the proposed strategy can be thus considered sustainability-oriented.

The aforementioned robust sustainability-oriented DRTO/NMPC-like methodology is configured as a multi-step approach that includes an offline and online phase. The offline phase, referred to as PHASE I, aims at optimally computing some key parameters that are subsequently employed in the online phase, indicated as PHASE II. A simplified graphical representation of how the overall strategy is configured is shown in Fig. 1.

Before going ahead, a preliminary introduction on the logics on which these two steps (PHASE I and PHASE II) are based is necessary.

PHASE I can be divided into two different blocks, i.e. the identification of a suitable set of scenarios, relating to the controlled system, and the optimal tuning of the abovementioned penalty terms. The two blocks must be carried out in series since the scenarios selection has a strong influence on the optimal tuning of the penalty terms. The detailed explanation of how the scenarios set is computed, based on the probability density function (PDF) of the uncertain parameters of the controlled system, is addressed in section [2.2]. Then the optimal tuning procedure for the penalty terms will be addressed in section [2.3].

PHASE II is much simpler than PHASE I and simply consists of the application of the properly configured robust sustainability-oriented DRTO/NMPC-like strategy to a controlled system in real-time. Since no relevant difficulties can be found in this phase, no detailed additional explanations will be added on this topic in the following.

By looking at Fig. 1, the reader should notice that the proposed robust sustainable online optimization and control framework must rely on a NMPC/DRTO-like algorithm. Here, this algorithm is chosen to be the BSMBO&C method (Rossi et al., 2014a, 2014c). A brief theoretical description of how this framework works is reported in section [2.1], but many more details can be found in the BSMBO&C-related references.

Finally, before starting to discuss the content of sections [2.1–2.3], let three remarks be introduced.

At first, observe that the proposed robust sustainability-oriented DRTO/NMPC-like strategy includes relevant novel contents. Indeed, it is able to provide an uncertain (fed-)batch process with sustainable operating conditions in real-time, allowing for the effect of any incoming external perturbation. This makes it unique up to now, at least for what concerns the authors' knowledge.

Secondly, note that the novel strategy proposed here is designed in a smart way as to concentrate all the computational-demanding operations in PHASE I, that is offline, thus preserving its real online applicability. Moreover, almost all the operations included in PHASE I can be parallelized, thus further reducing computational times also in the offline phase.

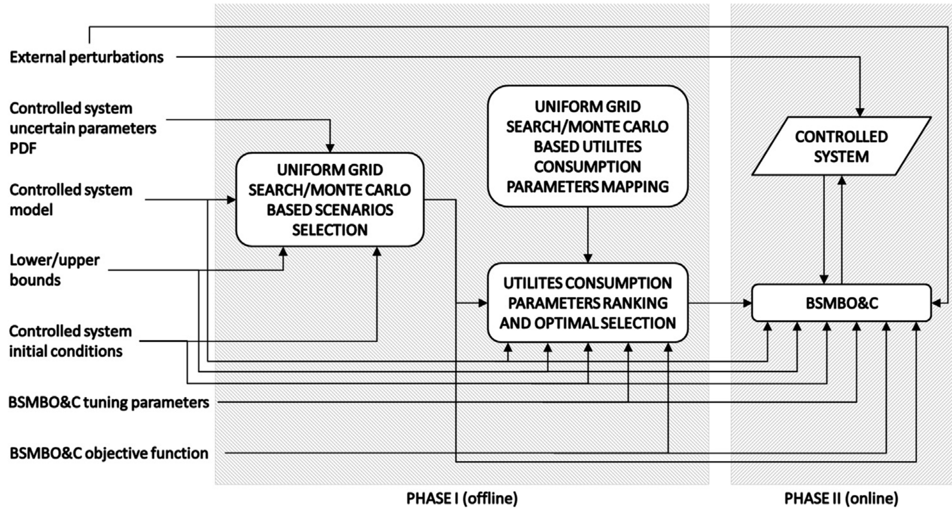

Fig. 1. Schematic representation of the robust sustainable optimization & control strategy (RSOCS).

Finally, notice that the reported novel strategy aims at dynamically and optimally balancing environmental impact and process performance, but the environmental impact is said to depend only on the level of utilities consumption. This limitation may seem relevant but could be theoretically removed as long as the resulting numerical complexity is reasonable. Indeed, the described strategy could be immediately generalized to measure process environmental impact including several different non-utilities-related sources like the production of harmful sub-products and toxic/dangerous effluents, the process energy consumption levels, etc. Detailed information on this generalization step will be probably addressed in detail in future works.

In conclusion, the proposed robust sustainability-oriented DRTO/NMPC-like framework is not only novel but also optimized in terms of computational burden and very flexible (at least in theoretical terms). This should make it suitable for real industrial applications in the near future.

2.1. The BSMBO&C algorithm: a brief theoretical insight

BSMBO&C (the acronym stands for Batch Simultaneous Model-Based Optimization and Control) is an advanced framework for the all-in-one online optimization and/or optimal control of (fed-) batch processes. In this work it will be employed in its integrated optimization and control mode but it might be also used as online optimizer or optimal controller only.

One of its specific and unique features is the capability of optimizing the performance of the controlled system by adjusting both its manipulated variables and its batch cycle time at the same time, based on a fully user-defined performance criterion (objective function). This typically allows it to ensure better performances than other existing tools for the NMPC and DRTO of (fed-)batch processes.

A simplified version of the algorithm, which aims at providing a simple but clear idea of how it is configured, is reported in Fig. 2. There BSMBO&C is described as a two-phase method including a first initialization phase and then a subsequent iterative phase. The initialization is executed only once and is used to provide the algorithm with the required user-supplied input data:

- the controlled system model;
- the objective function (i.e. two performance indicators);
- the tuning settings;
- the lower/upper bounds on the controlled system states, manipulated variables and batch cycle time.

The iterative phase consists of the repetition of one single iteration, also called BSMBO&C basic step, until a stopping condition is fulfilled, which implies that the optimal batch time has been reached. The basic step is constituted of several operations that are carried out in series:

- an optimization to evaluate the optimal values of the manipulated variables and the batch time in the next control action (optimization sub-step);
- the application of the optimal control action to the controlled process and the update of the control horizons of the manipulated variables;
- the measurement and analysis of the controlled system response;
- the convergence condition check and the consequent decision on whether to proceed with a new basic step.

Up to now, a simple but intuitive idea of how BSMBO&C operates has been conveyed. The interested reader can find many more details on the framework in its two reference papers (Rossi et al., 2014a, 2014c). However, some additional explanations on the mathematical structure of the algorithm's objective function must be added. BSMBO&C objective function is reported in Eq. (1) in a simplified fashion. Notice that it is made of two user-defined performance indicators (f and g) and two regulatory terms, i.e. an anti-ringing term (AR_T) and a slope control term (SC_T). The f and g functions are user-supplied data and must be defined such that the fg product measures the controlled system performance (the greater fg, the lower the controlled process performance and vice versa). The slope control and anti-ringing terms are introduced in order to prevent strong and repeated oscillations in the profiles of the controlled system states and manipulated variables, respectively. The precise formulation of AR_T and SC_T is not of interest for the purpose of this paper but can be found in the BSMBO&C reference papers. Instead, it is interesting to briefly describe the guidelines that can be used to choose f and g. The function g is the primary objective function and should account for the performance of a single batch cycle. f is the complementary objective function and should be used to handle multi-cycle problems as, for instance, scheduling-like problems. The importance of this additional

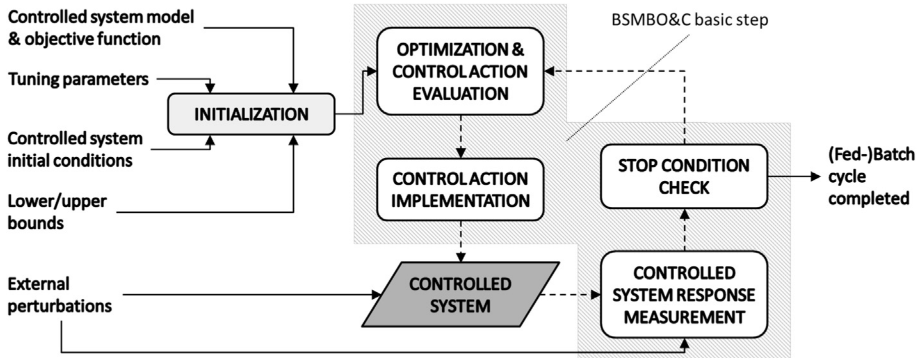

Fig. 2. Simplified graphical description of the BSMBO&C algorithm.

information on the user defined performance indicators will become clear in the following.

$$f_{obj}^{BSMBO\&C} = f(g + AR_T + SC_T) \tag{1}$$

One last remark on BSMBO&C concerns its numerical implementation. Its coding is realized in C++, relying on BzzMath library (Buzzi-Ferraris, 2014; Buzzi-Ferraris and Manenti, 2012) as numerical engine for both integration and optimization purposes. Since BzzMath integrators and optimizers are very performing and perfectly suitable to solve strongly non-linear problems, BSMBO&C can be successfully applied also to processes with strongly non-linear dynamics. This suggests its wider application range. This BSMBO&C feature, along with its effectiveness and efficiency, are the main reasons why this framework is selected as basic NMPC/DRTO-like strategy of the robust sustainability-oriented DRTO/NMPC-like approach.

2.2. The scenario-based approach for ensuring robustness and its integration into the BSMBO&C strategy

The scenario-based approach for ensuring robustness is a method that can be used to improve a NMPC/DRTO-like algorithm as to make it able to efficiently manage also uncertain controlled systems. In other words, it is a strategy to improve a NMPC/DRTO-like algorithm robustness. The idea on which it is based is quite simple. An online optimization/optimal control problem on an uncertain controlled process (i.e. a process whose model contains uncertain parameters) is converted into a problem of the same type but on a proper set of exact controlled processes. This artificial set of controlled process units is also referred to as scenarios set, thus the acronym multi-scenario that is used to refer to the methodology.

It is clear that the scenario-based approach for ensuring robustness is general and can be applied to any NMPC/DRTO-like algorithm. However, here the discussion is only limited to its application to the BSMBO&C framework.

Since the effectiveness of such a strategy is strongly influenced by the scenarios selection logic, this is the first topic to address. The methodology proposed here for the scenarios set evaluation is made of three steps in series:

- definition of a finite space from where to draw scenarios;
- identification of two scenarios, referred to as the nominal and worst case;
- definition of the additional scenarios to complete the set.

The identification of the finite space from which to draw scenarios can be readily done, assuming that the probability density function (PDF) of the uncertain parameters of the controlled system is known. It is only necessary to identify the region of the uncertain parameters space corresponding to a cumulative probability that equals a certain confidence threshold.

The identification of the nominal case is straightforward as it corresponds to the maximum of the PDF of the uncertain parameters. Instead, the worst case can be found via sensitivity analysis, performed on the controlled system uncertain parameters and manipulated variables. Indeed, the scenarios space can be mapped, using either Monte-Carlo methods or a uniform grid search, for the scenario that minimizes the distances between the controlled system states and their upper/lower bounds.

Finally, the additional scenarios can be chosen based on a mapping of the level surfaces of the PDF of the uncertain parameters using either Monte-Carlo or a uniform grid search. The choice of the first or the second mapping option depends on the number of uncertain parameters in the controlled system model.

Once the scenarios set is completely determined, all the controlled system models, corresponding to the selected scenarios, are assembled into a pseudo controlled process model that is supplied to the BSMBO&C as an input data. Moreover, the BSMBO&C performance functions are chosen as a weighted sum of the f and g functions referred to the single scenarios, where the weighting factors are defined as the normalized probability densities of the scenarios. All the concepts in this last paragraph are translated into mathematical expressions by Eq. (2) and Eq. (3).

$$\begin{cases} \mathbf{I}_M^s \dfrac{d\mathbf{w}^s}{dt} = \mathbf{h}^s(\mathbf{w}^s, \mathbf{m}, \mathbf{d}^*; \mu^s) \\ \mathbf{w}^s(t^*) = \mathbf{w}^{s,*} \end{cases} \xrightarrow[\mathbf{h}^R = \{\mathbf{h}^1 \ldots \mathbf{h}^s \ldots \mathbf{h}^{N_s}\}]{\substack{\mathbf{I}_M^R = \left\{\mathbf{I}_M^1 \ldots \mathbf{I}_M^s \ldots \mathbf{I}_M^{N_s}\right\} \\ \mathbf{w}^R = \left\{\mathbf{w}^1 \ldots \mathbf{w}^s \ldots \mathbf{w}^{N_s}\right\}}} \begin{cases} \mathbf{I}_M^R \dfrac{d\mathbf{w}^R}{dt} = \mathbf{h}^R\left(\mathbf{w}^R, \mathbf{m}, \mathbf{d}^*\right) \\ \mathbf{w}^R(t^*) = \mathbf{w}^{R,*} \end{cases} \tag{2}$$

$$\begin{cases} f^s \\ g^s \end{cases} \rightarrow \begin{cases} f^R = \sum_{s=1}^{N_s} p_s f^s \\ g^R = \sum_{s=1}^{N_s} p_s g^s \end{cases} \tag{3}$$

In Eq. (2) and Eq. (3), $\mathbf{I}_M^R$ is a diagonal singular/non-singular identity-like matrix, **w**, **m** and **d** represent the states, manipulated variables and external perturbations relating to the controlled system, μ identifies the uncertain parameters of the controlled system model and N_s is the total number of scenarios in the scenarios set. In addition, p_s indicates the normalized probability density of the generic scenario while superscript/subscript s refers to the generic scenario and superscript R refers to the entire set of scenarios.

As a final remark observe that typically this scenario-based approach ensures the same robustness guaranteed by the worst-case approach (i.e., the highest possible robustness) but takes to much higher performances of the controlled process unit. Therefore, this methodology can be considered a smart way to overcome the typical problem of the strategies for ensuring robustness, i.e. the loss in performance. This is why the scenario-based strategy for ensuring robustness is chosen to be merged with the BSMBO&C framework to protect it against controlled process uncertainty.

2.3. The utilities-usage-related penalty terms approach and its application to the BSMBO&C framework

The utilities-usage-related penalty terms approach is a simple way to force a NMPC/DRTO-like algorithm to provide its controlled system with sustainability-oriented (i.e. profitable but low-utilities-usage) online optimization/control policies. It works by adding a set of penalty terms to the objective function of the NMPC/DRTO-like strategy, which depend on the utilities usage and a set of tuning coefficients, referred to as utilities consumption parameters. These parameters can be used to specify the importance of the penalty terms, thus imposing the user's own concept of sustainability.

Similarly to section [2.2], the utilities-usage-related penalty terms approach could be applied to any NMPC/DRTO-like framework but here is addressed only limited to the application to the BSMBO&C.

The mathematical structure of the penalty terms to be added to the BSMBO&C objective function is reported in Eq. (4). There the arrows stand for replacement, i.e. f^R is not modified and g^R is replaced with the expression on the right of the corresponding arrow. Moreover, UI_h is the integral of the h-th controlled system utility flux, λ_h is the h-th utility consumption parameter and N_u is the number of utilities accessed by the controlled system.

$$\begin{cases} f^R \rightarrow f^R \\ g^R \rightarrow g^R + \sum_{h=1}^{N_u} \lambda_h UI_h \end{cases} \tag{4}$$

Notice that the only g^R function is modified. Indeed, adding penalties proportional to the utilities usage in this performance indicator is equivalent to add penalties to the overall BSMBO&C objective function (see the information included in section [2.1] on the BSMBO&C objective function and Eq. (1)).

Once the structure of the utilities-usage-related penalty terms has been described, the method for the evaluation of the utilities consumption parameters (λ) must be addressed. These parameters affect the function g^R that depends on the scenarios selected for the multi-scenario robustness strategy (see section [2.2]). Therefore, the methodology for their evaluation must depend on this scenarios set too. The authors of this work have found that an effective way to compute reasonably optimal values for the λ_h coefficients is the following:

- A set of λ guesses, including $\lambda = 0$, is chosen based on Monte Carlo or a uniform grid search algorithm;
- For each λ set, selected in the previous bullet, N_s multi-scenario BSMBO&C-driven optimization & control problems are solved in nominal conditions, i.e. no external perturbations are considered; these several simulations are performed with the same λ-dependent objective function (Eq. (4)) but different controlled systems that are chosen with the same features (i.e. values of the uncertain parameters) of the scenarios selected in section [2.2];
- Depending on the results coming from the nominal multi-scenario BSMBO&C-based simulations, each λ set is ranked based on a proper ranking index reported in Eq. (5) and described below (the lower the ranking index, the better the λ set and vice versa);
- The λ set with the best ranking is the one selected as optimal set of utilities consumption parameters.

The ranking index (RI), mentioned in the third bullet, is given by the combination of three different sub-indexes, each accounting for a certain property of a λ set. The first sub-index (RI_1) allows for the reduction in the utilities consumption compared to the $\lambda = 0$ case, the second (RI_2) accounts for the controlled system performance variation compared to the $\lambda = 0$ case and the third (RI_3) measures how homogeneous the utilities consumption reduction is among the N_s multi-scenario BSMBO&C-driven simulations (remind that for each λ set N_s multi-scenario BSMBO&C-based simulations are carried out). The mathematical representation of the ranking index and its three sub-indexes is reported in Eq. (5).

$$\begin{cases} RI = RI_1 RI_2 RI_3 \\ RI_1 = \sum_{h=1}^{N_u} \omega_h \dfrac{<UI>_h}{<UI^0>_h} \\ RI_2 = 1 + \chi \left| \dfrac{<fg> - <f^0 g^0>}{<f^0 g^0>} \right| \\ RI_3 = \sum_{h=1}^{N_u} \omega_h \sum_{s=1}^{N_s} p_s \left| \dfrac{\Delta UI_{hs} - \Delta <UI>_h}{\Delta <UI>_h} \right| \end{cases} \tag{5}$$

Each ranking sub-index contains global information, averaged on the results of all the N_s multi-scenario BSMBO&C-driven simulations, and local information, referred to each single multi-scenario BSMBO&C-based simulation. The rigorous mathematical description of these global and local informations is included in Eq. (6), Eq. (7) and Eq. (8). Inside these equations, UI_{hs} stands for the h-th utility consumption in the s-th multi-scenario BSMBO&C-based simulation performed with a non-zero λ set and UI_{hs}^0 is the equivalent of UI_{hs} but refers to a simulation where λ is null. Moreover, $(fg)_s$ is the product of the f and g functions related to the s-th multi-scenario BSMBO&C-based simulation performed with a non-zero λ set and $(f^0 g^0)_s$ is the equivalent of $(fg)_s$ but derives from a simulation where λ is null. Notice that UI_{hs}, UI_{hs}^0, $(fg)_s$, $(f^0 g^0)_s$ are all computed with the data derived from the optimal operation of the controlled systems (not the models of these controlled systems) related to the multi-scenario BSMBO&C-driven simulations. Moreover, the $(fg)_s$ and $(f^0 g^0)_s$ terms are computed based on the original f and g performance indicators, without the addition of the λ-based penalty terms.

$$\begin{cases} <UI>_h = \sum_{s=1}^{N_s} p_s UI_{hs} \\ <UI^0>_h = \sum_{s=1}^{N_s} p_s UI_{hs}^0 \end{cases} \tag{6}$$

$$\begin{cases} <fg> = \sum_{s=1}^{N_s} p_s (fg)_s \\ <f^0 g^0> = \sum_{s=1}^{N_s} p_s \left(f^0 g^0\right)_s \end{cases} \tag{7}$$

$$\begin{cases} \Delta UI_{hs} = \dfrac{UI_{hs} - UI_{hs}^0}{UI_{hs}^0} \\ \Delta <UI>_h = \dfrac{<UI>_h - <UI^0>_h}{<UI^0>_h} \end{cases} \tag{8}$$

The ranking sub-indexes also contain adaptive parameters, named ω_h and χ. The $\boldsymbol{\omega}$ coefficients are a set of user-defined parameters that can be used to account for the different importance of different utilities on the environmental impact of the controlled process. It is essential for these parameters to be normalized, i.e. their sum must equal one. Instead, χ is a coefficient that can be used to impose how important the controlled system performance is in terms of ranking index. In other words, by changing χ it is possible to define which operating regions of the controlled system can be considered sustainable. The selection of the ω_h and χ coefficients must be carried out by the user of the robust sustainability-oriented DRTO/NMPC-like strategy and, unfortunately, no general rules can be defined to guide this specific choice. The best values for these coefficients are too problem dependent.

A final remark must be added on the strategy for the evaluation of the utilities consumption parameters. It is typically the most computational demanding block of the entire PHASE I. However, its configuration is such that all its operations can be executed in parallel, thus significantly reducing the required computational time. A precise reader might ask why the optimal λ set evaluation is not handled via optimization. The answer stands in the multi modal-nature of the optimization problem that is, for this reason, almost impossible to solve with reasonable effort. In the end, this is one of the cases in which the simple beats the complex.

3. A case study: the Williams–Otto fed-batch process

The robust sustainability-oriented DRTO/NMPC-like strategy, proposed in this paper and described in its theoretical concepts in section [2], is now applied to a case study. Observe, once again, that the DRTO/NMPC-like algorithm, which the strategy relies on, is the BSMBO&C framework. Coming back to the case study description, it employs a Williams–Otto fed-batch reactor as target system, whose model is supposed to contain uncertainties in the refrigeration apparatus. The fed-batch reactor is modelled as described in section [3.1]. Moreover, the process performance measure is a user-supplied information (see section [2.1]) and is reported in section [3.1] too.

The test case is designed to demonstrate the effectiveness of the robust sustainable DRTO/NMPC-like strategy in itself and compared to a standard robust optimization & control strategy, which does not provide any sustainability guarantee. Therefore, all the test simulations are performed twice, once with the complete methodology described in section [2] and once with the only BSMBO&C framework coupled with the scenario-based robustness strategy (multi-scenario BSMBO&C). The simulations couples are then compared. Moreover, since the Williams–Otto fed-batch reactor to be managed is subject to uncertainties, several simulations are performed for different real reactors, i.e. supposing different controlled processes.

Finally, in order to provide a reasonably accurate validation, two different cases are considered. In the first (2Δ case), two unexpected process perturbations are supposed to influence the controlled fed-batch reactor while in the second (1Δ case) a single critical perturbation is supposed to occur. These two different cases are used to demonstrate the effectiveness of the proposed strategy in both every-day and unlikely/unusual process conditions (for each of the two cases the whole set of simulations mentioned above is repeated).

The detailed description of the numerical results of the test case is reported in sections [3.2] and [3.3]. In detail, section [3.2] contains information on both the selected scenarios for the scenario-based robustness strategy and the selected optimal set of utilities consumption parameters. Instead, section [3.3] includes all the results concerning the case study simulations with both the 2Δ and 1Δ perturbations set.

3.1. Williams–Otto fed-batch reactor: modelling and related process performance measures

The Williams–Otto fed-batch process is a well-known literature process that is commonly used to test model-based online optimization and/or control systems. Here the fed-batch reactor, in which the process is carried out (Fig. 3), is modelled by means of some assumptions: single phase reacting mixture, perfectly mixed reactor vessel and cooling jacket, temperature-independent thermodynamic properties of the reacting medium. Under these assumptions, the achieved model equations are those shown in Eq.(9) and include a complete set of component material balances (first ODE), a global material balance (second ODE) and the reactor and cooling jacket thermal balances (third and fourth ODEs). In Eq.(9):

- N_R and N_C are the number of chemical reactions and components;
- R_l, ν_{il} and $\Delta H_{R,l}$ are the rate of the l-th reaction, the stoichiometric coefficient of the i-th component in the l-th reaction and the heat of the l-th reaction;
- U is the global heat transfer coefficient between the reacting mixture and the jacket cooling fluid;

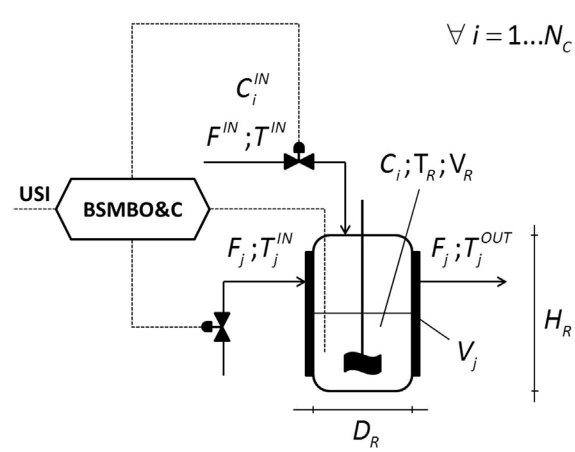

Fig. 3. Williams–Otto fed-batch reactor layout (USI stands for user-supplied information).

- Cp_i, Cp_j and ρ_j are the specific heat of the i-th component in the reacting mixture, the coolant specific heat and the coolant density.

The meaning of all the other symbols can be directly and clearly inferred from Fig. 3.

and F^{IN} as the only adjustable inputs and will consider the coolant fluid as the only process utility.

Once the model and the features of the Williams–Otto fed-batch reactor have been conveyed, it is necessary to define the performance indicators with respect to which the reactor must be optimally managed. Here a set of economic f and g functions is

$$
\begin{cases}
\dfrac{dC_i}{dt} = \dfrac{F^{IN}}{V_R}\left(C_i^{IN} - C_i\right) + \displaystyle\sum_{l=1}^{N_R} \nu_{il} R_l \quad \forall i = 1 \ldots N_C \\
\dfrac{dV_R}{dt} = F^{IN} \\
\dfrac{dT_R}{dt} = \dfrac{4U}{D_R \displaystyle\sum_{i=1}^{N_C} C_i Cp_i}\left(T_j^{OUT} - T_R\right) + \dfrac{F^{IN} \displaystyle\sum_{i=1}^{N_C} C_i^{IN} Cp_i}{V_R \displaystyle\sum_{i=1}^{N_C} C_i Cp_i}\left(T^{IN} - T_R\right) - \dfrac{\sum_{l=1}^{N_R} \Delta H_{R,l} R_l}{\sum_{i=1}^{N_C} C_i Cp_i} \\
\dfrac{dT_j^{OUT}}{dt} = \dfrac{F_j}{V_j}\left(T_j^{IN} - T_j^{OUT}\right) + \dfrac{4UV_R}{D_R V_j \rho_j Cp_j}\left(T_R - T_j^{OUT}\right)
\end{cases}
\tag{9}
$$

Some essential complementary information to Eq. (9) must be added. The Williams–Otto process initial conditions, operational constraints (lower/upper bounds) and kinetic scheme are the first of these additional data and are summarized in Table 1. Another essential information that is needed is the nature of the uncertainty located in the heat transfer apparatus. Here this uncertainty is

chosen, since g is set to the inverse of the dimensionless net income per batch cycle (see Eq. (10)). Inside this equation, the subscripts/superscripts BC are applied to a variable to identify its value at the end of a batch cycle, i.e. in t_{BC}. The meaning of all the other symbols can be either inferred from Table 1 or has already been explained.

$$
\begin{cases}
f = 1 \\
g = \dfrac{\left[\begin{array}{l} V_R^0\left(C_A^0 PM_A EV_A + C_B^0 PM_B EV_B\right) + C_B^{IN} PM_B EV_B \displaystyle\int_0^{t_{BC}} F^{IN} dt - \\ + V_R^{BC}\left(C_C^{BC} PM_C EV_C + C_E^{BC} PM_E EV_E + C_G^{BC} PM_G EV_G + C_P^{BC} PM_P EV_P\right) + \end{array}\right]}{C_A^0 V_R^0 (PM_C EV_C - PM_A EV_A - PM_B EV_B)}
\end{cases}
\tag{10}
$$

supposed to be concentrated into the heat transfer coefficient, thus being the only uncertain parameter of the fed-batch reactor model. In detail, U is considered normally distributed with assigned mean and variance. All the U-related statistical data can be found in Table 1 too. Finally other essential miscellaneous data consist of the required thermodynamic properties, the fed-batch reactor vessel sizing and so on. All these remaining information is, once again, included in Table 1.

As a last remark on the Williams–Otto fed-batch reactor, observe that the only two independent variables that can be used to influence its operation are the coolant flow (F_j) and the feed flow (F^{IN}) while its only utility flux is F_j. Therefore, the proposed robust sustainability-oriented optimization and control strategy will use F_j

In conclusion, notice that the function f is set to one in Eq. (10). This means that the users, i.e. the authors of the paper, want the performance of the Williams–Otto fed-batch reactor to be optimized on the single batch cycle. No scheduling-like problems are addressed in this case study.

3.2. The scenarios and utilities consumption parameters selection: numerical results

Thanks to the previously conveyed information on the Wiliams–Otto process/fed-batch reactor, PHASE I of the proposed robust sustainability-oriented optimization & control approach (see Fig. 1) can be performed. Notice that the confidence

Table 1
Williams–Otto process/fed-batch reactor data.

Kinetic scheme	$A + B \rightarrow C$	(1)	$R_1 = k_1^0 \exp\left(-\frac{E_1}{T_R}\right) C_A C_B$	$k_1^0 = 1.3833\text{E}+5$; $E_1 = 6.45\text{E}+3$
	$B + C \rightarrow P + E$	(2)	$R_2 = k_2^0 \exp\left(-\frac{E_2}{T_R}\right) C_B C_C$	$k_2^0 = 6.0098\text{E}+7$; $E_2 = 8.7785\text{E}+3$
	$C + P \rightarrow G$	(3)	$R_3 = k_3^0 \exp\left(-\frac{E_3}{T_R}\right) C_C C_P$	$k_3^0 = 2.2288\text{E}+11$; $E_3 = 1.1155\text{E}+4$
Heats of reaction	$\Delta H_{R,1} = -1.8510\text{E}+5$; $\Delta H_{R,2} = -2.5765\text{E}+5$; $\Delta H_{R,3} = -5.053\text{E}+5$			
Specific heats and densities (reacting mixture and coolant)	$Cp_A = 321.204$; $Cp_B = 127.14$; $Cp_C = 352.288$; $Cp_E = 166.212$; $Cp_G = 844.132$; $Cp_P = 426.617$; $Cp_j = 4.186$; $\rho_j = 1\text{E}+3$			
Molecular weights (reacting mixture)	$PM_A = 142$; $PM_B = 60$; $PM_C = 202$; $PM_E = 81$; $PM_G = 383$; $PM_P = 181$			
Reactor structure	$D_R = 1$; $H_R = 3.5$; $V_j = 0.8236$			
Global heat transfer coefficient	$U_{ave} = 0.8$; $U_{std\,dev} = 0.1$ (U is normally distributed)			
Relevant lower/upper bounds	$F^{IN,MAX} = 1\text{E}-3$; $F_j^{MAX} = 1\text{E}-2$; $T_R^{MAX} = 335$; $V_R^{MAX} = 2.15$			
Initial conditions	$C_A^0 = 1.5$; $C_B^0 = 0.25$; $C_{i \neq A,B}^0 = 0$; $V_R^0 = 1$; $T_R^0 = 308$; $T_j^{OUT,0} = 308$			
Feed conditions and coolant inlet temperature	$C_B^{IN} = 1$; $C_{i \neq B}^{IN} = 0$; $T^{IN} = 298$; $T_j^{IN} = 308$			
Reactants/products price	$EV_A = 25$; $EV_B = 75$; $EV_C = 200$; $EV_E = 0$; $EV_G = 0$; $EV_P = 40$			
Units of measure	amount of substance [kmol]; mass [kg]; length/area/volume [m]/[m^2]/[m^3]; time [s]; temperature [K]; energy [kJ]; prices [€]			

Table 2
Principal numerical results coming from the scenarios and utility consumption parameters selection.

Selected scenarios	Nominal case $U = 0.8$	Worst case $U = 0.48$	Other scenarios $U = 0.58667$ $U = 0.69333$ $U = 0.90667$ $U = 1.01333$ $U = 1.12$
Optimal utilities consumption coefficients	$\lambda_j = 4.122\text{E}-4$ (there is only one utility consumption parameter and it relates to F_j)		
Units of measure	See Table 1 for further information		

threshold, required for the first step of the scenarios selection procedure (see section [2.2]), is set to 99.9%. Moreover, both for the third step of the scenarios selection procedure and for the utilities consumption parameters mapping the uniform grid search option is preferred to Monte Carlo method. This choice appears reasonable because there is only one uncertain parameter in the fed-batch reactor model and only one utility flux to be considered in this version of the Williams–Otto process. Finally, it has to be highlighted that the scenario selection procedure is limited to choose only seven scenarios, in order to preserve the online applicability of the proposed robust sustainability-oriented DRTO/NMPC-like strategy.

The numerical results, achieved through the aforementioned operations, are summarized in one table (Table 2) and two figures (Figs. 4 and 5). Some interesting remarks can be added based on these results. These comments are detailed in the following lines.

Dealing with the outcomes coming from the scenarios selection procedure, observe that:

- the worst case scenario corresponds to the minimum allowed value of the heat transfer coefficient based on the 99.9% confidence threshold (this is expected and reasonable);
- The selected confidence threshold (for the first step of the scenarios selection procedure) and number of scenarios seem to guarantee a reasonably accurate description of the uncertainty in the Williams–Otto process model (see the chart in Fig. 4).

As a last comment, note that the two aforementioned bullets suggest that the scenarios selection procedure appears to require only a limited number of scenarios to ensure reasonable robustness in PHASE II. This indirectly confirms that the proposed robust sustainability-oriented DRTO/NMPC-like method can be applied in real-time not only in paper but also in real life.

Coming now to the results of the evaluation of the optimal utilities consumption parameters, the following comments can be made:

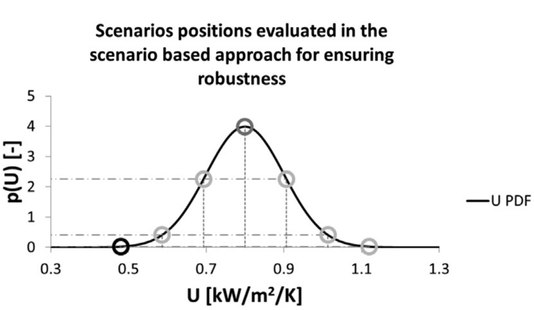

Fig. 4. Graphical representation of the scenarios selection step output (p(U) identifies the heat transfer coefficient probability density function (PDF) while the black, dark grey and light grey circles stand for worst case, nominal case and additional scenarios).

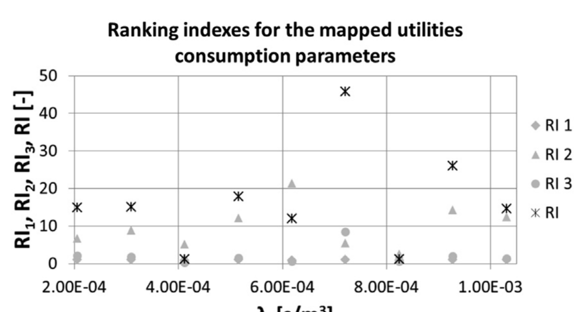

Fig. 5. Trends of the ranking index and sub-indexes for the only employed utility consumption parameter (λj).

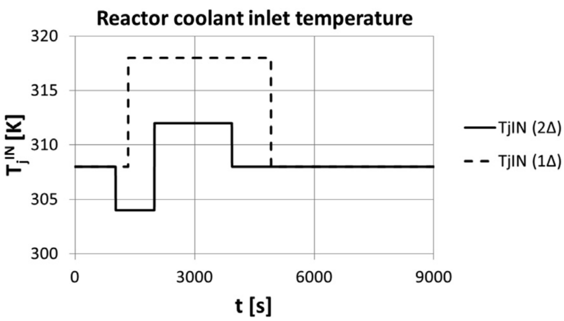

Fig. 6. External perturbations imposed in the 2Δ and 1Δ cases.

- Fig. 5 confirms that the ranking index (RI) and sub-indexes (RI_1, RI_2, RI_3) trends for the only utilities consumption parameter (λ_j) are multimodal as already anticipated in section [2.3] (λ_j refers to the Williams–Otto fed-batch reactor cooling medium);
- Fig. 5 also suggests that different λ_j values might take to very similar RI values, i.e. several λ_j might take to similar effects (the λ_j value reported in Table 2 is evidently that corresponding to the minimum RI).

These remarks convey the idea that the identification of the best values for the utilities consumption parameters is not trivial and might require a very fine (uniform/random) search grid. However, this is not a serious problem since PHASE I of the proposed robust sustainability-oriented DRTO/NMPC-like methodology has to be executed offline and could take up to relevant time to be completed without negatively affecting the real-time applicability of PHASE II (the only online phase).

3.3. The simulations results: a sustainability comparison

By employing the results belonging to PHASE I, PHASE II can be carried out (see the beginning of section [3] for details on the simulations performed here). The only additional information that is needed is the nature of the external perturbations affecting the Williams–Otto fed-batch process unit. These data are shown in Fig. 6. Notice that the only coolant inlet temperature is used as external disturbance. This choice is reasonable because this vari-able is the most influential on the fed-batch reactor operation.

The results achieved in the execution of PHASE II are summarized in several different charts, shown in Figs. 7–10. In detail, Fig. 7 contains the optimal Williams–Otto fed-batch reactor operation supposing its heat transfer coefficient (U_{real}) to equal 0.7125 kW/m^2/K. Figs. 8 and 9 show the same data included in Fig. 7 but for different U_{real} values, i.e. 0.8 kW/m^2/K and 0.8875 kW/m^2/K, respectively. By looking at these three figures, important remarks can be drawn:

- in all the three circumstances the proposed robust sustainability-oriented DRTO/NMPC-like strategy is able to significantly reduce the coolant consumption (F_j^{int}) while limited changes can be observed in the optimal temperature profile (and in the optimal composition profiles, even though not explicitly reported) of the fed-batch reactor;
- the trend highlighted in the previous bullet is preserved both in the case of every-day process perturbations (2Δ case) and in the case of unexpected critical disturbances (1Δ case);
- the application of the utilities-usage-related penalty terms approach does not introduce significant additional oscillations in the optimal profiles of the manipulated variables (F_j and F^{IN}) (the oscillations in F_j and F^{IN} optimal trajectories might seem important but it is only a false impression due to the charts abscissa scale);
- the application of the utilities-usage-related penalty terms does not take towards easier bounds violations (no bounds violations are observed with and without the employment of these penalty terms).

All these remarks bring to several conclusions. First, the proposed robust sustainable optimization & control framework seems

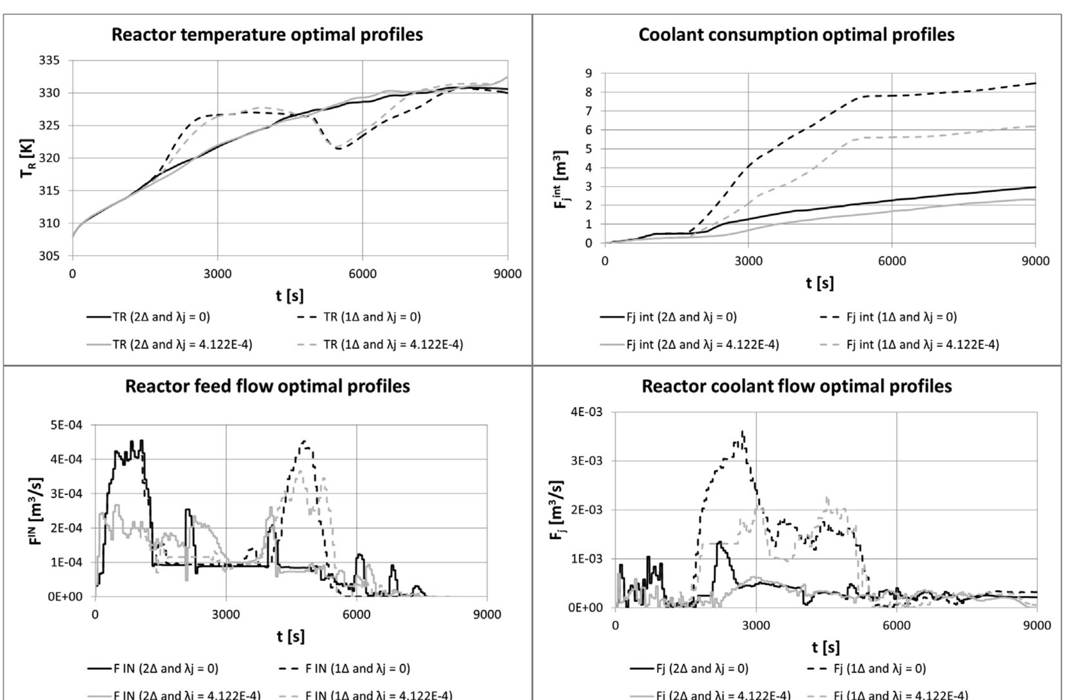

Fig. 7. Williams–Otto fed-batch reactor optimal operation with ($\lambda_j \neq 0$) and without ($\lambda_j = 0$) the employment of the utilities-usage-related penalty terms approach ($U_{real} = 0.7125$ kW/m^2/K).

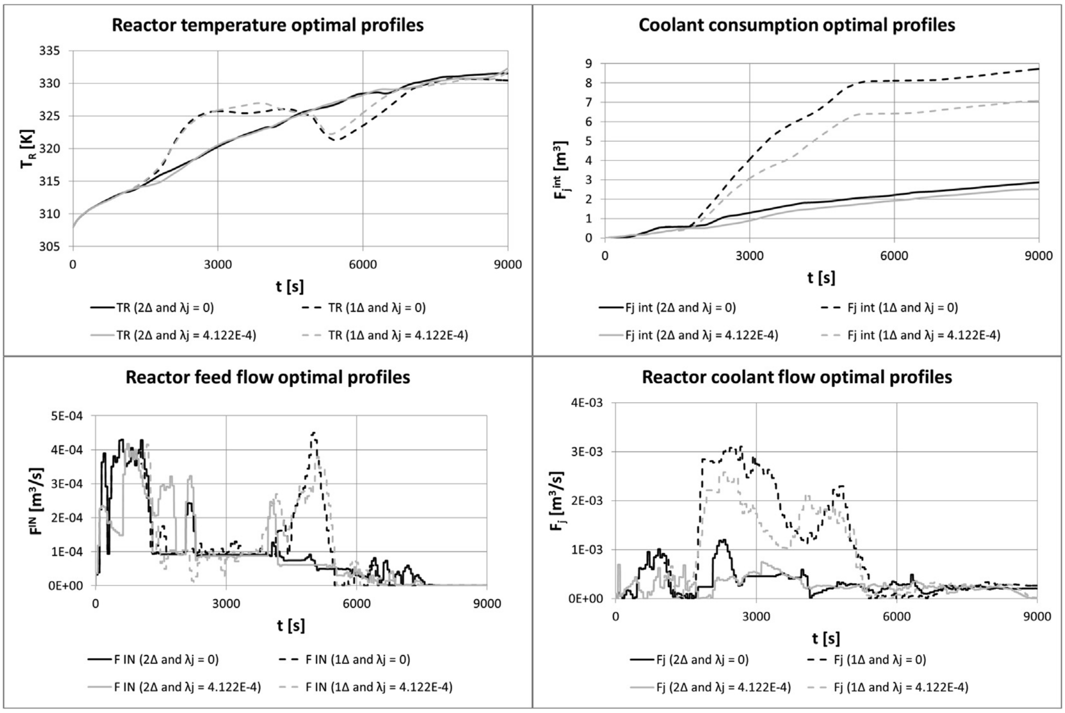

Fig. 8. Williams–Otto fed-batch reactor optimal operation with ($\lambda_j \neq 0$) and without ($\lambda_j = 0$) the employment of the utilities-usage-related penalty terms approach ($U_{real} = 0.8$ kW/m^2/K).

to be able to significantly reduce the process coolant consumption (i.e. the environmental impact) per batch cycle without seriously affecting the process performance in each batch cycle. On the one hand, it means that the proposed framework seems effective in itself because it seems to be able to optimally manage a process aiming at its maximum sustainability. On the other hand, it means that the proposed framework can provide its controlled system with much better management policies, in terms of process sustainability, than a standard robust optimization & controlled strategy. Second, no harmful effects (increased instability, increased probability of bounds violations, increased risk of control losses, etc.) are introduced through the application of the proposed

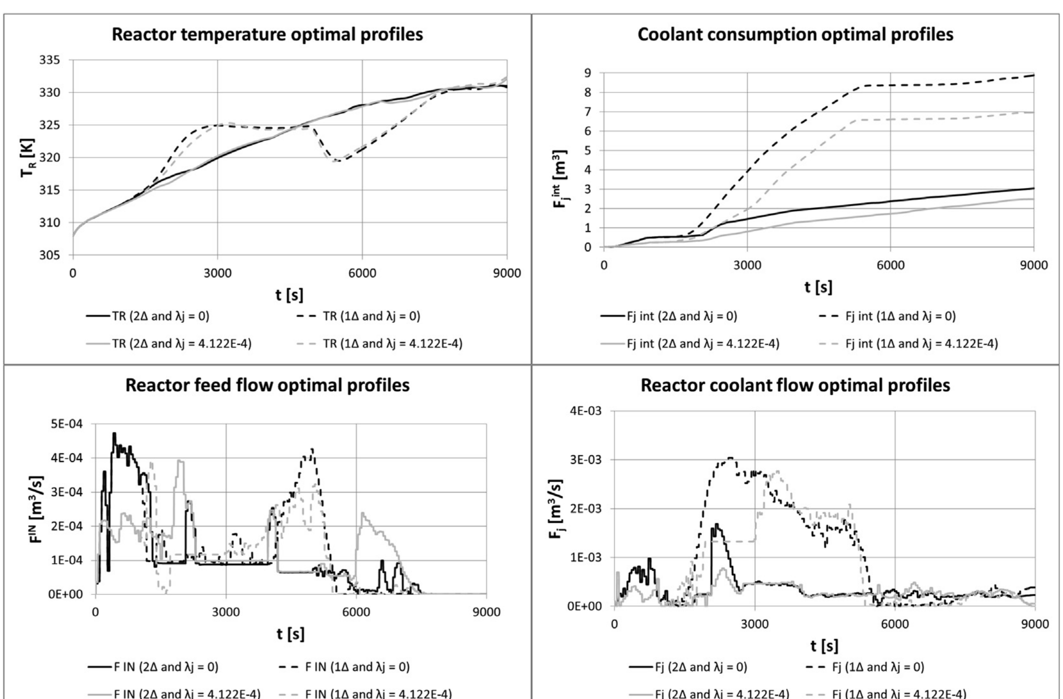

Fig. 9. Williams–Otto fed-batch reactor optimal operation with ($\lambda_j \neq 0$) and without ($\lambda_j = 0$) the employment of the utilities-usage-related penalty terms approach ($U_{real} = 0.8875$ kW/m^2/K).

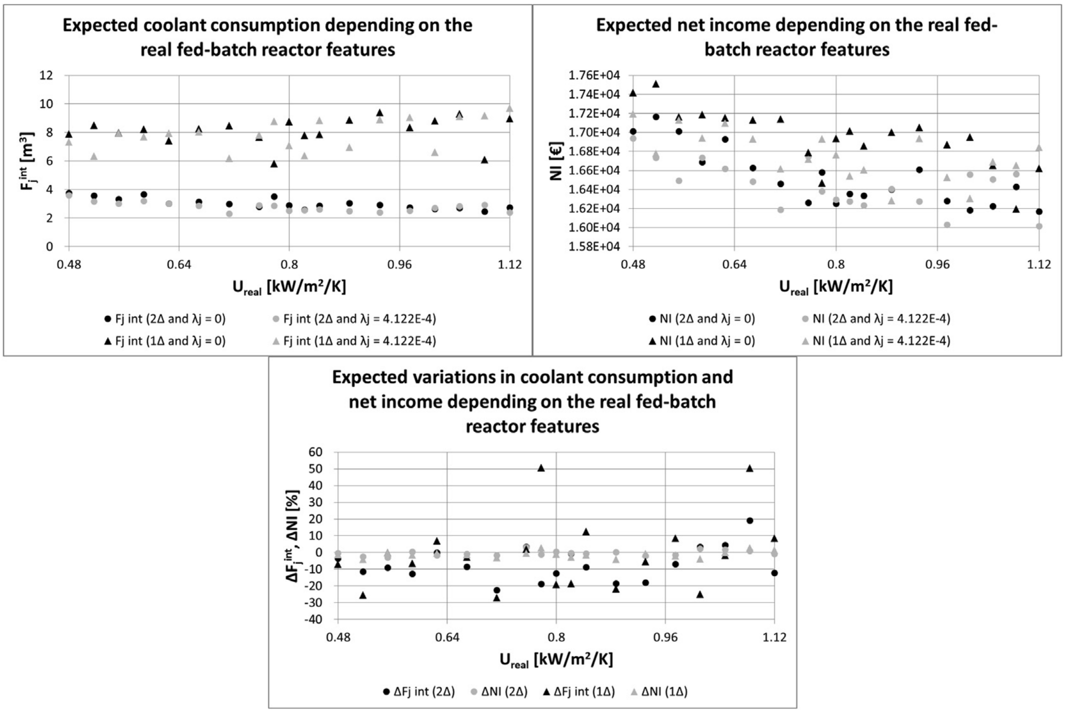

Fig. 10. Effect of the employment of the utilities-usage-related penalty terms approach on the performance and sustainability in the optimal operation of the Williams–Otto fed-batch reactor.

strategy. Third, the proposed strategy seems to fairly operate even in the case of critical process disturbances. This means that no safety hazards, e.g. thermal runaways, explosions, etc., can be promoted even in the case of huge process perturbations.

The first conclusion is supported by the data shown in Fig. 10. There the variation in the coolant consumption (F_j^{int}) and net income (NI) per cycle, with respect to the situation achieved when a standard robust optimization & control framework is applied, is reported as a function of U_{real}. Indeed, observe that almost for any possible controlled fed-batch reactor the coolant consumption is significantly reduced while the net income per cycle is almost unchanged. Unfortunately, Fig. 10 also highlights that the proposed robust sustainability-oriented optimization & control framework is not always effective in the case of critical unexpected perturbations affecting the controlled system. Indeed, in the 1Δ case, the coolant consumption is significantly increased in correspondence with about one fourth of the map-ped values of U_{real}. This ineffectiveness depends on the method employed for the selection of the utilities consumption param-eters, which is based on nominal multi-scenario BSMBO&C simulations. Future works will be aimed at removing this weakness.

Nevertheless, the proposed robust sustainability-oriented optimization & control framework demonstrates to be effective in promoting process sustainability in itself and compared to a standard robust optimization & control strategy in the case of standard process operation. Moreover, it shows the same effectiveness, in about 75% of cases (on a statistical basis), even when critical disturbances are encountered. Finally, it shows to be reliable and safe since it does not promote oscillations in the controlled system independent inputs, easier bounds violations, etc.

In the end, the proposed robust sustainable optimization & control framework seems a well-performing approach that would deserve to be tested on real lab scale/industrial equipment in the future.

4. Conclusions

In this work, a robust sustainability-oriented online optimization & control framework for fed-batch processes is proposed, described and tested on a well known benchmark for this type of algorithms, a Williams–Otto fed-batch process. The framework is designed to provide its uncertain controlled system with an online management policy aimed at the best trade-off between process performance and utilities consumption, i.e. process environmental impact. In simpler words, it is aimed at ensuring real-time process sustainability under uncertainty. This latter capability represents the real novelty of the proposed approach. The results coming from the validation case study suggest that the framework is very effective in case of typical process operation while it is partially effective in the case of unusual/unlikely critical process disturbances (future works will go towards the removal of this weakness). As a consequence, the proposed robust sustainability-oriented online optimization & control framework probably deserves to be applied to lab scale/industrial processes to check its real effectiveness in real life applications.

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