Online model-based optimization and control for the combined optimal operation and runaway prediction and prevention in (fed-)batch systems

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1. Introduction

Batch/fed-batch processes are employed in several industrial sectors including, for instance, the pharma contest, the fermentation of sugars towards bio-chemicals and bio-fuels, the polymers production, the manufacturing of ultrapure materials for micro-electronics, etc. On the one hand, many of these sectors produce high added-value products but, on the other hand, the related safety risks are relevant too. Indeed, especially thermal runaways may be quite common in this kind of productions. Because of these twofold nature of (fed-)batch processes, authors are typically divided between those studying efficient and reliable solutions for their economic optimization and/or optimal control and those investigating robust approaches to ensure their stability and safety.

The research work aimed at finding suitable options for the optimization and optimal control of discontinuous equipment is traditionally related to the non-linear model predictive control strategies (NMPC) and the dynamic real-time optimization approaches (DRTO). NMPC/DRTO-like algorithms have been studied since the 90s (Eaton and Rawlings, 1991) but their application to the (fed-)batch world is much more recent. For instance, the dynamic optimization of a batch distillation column in addressed in (Greaves et al., 2003) while the optimal control of a Nylon-6,6 production equipment, a CVD reactor and a PMMA production process is studied in (Joly and Pinto, 2004; Viganò et al., 2010; Lima et al., 2013). Moreover, approximately during the last decade, some general NMPC methods for (fed-)batch systems have been developed (Nagy and Braatz, 2003), along with some guidelines on how to tune them (Vallerio

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et al., 2014), and some studies have also been performed on the most suitable control strategies to be coupled to the DRTO frameworks (Pahija et al., 2014). Finally, in very recent times, some unconven-tional sustainability-oriented optimization and control strategies and some robust optimal control methodologies for batch systems have been broached too (Rossi et al., 2014b; Logist et al., 2011; Santos et al., 2012; Vallerio et al., 2014). The stability of all of these algorithms has also been deeply investigated. Papers like (Srinivasan and Bonvin, 2007; Zavala and Biegler, 2009) report these stability studies for both batch and continuous processes.

On the contrary, the research activity concerned with runaways prediction and prevention in batch/fed-batch equipment typically consists of the development of proper safety diagrams that can be used to identify either possible hazardous situations or safe and productive operating conditions, depending on the constitutive parameters of the target system. These maps are often expressed as a function of certain dimensionless numbers, relating to the heat produced by the reacting phenomena and that removed by the cooling apparatus. Several examples of such an approach can be found in the literature in papers like (Zaldívar et al., 2003; Westerterp and Molga, 2004; Molga et al., 2007; Maestri et al., 2009a, 2009b; Copelli et al., 2010, 2013a, 2013b), where the safe operation of potentially runaway (fed-)batch systems is investigated in the case of simple, series and arbitrary kinetic schemes. Moreover, additional safety-diagrams-related methodologies can also be found in (Milewska et al., 2005), where CFD calculations are employed to replace the standard batch/fed-batch reactor models, based on perfect mixing assumptions. Even performance comparisons among several of these safety-diagrams-based strategies are now available in some literature works, like for example (Casson et al., 2012). Recently, some methods have also been proposed to predict in real-time whether a control loss is likely to occur inside a target system in the near future (Nomen et al., 2005; Varga et al., 2010; Venka-tasubramanian, 2011; Monroy et al., 2012). These approaches can be successfully applied also to (fed-)batch equipment and go towards the idea of monitoring the target system safety not only in terms of recipe formulation but also during the operation phase.

It appears that the study of online optimization and/or optimal control strategies for (fed-)batch process units is a well-established research topic and the same applies to the methodologies for runaway online prediction and offline prevention. However, almost no successful attempts to merge the two research fields (DRTO/NMPC and runaway prediction/prevention) have been done until now. Indeed, to the knowledge of the authors of this work, the only material published towards this specific aim is that reported in (Kühl et al., 2007), where the authors employ a modified NMPC scheme to provide a fed-batch reactor with a safe control policy, thus avoiding the risk for unexpected runaway. In this work, possible runaways are avoided by adding a further constraint to the standard optimal control algorithm, which keeps the reactor inside an operating region where runaway is predicted to be impossible based on its energy balance and independently of the external perturbations affecting it. The work of Kühl et al. is certainly pioneering but suffers from at least a couple of drawbacks:

- the modified NMPC framework cannot really predict and prevent runaways but it is able to avoid them only because it forces the controlled system to operate in those regions where control losses are always impossible;
- poor controlled system performance might be achieved with respect to a standard NMPC scheme, eventually taking to compromised economic sustainability of the process.

Therefore, finding ways for simultaneously providing a (fed)-batch system with profitable online optimization and/or optimal control policies along with safety guarantees against possible runaways, still remains an open issue.

This paper tries to give an answer to this latter issue by relying on a general and advanced algorithm specifically designed for the online optimization and/or optimal control of (fed-)batch systems, the BSMBO&C (Rossi et al., 2014a, 2014c). In detail, the aim is that of showing that it is simultaneously possible to:

- provide a potentially runaway controlled system with a profitable online optimization/optimal control policy, based on a user-defined performance measure (objective function);
- ensure process safety in terms of runaway prediction and prevention, intended as the capability of foreseeing, in real-time, possible future dangerous situations in advance and automatically deciding whether and when to (optimally) stop a production cycle in order to prevent them.

In the opinion of the authors, this paper includes two relevant novelties:

- the heuristic demonstration of the tangible possibility of employing proper NMPC/DRTO-like algorithms for the real runaways prediction and prevention in real-time;
- the heuristic proof that it is possible to provide batch/fed-batch systems with profitable but still safe online optimization/optimal control policies, thus preserving process economic sustainability.

In terms of paper contents, first the BSMBO&C framework is briefly introduced and the conceptual guidelines for its application to runaway discontinuous processes are addressed along with the explanation of why it is such effective for this kind of equipment. Subsequently, this conceptual architecture is applied to a case study aimed at demonstrating the attainability of the aforementioned work goals. The test case is based on a well-known runaway (fed-)batch process, i.e. the oxidation of 2-octanol to 2-octanone with nitric acid in aqueous mixture (Van Woezik and Westerterp, 2002) and includes simulations characterized by both critical process disturbances and cooling system failures. The achieved results show that online runaways prediction and prevention along with safe and profitable online optimization/control policies are goals that can be simultaneously attained.

2. BSMBO&C framework description: basic concepts

The BSMBO&C (Batch Simultaneous Model-Based Optimization and Control) is an advanced framework for the simultaneous online optimization and/or optimal control of (fed-)batch processes. Unlike several common alternatives, e.g. standard NMPC/DRTO-like frameworks, it allows:

- optimizing the performance of the controlled system by simultaneously adjusting both its manipulated variables and its batch cycle time (the batch cycle time is effectively re-optimized in the evaluation of each control action along with the manipulated variables, in fully integrated fashion);
- supporting fully user-defined performance indicators as objective function;
- merging the regulatory control and optimization layers into a single optimization and control level simultaneously accounting for both aspects (this means that there is no more need for a regulatory control system as in standard DRTO frameworks).

Its flexibility in the objective function selection and capability of treating the batch time as an additional independent variable will later demonstrate to be essential for the aims of the paper.

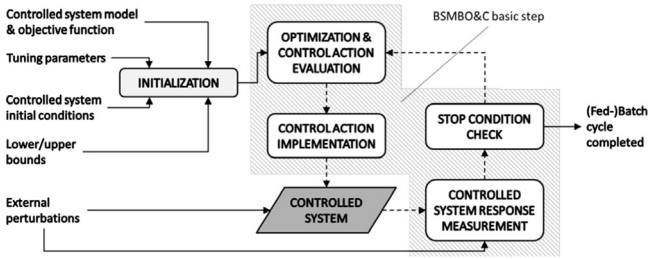

Fig. 1. BSMBO&C framework simplified structure.

A simplified version of the algorithm, which aims at providing a simple but clear idea of how it is designed, is reported in Fig. 1. There BSMBO&C is presented as a two-phase method including a first initialization phase and then a subsequent iterative phase. The initialization phase (initialization box in Fig. 1) is performed only once and is used to provide the algorithm with the required user-defined input data:

- the controlled system model;
- the objective function (performance indicator);
- the tuning settings;
- the lower/upper bounds on the states, the manipulated variables and the batch cycle time relating to the controlled system.

The iterative phase (shaded region in Fig. 1) consists of the repetition of one single iteration, also called *basic step*, until a stopping condition is satisfied, which implies that the optimal batch time has been reached. The *basic step* is made of four operations in series:

- an optimization to compute the optimal values of the manipulated variables and the batch time in the next control action (*optimization sub-step*);
- the implementation of the optimal control action to the controlled process (here the update of the control horizons of the manipulated variables is preformed too);
- the measurement of the controlled system response;
- the convergence condition check and the subsequent decision on whether to perform another *basic step*.

Up to now, a simple but intuitive idea of how BSMBO&C works has been conveyed. Despite the aim of this section is only that of providing a simplified description of the BSMBO&C method (all the details can be found in (Rossi et al., 2014a, 2014c), some additional specific information on the *optimization sub-step* must be provided. Indeed, this is an essential prerequisite to fully understand the concepts described in Sections 3 and 4. In detail, it is essential to analyze some key concepts referring to the formulation of the BSMBO&C objective function, whose simplified representation is reported in Eq. (1).

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

Notice that this objective function is made of two user-defined performance indicators (f and g), an anti-ringing term (AR_T) and a slope control term (SC_T). The f and g functions must be set by the user such that the fg product measures the controlled system performance (the greater fg, the lower the controlled process performance and vice versa). Instead, the slope control and anti-ringing terms are introduced in order to prevent strong and repeated oscillations in the trends of the controlled system states and manipulated variables, respectively. The exact formulation of AR_T and SC_T is not a subject of interest for the aims of this article and can be found in the BSMBO&C reference papers. However, it is essential to notice that the relative importance of both AR_T and SC_T terms inside $f_{obj}^{BSMBOC\&C}$ can be adjusted by changing two sets of tuning coefficients, named ***ARc*** and ***Dc***, respectively. In detail, by increasing the values in ***ARc*** and ***Dc*** vectors, BSMBO&C framework applies a smoother and more robust management policy to the controlled process while the opposite is achieved when ***ARc*** and ***Dc*** elements are reduced. It can be already inferred that the selection of ***ARc*** and ***Dc*** is critical when the controlled system may be subject to runaway. Especially the slope control term plays a key role on the BSMBO&C effectiveness in these situations. Efficient rules for fairly tuning the BSMBO&C in these cases will be addressed in Section 3 but it is now clear why this excursus on the formulation of the BSMBO&C objective function is needed before going ahead.

One last remark on the BSMBO&C concerns its numerical implementation. Its coding is realized in C++, employing BzzMath library (Buzzi-Ferraris and Manenti, 2012; Buzzi-Ferraris, 2014) as numerical engine for both integration and optimization purposes. Since BzzMath integrators and optimizers are very efficient and perfectly suitable to solve also strongly non-linear problems, BSMBO&C can be successfully applied also to processes characterized by strongly non-linear dynamics. Consequently, this framework is very suitable to manage runaway systems also from the numerical point of view, since their dynamics are strongly non-linear by definition.

Up to now, a simplified description of the BSMBO&C has been conveyed. All the information that is selectively included in this section is only that needed to understand the content of rest of the paper. Starting from this general description of the BSMBO&C features, its specific application to runaway process units will be detailed in Sections 3 and 4.

3. BSMBO&C method for the optimal management of runaway systems

The BSMBO&C framework has already been introduced in the previous section. Here the conceptual guidelines for its application to runaway batch/fed-batch processes are addressed along with the explanation of why it is such effective for this kind of equipment.

The latter of these concepts is detailed in Section 3.1. The first, instead, consists of the definition of proper performance indicators (f and g) and smart tuning settings (***ARc*** and ***Dc***), which ensure good performances when the controlled system may be subject to runaway. These topics are addressed in Sections 3.2 and 3.3.

Before going ahead, notice that, throughout all this work, it will be always assumed that a very accurate controlled system model is available. Therefore, model mismatch is supposed to be negligible. If this assumption does not hold, then different actions must be taken. Future works will be aimed at investigating such situations, thus going towards the study of robust model-based runaway prediction and prevention strategies.

3.1. BSMBO&C for safe and profitable online optimization and/or optimal control of runaway processes: the conceptual insight

BSMBO&C software is very suitable to be applied to runaway (fed-)batch processes because of its mathematical structure through which, under proper configuration settings, it is able to push the performance of the controlled system to the limit while ensuring process safety, i.e. runaway risk removal.

The capability of automatically predicting and preventing runaways, in real-time and in any circumstance, derives from a peculiar feature of its implementation, i.e. the ability of treating the batch cycle time as an additional independent variable (see Section 2). Indeed, once a set of suitable bound constraints is specified and a proper set of performance indicators (f and g) is chosen, BSMBO&C can dynamically determine whether and when

it is convenient to stop a production cycle, based on the value of the *fg* product and provided that bounds are satisfied (see Section 2). It is clear that if a runaway occurred, bounds would never be fulfilled. Therefore, BSMBO&C automatically avoids driving the controlled system to runaway conditions, independently of the reason that forces the control loss, simply because these conditions are infeasible based on the bound constraints. Notice that many NMPC/DRTO-like algorithms, where the batch operation time is fixed a-priori, fail in avoiding runaways in some circumstances. In detail, this happens when it is impossible to prevent the loss of control by simply modifying the manipulated variables of the controlled system. On the contrary, BSMBO&C can efficiently avoid control losses also in these cases by automatically selecting a batch cycle time that is lower than that at which the unavoidable runaway occurs.

It is now clear that BSMBO&C is really able to automatically predict and prevent runaways online while most of the available NMPC/DRTO-like methods can only predict, but not directly prevent, control losses. This qualitative reasoning conveys the idea that it is possible to employ properly structured DRTO/NMPC-like algorithms, as the BSMBO&C, to predict and prevent safety hazards.

However, that reported above is not the only reason why the BSMBO&C is very suitable to be applied to (fed-)batch processes that may be subject to runaway. Indeed, the BSMBO&C can also ensure its controlled system to operate in the most profitable conditions because the control actions are taken as to optimize its performance with respect to the f and g functions. No performance losses are observed, which are related to the unstable nature of the controlled process unit. Observe that the same does not apply to many common NMPC/DRTO-like strategies and the Kühl et al. method, where additional constraints must be added for safety reasons, i. e. to keep the controlled system stable, independently of the external perturbations.

In conclusion, the BSMBO&C and BSMBO&C-like methods (if there exists one) appear to be capable of providing a batch/fed-batch process with both profitable and safe, i.e. runaways-free, operating conditions, at least in abstract terms. This suggests that the aims of this work are reasonable and can be conceptually achieved. Section 4 will provide some practical evidences of this.

3.2. The objective function selection

The selection of the f and g functions must be carefully addressed when the controlled system may be subject to runaway. Indeed, those functions should be formulated such that their product increases when the controlled process goes towards a control loss. This feature is not mandatory because the BSMBO&C is be able to optimally manage a (fed-)batch process unit with respect to any user-supplied performance criterion. However, it can be considered as a further safety assurance that allows not driving the controlled process too close to runaway conditions. Indeed, remind that a very limited model mismatch is always unavoidable.

Typically, each selection of the user-defined performance indicators respects the aforementioned property, i.e. the *fg* product increases towards runaway conditions. For example, this applies when the f and g functions are based on process economics, production and yields. Indeed, runaway is always unwanted for safety reasons but it often negatively affects process profitability too.

However, in the rare event that a couple of performance functions are selected, whose *fg* product does not increase towards runaway conditions, it is advisable to properly modify them by adding an event-based penalty term that activates only in the very proximity of a control loss occurrence. This change takes to a discontinuous user-defined performance criterion but this is not troublesome at all since the BSMBO&C can also handle discontinuous objective functions (the *optimization sub-step* is based on a derivative-free optimizer). Thanks to the event-based penalty terms approach, the unconventional f and g functions are reduced to a form that resembles that of a conventional set of performance indicators, where the *fg* product increases towards runaway conditions. The adaptation strategy described in these lines is formalized in Eq. (2).

$$\begin{cases} f \rightarrow f \\ g \rightarrow g + b_{runaway}\psi(1+|g|) \end{cases} \tag{2}$$

In terms of notation, the arrow stands for replacement, i.e. f is not changed but g is replaced with the reported expression. Moreover, f and g are the original unconventional performance functions and $b_{runaway}$ is a boolean term that is set to one when the controlled system is close to runaway and is set to zero otherwise. The statement "close to runaway" must be translated into a quantitative criterion accordingly to the specific case. Finally, ψ is the dimensionless penalty factor that must be greater than one (a value of two to five seems a good choice).

As a final remark, notice that only the g function is modified with the event-based penalty term, while the f function remains unchanged. Indeed, the aim of the event-based penalty terms is that of making the *fg* product increase towards runaway conditions. This goal can be achieved also by varying only the g function. This is the reason why only g is adjusted.

3.3. The tuning settings

The choice of the ***ARc*** and ***Dc*** parameters is critical when the controlled process unit may be subject to runaway. Especially the ***Dc*** values must be properly assigned. An effective and simple criterion that can be used to select proper anti-ringing (***ARc***) and slope-control (***Dc***) coefficients is partially heuristic and relies on two steps in series:

- the evaluation of good first guesses of the aforementioned coefficients by means of Eqs. (3) and (4);
- the refinement of these first estimates via sensitivity analysis.

The first step is the most critical because it suggests the region where reasonable values of ***ARc*** and ***Dc*** should be contained. Instead, the second step is much easier because it is purely mechanical and requires almost no arbitrary choices. Therefore, only the first step is the one that deserves attention and will be detailed in the rest of the current section.

Before describing how to properly exploit Eqs. (3) and (4) to efficiently address this first step, it is essential to convey some information on both the notation employed in these two equations and the idea on which they are based. In terms of notation, ARc_i is the i-th element of the ***ARc*** vector, i.e. the anti-ringing coefficient referring to the i-th controlled system manipulated variable. Instead, Dc_k is the k-th element of the ***Dc*** vector, i.e. the slope control coefficient relating to the k-th controlled system state. Moreover, g^{MO} is the order of magnitude of the g function, $\Delta m_i^{MAX,MO}$ is the order of magnitude of the maximum allowed variation of the i-th manipulated variable between adjacent control actions and $\Delta w_k^{MAX,MO}$ has the same meaning of $\Delta m_i^{MAX,MO}$ but refers to the k-th state. Finally, $\Delta t_{CI}^{0,i}$ represents the initial length of the discretization intervals employed in the approximation of the temporal trend of the i-th manipulated variable and α_i and β_k are user-supplied parameters. For any additional detailed information on the notation, please refer to the BSMBO&C reference papers, where the adopted symbols are fully compliant with those selected here. Coming now to the conceptual foundation of Eqs. (3) and (4), the idea is to derive a formula that allows computing the ***ARc*** and ***Dc*** parameters so that:

- the g function is approximately increased by the $100\alpha_i\%$ when the variation in the i-th manipulated variable, between consecutive control actions, equals $\Delta m_i^{MAX,MO}$;

- the g function is approximately increased by the $100\beta_k$% when the variation in the k-th state, between consecutive control actions, equals $\Delta w_k^{MAX,MO}$.

The mathematical reason why the listed concepts are embodied by the expressions in Eqs. (3) and (4) is not explained in detail. However, the interested reader can easily understand it by looking at the structure of the AR_T and SC_T terms inside the BSMBO&C objective function, reported in the BSMBO&C reference papers.

$$ARc_i = \alpha_i g^{MO} \left(\frac{\Delta t_{CI}^{0,i}}{\Delta m_i^{MAX,MO}} \right)^2 \tag{3}$$

$$Dc_k = \beta_k g^{MO} \left[\frac{\underset{i}{Min}\left(\Delta t_{CI}^{0,i}\right)}{\Delta w_k^{MAX,MO}} \right]^2 \tag{4}$$

It is now possible to address the application of Eqs. (3) and (4) in the evaluation of good first guesses for the BSMBO&C tuning coef-ficients, when runaway controlled processes have to be managed. The idea is to define the first guess ***ARc*** as to avoid infeasible repeated oscillations in the temporal profiles of the manipulated variables of the controlled process. This can be achieved by applying Eq. (3) with α_i inside the range [0.15–0.2] (typically, instead, values of α_i close to 0.35 are recommended). Indeed, for these specific type of controlled process units, it is always better not to tighten the anti-ringing too much because this might result in a higher prob-ability of aborting a production cycle due to unavoidable runaways. The evaluation of the first guess ***Dc*** is more critical. It is essential to set all the Dc_k parameters, referring to state variables that are markers of a control loss occurrence, to a proper non-zero value (for standard controlled systems ***Dc*** is a null vector, thus β_k equals zero for all the states). These proper values derive from the application of Eq. (4) where β_k belongs to the range [0.25–0.4]. The choice of non-zero values for the specific set of slope control coefficients (Dc_k) mentioned above allows to prevent the unwanted situation in which the BSMBO&C may suggest to stop a batch cycle at a certain time and a runaway would occur in a negligible additional time. This type of operation is clearly infeasible because there would not be enough time to unload the batch content before the control loss occurrence. It is now clear how important the choice of ***Dc*** is when possible runaway fed-batch equipment has to be managed.

The tuning criterion described in this section will be applied in the article case study (Section 4). At that point, the effectiveness and simplicity guaranteed by this approach will be clearly understood.

4. The case study: oxidation of 2-octanol with nitric acid

The conceptual background concerning the BSMBO&C and its application to runaway (fed-)batch systems has already been explained in Sections 2 and 3. Here, a case study is presented that applies this abstract structure to a well-known example of runaway fed-batch process: the oxidation of 2-octanol with nitric acid. The aim is to show even in practice what has already been conceptually detailed in Section 3.1, i.e. the possibility of providing a runaway fed-batch process with performing optimization/control policies while ensuring automatic and online runaway prediction and prevention. In order to have a means of comparison, the simulations of the case study are performed with both the BSMBO&C framework and a conventional PID controller as reactor control/optimization devices. The PID controller serves as the industrial state-of-the-art in the batch units control.

In order to perform the aforementioned case study, a suitable fed-batch reactor layout must be chosen and the relating reactor model must be built. These operations are described in Section 4.1 along with some general details on the 2-octanol oxidation process with nitric acid. Moreover, the BSMBO&C optimal configuration settings for this specific process must be evaluated based on the guidelines of Section 3. The same applies to the PID controller, but based on a suitable tuning method. These tuning/configuration operations are addressed in Section 4.2. Finally, the developed fed-batch reactor model and BSMBO&C/PID configuration/tuning settings are applied in a couple of different scenarios reported in Sections 4.3 and 4.4 and the relating computational effort statistics are shown in Section 4.5. The two scenarios are properly selected as to make the case study meaningful for the aims of the work.

4.1. The fed-batch reactor layout and modelling

The first aim of this section is to choose the features of a fed-batch reactor where to perform the 2-octanol oxidation with nitric acid while the second objective is the modelling of this reacting system. However, in order to complete these two tasks, it also is essential to convey some basic information on the nature of the 2-octanol oxidation process. Therefore, before analyzing reactor layout and/or modelling related problems, a brief description of this process is reported. For details on this topic please refer to (Van Woezik and Westerterp, 2002) or similar works.

The oxidation of 2-octanol (A) to 2-octanone (C) with a mixture of nitric acid (N) and water (Q) is a very exothermic process, whose most simplified but still sufficiently accurate representation can be achieved with a kinetic scheme of only two reactions (Eq. (5)). Notice that the reacting mixture decomposition reactions are neglected as a first but feasible approximation. The primary reaction, whose rate is named R_1, embodies the partial oxidation of the alcohol to the ketone, which is the target product. Instead, the side-reaction, whose rate is R_2, models a further ketone oxidation to a mixture of car-boxylic acids (X), which represent the sub-products. These acids can be modeled as the only hexanoic acid. An essential active species for both reactions is the NO_2^+ ion (B) that is generated as a product of the main reaction or by chemical interaction between nitric acid and an initiator. Typically, this initiator is only used to start the reacting process that is then self-sustaining. Aside from the kinetic scheme structure, notice that the side-reaction is approximately three times more exothermic than the primary reaction. By keeping in mind this aspect and observing that the main reaction is autocatalytic, it can be easily understood that this reacting process may be subject to thermal runaway. Therefore, its employment in this case study is perfectly in line with the aims of the work. The last relevant feature of the oxidation of 2-octanol with nitric acid to be mentioned concerns the phases in which the two reactions (Eq. (5)) occur. Indeed, a reacting system containing A, B, C, X, N and Q is intrinsically two-phase (Fig. 2). Therefore the reacting mixture is made of an organic liquid phase, rich in A, C and X and an aqueous phase, rich in B, N and Q. Since the solubility of the compounds belonging to one phase is negligible into the other phase, the chemical reactions occur at the liquid–liquid interface. Therefore, in order to perform this kind of

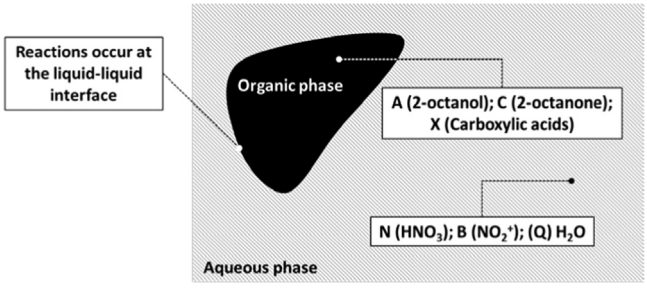

Fig. 2. Schematic representation of the two phase system in which the oxidation of 2-octanol with nitric acid has to be performed.

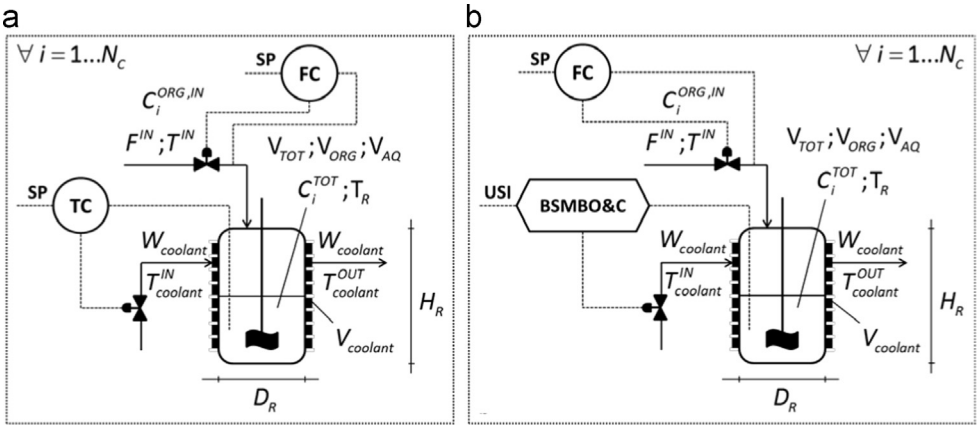

Fig. 3. Fed-batch reactor drawing and optimization/control systems layout.

process in chemical regime, it is essential to keep the reacting medium strongly agitated.

$$\begin{aligned} A+B+N &\xrightarrow{R_1} C+2B \\ C+B+N &\xrightarrow{R_2} X \end{aligned} \tag{5}$$

All the aforementioned characteristics of the 2-octanol oxidation with nitric acid have to be considered when it comes to deciding how to configure a fed-batch reactor for such a process. It can be clearly understood that using this kind of reactor is probably the best choice here for several reasons:

- the reacting process is very exothermic thus the temperature control is critical;
- it is essential to slowly add one reactant into the reacting medium to minimize safety risks;
- it is advisable to work on relatively low volumes of reactants as to minimize damages in the unfortunate occurrence of a control loss.

Indeed, a fed-batch reactor is the typical unit used in the industrial practice for these nitric-acid-driven oxidations. In terms of configuration, the reactor has to be equipped with a refrigerating apparatus made of C-tubes. The cooling jacket is avoided since the C-tubes allow reaching higher overall heat transfer coefficients, thus taking to a more easily manageable system. Finally, the largest available height to diameter ratio for the reactor will be selected to increase the heat exchange area, once again with the aim of improving the process manageability.

Up to know, the first aim of this section has been reached, but it is now necessary to derive a model of the fed-batch reactor for the 2-octanol oxidation. This is addressed in the following lines. However, before entering into the details of the model equations, let the employed notation be introduced and explained:

- V_{TOT}, V_{ORG} and V_{AQ} stand for total, organic and aqueous volume of the reacting mixture while $V_{coolant}$ represents the C-tubes section volume;
- C_i^{ORG}, C_i^{AQ} and C_i^{TOT} are the i-th component concentrations in the reacting mixture, referred to the organic phase, aqueous phase and both phases, while $C_i^{ORG,IN}$ is the i-the component concentration in the reactor feed, referred to the organic phase;
- n_i^{ORG}, n_i^{AQ} and n_i^{TOT} identify the i-th component moles in the reacting mixture, relating to the organic phase, aqueous phase and both phases;
- T^{IN} and T_R represent the reactor feed temperature and the reactor temperature while $T_{coolant}^{IN}$ and $T_{coolant}^{OUT}$ are the cooling fluid inlet and outlet temperatures;
- F^{IN} stands for reactor feed volumetric flow while $W_{coolant}$ stands for coolant mass flow;
- ρ_{ORG} and ρ_{TOT} are the densities of the reacting mixture, referring to the organic phase only and the overall pseudo-phase, $\rho_{coolant}$ is the cooling fluid density and ρ_{ORG}^{IN} is the density of the reactor feed, referring to the organic phase;
- Cp_{TOT} and $Cp_{coolant}$ are the constant pressure heat capacities of the whole reacting mixture (as a pseudo-phase) and the cooling fluid (at the outlet conditions) while Cp_{ORG}^{IN} and $Cp_{coolant}^{IN}$ are the heat capacities of the reactor feed (as the organic phase only) and the cooling fluid (at the inlet conditions);
- $\Delta H_{R,j}$ identifies the enthalpy of reaction for the j-th reaction;
- N_R represents the number of reactions occurring inside the reactor;
- υ_{ij} stands for stoichiometric coefficient of the i-th component in the j-the reaction, R_j is the j-th reaction rate and k_j^{eff} is the j-th reaction rate constant;
- U is the global heat transfer coefficient while A_{exc} is the thermal exchange area between the reactor vessel and the C-tubes section;
- D_R is the reactor diameter.

Once the explanation of the chosen notation is complete, the model of the fed-batch reactor for the 2-octanol oxidation can now be detailed (refer to Fig. 3 for a reactor drawing). First of all, let the more relevant simplifying assumptions be introduced. The reactor is supposed to be perfectly mixed since the agitation provided by the stirrer is typically very effective in these oxidation units. Moreover, the C-tubes refrigerating section is supposed to be perfectly mixed too. This is not such a good assumption, but it is conservative since it eventually takes to an underestimation of the heat removal efficiency. In addition, the effect of the reactor metal mass on its thermal behavior is neglected. Finally, the enthalpy of reaction is considered constant and the dp/dt-like terms are considered negligible. Coming now to the description of the model equations, several global and component material balances along with two energy balances have to be written. The global material balances include an overall conservation equation (Eq. (6)) and the material conservation on the only organic phase (Eq. (7)). Of course the material balance on the aqueous phase is unnecessary since the aqueous volume can be simply evaluated via the Eq. (8). Observe that, in these three expressions, the inlet flows are identified as an organic phase only. This is because the reactor is supposed to be fed only with organic compounds (for the current case 2-octanol).

$$\frac{dV_{TOT}}{dt} = \frac{\rho_{ORG}^{IN}}{\rho_{TOT}} F^{IN} \tag{6}$$

$$\frac{dV_{ORG}}{dt} = \frac{\rho_{ORG}^{IN}}{\rho_{ORG}} F^{IN} \tag{7}$$

$$V_{AQ} = V_{TOT} - V_{ORG} \tag{8}$$

Instead, the component material balances can be formulated as it is shown in Eq. (9). These balances must be written for all the reacting mixture components (A, B, C, N, X, Q). Once again, a pure organic reactor feed is supposed.

$$\frac{dC_i^{TOT}}{dt} = \frac{F^{IN}}{V_{TOT}}\left(C_i^{ORG,IN} - \frac{\rho_{ORG}^{IN}}{\rho_{TOT}} C_i^{TOT}\right) + \sum_{j=1}^{N_R} \upsilon_{ij} R_j \tag{9}$$

In order to ease the understanding of the expression in Eq. (9), the definitions of all the possible concentrations, depending on the reference phase, are summarized in Eq. (10). Moreover, the expressions for the reaction rates are reported in Eq. (11). The kinetic constants (k_j^{eff}) definitions will be provided in the following.

$$C_i^{ORG} = \frac{n_i^{ORG}}{V_{ORG}}; \quad C_i^{AQ} = \frac{n_i^{AQ}}{V_{AQ}}; \quad C_i^{TOT} = \frac{n_i^{TOT}}{V_{TOT}} \tag{10}$$

$$R_1 = k_1^{eff} C_A^{TOT} C_B^{TOT} \frac{V_{TOT}}{V_{ORG}}; \quad R_2 = k_2^{eff} C_C^{TOT} C_B^{TOT} \frac{V_{TOT}}{V_{ORG}} \tag{11}$$

Finally, let the energy conservation equations be introduced. The reactor energy balance is described in Eq. (12) while the C-tubes section energy balance is shown in Eq. (13). Consider that Eq. (13) supposes that the material dynamics of the C-tubes section itself is negligible. Indeed, the coolant is a mixture of water and propylene glycol in equal amounts, thus being reasonably uncompressible. The only relevant additional remark on the energy conservation equations relates to the evaluation of the heat transfer area. This area changes with the total volume of mixture inside the reactor according to Eq. (14). Notice that this equation computes the heat exchange surface by considering only the reactor lateral surface as an active element in the heat exchange process. Indeed, C-tubes cannot be installed on the bottom of a vessel.

$$\frac{dT_R}{dt} = \frac{1}{V_{TOT}\rho_{TOT}Cp_{TOT}}\left[F^{IN}\rho_{ORG}^{IN}\left(\frac{Cp_{ORG}^{IN} + Cp_{TOT}}{2}\right)\left(T^{IN} - T_R\right) + \right.$$
$$\left. - V_{AQ}\sum_{j=1}^{N_R}\Delta H_{R,j} R_j + UA_{exc}\left(T_{coolant}^{OUT} - T_R\right)\right] \tag{12}$$

$$\frac{dT_{coolant}^{OUT}}{dt} = \frac{1}{V_{coolant}\rho_{coolant}Cp_{coolant}}$$
$$\left[\begin{array}{l} W_{coolant}\left(\frac{Cp_{coolant}^{IN} + Cp_{coolant}}{2}\right)\left(T_{coolant}^{IN} - T_{coolant}^{OUT}\right) \\ + UA_{exc}\left(T_R - T_{coolant}^{OUT}\right) \end{array}\right] \tag{13}$$

$$A_{exc} = 4\frac{V_{TOT}}{D_R} \tag{14}$$

Now, by putting together Eqs. (6)–(14), the model of the fed-batch reactor for the oxidation of 2-octanol is formally complete (of course a proper set of initial conditions must be coupled to the model equations before being able to solve them). It is now necessary to deal with how to compute the physical properties of the reacting mixture, the reactor inlet feed and the cooling fluid along with the global heat transfer coefficient. The pure-component physical properties are evaluated by means of temperature-dependent correlations derived from several handbooks, among which the most famous is Perry's Chemical Engineering Handbook (Perry and Green, 2008). The same handbooks are also used to choose proper correlations to compute the mixture physical properties from the pure-component ones. Notice that, since a very efficient agitation is typically achieved in these oxidation reactors, the mixture physical properties are estimated thanks to a pseudo-single-phase approach. Instead, the heat transfer coefficient estimation is handled via the combination of different thermal resistance sources:

- the reacting mixture resistance (due to the internal boundary layer) and C-tubes coolant resistance (due to the external boundary layer);
- the metal wall resistance;
- the fouling resistance.

The first two terms are estimated thanks to common stirred vessels and C-tubes sections correlations, the metal wall resistance is derived from the stainless steel thermal conductivity and the fouling data come from specific handbooks. The detailed explanation of all the equations/correlations employed in the heat transfer coefficient and physical properties estimation is not reported for the sake of brevity. However, this is well-established content. Therefore, the interested reader can easily search and find all the related material.

Up to know the model of the fed-batch reactor for the 2-octanol oxidation has been described. Notice that this model is quite general and can also be employed to simulate other nitric acid oxidations of organic compounds. However, limited to the case of the 2-octanol oxidation, some numerical data on the process itself and on the reactor structure must be conveyed. These data will be used in Sections 4.3 and 4.4 to perform all the numerical simulations. Table 1 summarizes the aforementioned data. Some additional symbols, employed in this Table must be detailed:

- V_{ORG}^{IN} is the total volume of organic mixture to be fed to the reactor;
- PMiis the i-th component molecular weight while $PMcoolant$ is the cooling liquid molecular weight;
- $W_{coolant}^{0}$ is the zero-time coolant flowrate;
- $W_{coolant}^{MIN}$, $W_{coolant}^{MAX}$, $T_{coolant}^{OUT,MIN}$, $T_{coolant}^{OUT,MAX}$, T_R^{MIN}, T_R^{MAX} identify the lower and upper bounds on the coolant flow, the coolant outlet temperature and the reactor temperature;
- V_{ORG}^{0}, V_{TOT}^{0}, $C_i^{TOT,0}$, T_R^{0}, $T_{coolant}^{OUT,0}$ represent the zero-time values for the corresponding reactor states, i.e. the initial conditions of the abovementioned reactor model;
- $€_i$ is the i-th component dimensionless economic value while $€_{N-Q}^{mix,0}$ is the dimensionless economic value of the water–nitric acid mixture that is initially loaded into the reactor;
- K_R is the reactor vessel thermal conductivity;
- H_R and s_R are the reactor vessel height and thickness;
- H_{CT}, s_{CT} and N_{CT} are the single C-tube height, the single C-tube thickness and the number of spirals in the C-tubes section;
- D_I, z_I and rpm_I stand for impeller diameter, elevation (with respect to the vessel bottom) and rounds per second.

Notice that only those symbols that will be used in the next sections are listed here. The acronyms that are local to Table 1 are not explained in detail since there is no need for that.

4.2. BSMBO&C/PID configuration for the 2-octanol oxidation reactor

The principal features of the 2-octanol oxidation process and the layout of the fed-batch reactor, where to carry on it, have already been described in Section 4.1. Now it is essential to discuss how the BSMBO&C and the standard PID-based control system (PID-CS) are applied to the oxidation reactor. First of all, the selected manipulated and controlled variables have to be mentioned and then the employed configuration settings (PID controller tuning parameters and additional configuration features, BSMBO&C objective function and tuning coefficients) have to be conveyed.

The manipulated and controlled variables selection can be inferred from Fig. 3 but, before going ahead, some new symbols need to be explained. In detail, N_C is the number of components in

Table 1
2-octanol oxidation process data and fed-batch reactor features.

Process kinetic scheme			
Rate constants equations and kinetic parameters	$k_1^{eff} = k_1^{eff,0}\exp\left[-\frac{E_1^*}{T_R}+m_1 H\right]$		$k_1^{eff,0} = 1E+5$ [m^3/kmol/s] $E_1^* = 1.13E+4$ [K] $m1 = 6.6$ [dimensionless]
	$k_2^{eff} = k_2^{eff,0}\exp\left[-\frac{E_2^*}{T_R}+m_2 H\right]$		$k_2^{eff,0} = 1E+10$ [m^3/kmol/s] $E_2^* = 1.2E+4$ [K] $m2 = 2.2$ [dimensionless]
Hammett acidity function	$H = \lambda+\mu\frac{C_N^{TOT}PM_N}{C_N^{TOT}PM_N+C_Q^{TOT}PM_Q}$		$\lambda = 0.4$ [dimensionless] $\mu = 5$ [dimensionless]
Thermodynamic parameters			
Enthalpy of reaction	$\Delta H_{R,1} = -1.6E+5$ [kJ/kmol]		$\Delta H_{R,2} = -5.2E+5$ [kJ/kmol]
Other properties	*all the other thermodynamic properties can be easily found in chemical engineering handbooks		
Molecular weights			
$PM_A = 130$ [kg/kmol]	$PM_Q = 18$ [kg/kmol]		$PMC = 128$ [kg/kmol]
$PM_N = 63$ [kg/kmol]	$PM_X = 116$ [kg/kmol]		$PMcoolant = 47$ [kg/kmol]
Inlet mixture properties	$T^{IN} = 298$ [K]	$V_{ORG}^{IN} = 0.6$ m^3	$C_{i\neq A}^{ORG,IN} = 0$ [kmol/m^3] $C_A^{ORG,IN} = 6.333$ [kmol/m^3]
Inlet coolant properties	$T_{coolant}^{IN} = 261$ [K]		$W_{coolant}^0 = 11.8$ [kg/s]
Process physical bound constraints			
Inlet coolant flow	$W_{coolant}^{MIN} = 0$ [kg/s]		$W_{coolant}^{MAX} = 25$ [kg/s]
Reactor and coolant temperatures	$T_{coolant}^{OUT,MIN} = 255$ [K] $T_R^{MIN} = 255$ [K]		$T_{coolant}^{OUT,MAX} = 275$ [K] $T_R^{MAX} = 283$ [K]
Process initial conditions			
$T_R^0 = 261$ [K]	$T_{coolant}^{OUT,0} = 261$ [K]	$V_{TOT}^0 = 1.5$ [m^3]	$V_{ORG}^0 = 1.58E-4$ [m^3]
$C_A^{TOT,0} = 1E-3$ [kmol/m^3]	$C_C^{TOT,0} = 0$ [kmol/m^3]		$C_B^{TOT,0} = 3.52E-02$ [kmol/m^3]
$C_Q^{TOT,0} = 30.02$ [kmol/m^3]	$C_X^{TOT,0} = 0$ [kmol/m^3]		$C_N^{TOT,0} = 12.83$ [kmol/m^3]
Reactants/products dimensionless economic values			
$€_{N-Q}^{mix,0} = 0.11$ [dimensionless]	$€_A = 0.633$ [dimensionless]	$€_C = 1$ [dimensionless]	$€X = 0.02$ [dimensionless]
Reactor features			
C-tubes sizing	$H_{CT} = 0.0933$ [m]	$s_{CT} = 0.0035$ [m]	$N_{CT} = 15$ [dimensionless] *The C-tubes are half-cilynders
Vessel sizing and thermal conductivity	$D_R = 1.4$ [m]	$H_R = 1.4$ [m]	$s_R = 0.01$ [m] $K_R = 20$ [W/m/K]
Impeller data	$D_I = 0.7$ [m]	$z_I = 0.3$ [m]	$rpm_I = 200$ [rpm]

the reacting mixture, *FC* and *TC* stand for flow and temperature controller, *SP* and *USI* stand for set-point and BSMBO&C user-supplied input data. Fig. 3 suggests that the 2-octanol oxidation reactor owns only one independent variable, i.e. the cooling fluid flowrate ($W_{coolant}$), because the other possible degree of freedom (the reactor feed flow (F^{IN})) is supposed to be assigned. Therefore, the BSMBO&C is configured to adjust the coolant flow and the batch cycle time while the PID-CS is set up as to control the reactor temperature (T_R) with $W_{coolant}$. As an additional and complementary remark on this topic, Fig. 3 highlights the presence of a flow controller on the reactor feed too. However, the relating control loop is considered perfect because F^{IN} is an almost incompressible liquid stream. Thus this *FC* is only inserted for the sake of completeness. Notice that, despite a controller is placed on F^{IN}, this variable remains fixed and the controller itself is only used to practically set its value.

Dealing now with the PID-CS tuning procedure, it is a standard PID controller tuning problem and is addressed via the ISE (integral square error) minimization followed by a rounding step. The optimal values of K_c (proportional gain), τ_I (integral time) and τ_D (derivative time), achieved with the abovementioned procedure, are reported in Table 2. In order to avoid confusion in the definition of these PID tuning parameters, the mathematical formulation of the PID control law, employed in this case study, is presented in Eq. (15). In this expression, y and y_{SP} are the controlled variable and its set-point while m and m_{bias} are the manipulated variable and its bias.

$$m = m_{bias}+K_C\left[(y-y_{SP})+\frac{1}{\tau_I}\int_0^t (y-y_{SP})dt+\tau_D\frac{d}{dt}(y-y_{SP})\right] \quad (15)$$

An additional configuration detail is worth mentioning. The PID-CS is not equipped with an anti-windup protocol. This choice seems strange but the anti-windup algorithm does not ensure significant advantages in this case (several tests have been carried out to check it). This is probably due to the relevant additional complexity in tuning the PID-CS when it is coupled with an anti-windup strategy. As a consequence, some saturation effects may be found later on.

Finally, coming to the BSMB&C configuration, it is more complex. It is performed based on the rules explained in Sections 3.2 and 3.3. In this case, its performance functions (f and g) are selected as economic net-income-based indices (Eq. (16)). In Eq. (16), t_{BC} represents the end time of a batch cycle while $C_i^{(TOT,BC)}$ and V_{TOT}^{BC} identify the corresponding variables (C_i^{TOT} and V_{TOT}) evaluated at the end of a batch cycle, i.e. in t_{BC}. Note that, because of this f and g choice, there is no need for using the strategy reported in Eq. (2) to force the BSMBO&C objective function to increase in the very proximity of a control loss.

$$\begin{cases} f = 1 \\ g = \left[\begin{array}{l}\left(C_N^{TOT,0}PM_N+C_Q^{TOT,0}PM_Q\right)V_{TOT}^0€_{N-Q}^{mix,0}+C_A^{ORG,IN}PM_A€_A\int_0^{t_{BC}}F^{IN}dt+ \\ -\left(C_C^{TOT,BC}PM_C€_C+C_X^{TOT,BC}PM_X€_X\right)V_{TOT}^{BC}\end{array}\right] \end{cases} \quad (16)$$

Moreover, the optimal values of the ***ARc*** and ***Dc*** vectors are reported in Table 2. The reader can immediately notice that the only ***Dc*** element corresponding to T_R is non-zero. This is in line with the contents included in Section 3.3, where it is highlighted that the only ***Dc*** elements relating to runaway markers need to be set to non-zero values. Another interesting point is that also the ***ARc*** and ***Dc*** achieved with the simple application of Eqs. (3) and (4) are reported in Table 2. This is done to show that the heuristic formulas contained in Eqs. (3) and (4) can provide a good first guess for BSMBO&C tuning coefficients.

Table 2
PID-CS and BSMBO&C tuning settings.

PID-CS tuning parameters							
Temperature controller (TC)	K_C=0.85 [kg/s/K]		τ_I=560 [s]			τD=7.5E+3 [s]	
BSMBO&C tuning coefficients							
Tuning coefficients first guess		C_i^{TOT} $\forall i = 1...N_C$	V_{TOT}	V_{ORG}	T_R	$T_{coolant}^{OUT}$	$W_{coolant}$
	Dc	0	0	0	4.8E+4	0	–
	ARc	–	–	–	–	–	1.1E+5
Optimal tuning coefficients (after refinement)		C_i^{TOT} $\forall i = 1...N_C$	V_{TOT}	V_{ORG}	T_R	$T_{coolant}^{OUT}$	$W_{coolant}$
	Dc	0	0	0	2.25E+4	0	–
	ARc	–	–	–	–	–	2.5E+5
Miscellaneous data for applying Eqs. (3) and (4)	$\Delta t_{CI}^{0,W_{coolant}} = 60$ [s]	$g^{MO} = 100$ [kg]		$\alpha_{W_{coolant}} = 0.15$ [dimensionless]		$\beta_{T_R} = 0.3$ [dimensionless]	
	$\Delta m_{W_{coolant}}^{MAX,MO} = 0.7$ [kg/s]			$\Delta w_{T_R}^{MAX,MO} = 1.5$ [K]			

This section has reported the configuration of the BSMBO&C and the PID-CS for the current case study (2-octanol oxidation). It is now possible to proceed to the detailed description of the results coming for the simulated scenarios.

4.3. The case of the reactor feed step-change

This first scenario aims at investigating the response of the 2-octanol oxidation reactor, equipped either with the BSMBO&C or with the PID-CS, to a critical process disturbance that is chosen as a strong variation in F^{IN}. Therefore, in this section, two simulations are carried out, one with the BSMBO&C and one with the PID-CS as optimization and/or control suites. In each of them, the same delta F^{IN} is applied to the 2-octanol oxidation reactor and the achieved responses are analyzed and compared on some aspects.

Before going to the results description, some additional information on the simulations must be discussed. In detail, it is needed to convey the feeding policy for the fed-batch reactor and select the batch cycle time and reactor temperature set-point for the PID-CS. Starting with the first point, the initial value of F^{IN}, indicated as $F^{IN,0}$, is chosen as to ensure a homogeneous addition of the 2-octanol to the reacting mixture during ten hours (the total volume of 2-octanol fed to the oxidation reactor equals V_{ORG}^{IN}). Then, starting from 2.75 h after the beginning of the batch cycle, F^{IN} is supposed to increase by 2.5 times, thus significantly enlarging the feeding speed (of course, F^{IN} is shut off once all V_{ORG}^{IN} is fed to the reactor). This abnormal increase in F^{IN} is the unexpected process disturbance. Instead, concerning the second aforementioned point, the batch cycle time for the PID-CS is fixed to that achieved through a BSMBO&C-driven simulation with no perturbations while the T_R set-point for the same control system (PID-CS) is fixed to the average temperature coming from the same perturbations-free BSMBO&C-driven simulation. This T_R set-point assignment is evidently not optimal, but this is not relevant for the aims of this work. Indeed, the idea is to use the PID-CS to mime the industrial state-of-the-art in terms of control systems for fed-batch units with the principal aim of showing how unsafe, and not how profitable, these standard control systems might be.

Coming now to the results description, some key dynamic profiles, concerning the operation of the 2-octanol oxidation reactor in the aforementioned conditions, are shown in Fig. 4. Notice that the control system representing the industrial state-of-the-art (PID-CS) is not able to avoid a dangerous control loss that drives the reactor to a runaway. Instead, the BSMBO&C is perfectly able to prevent this safety problem (the coolant flow oscillations may seem critical but it is only a problem of charts scale). Moreover, observe that the BSMBO&C decides to reduce the batch time with respect to a perturbations-free situation. This batch time reduction is due to the F^{IN} increase, which simply accelerates the conversion of 2-octanol to the desired but also undesired products, and may be aimed at both producing the lowest possible amount of low-price carboxylic acids and avoid possible safety risks. Aside from safety issues, some economic data, relating to this scenario and to the ideal situation where no perturbations affect the fed-batch reactor, are reported in Table 3 (in this Table, χ_i stands for i-th component conversion, η_i stands for i-th component yield, Ern_{real} and Ern_{max} stand for the real achieved revenues and the maximum possible revenues). These data suggest that the BSMBO&C can provide the fed-batch oxidation reactor with a profitable optimization/control policy. Indeed, the revenues obtained when it is applied are up to the 90% of the maximum possible earnings, in both the perturbations-free and the current situation. The maximum profit is evaluated considering that the re-oxidation of 2-octanone to carboxylic acids is not possible. On the contrary, the corresponding economic data relating to the PID-CS clearly show that this scheme is not able to provide almost any revenue (however, remind that the PID-CS scheme set-point is not optimized). This is consistent with the fact that it drives the fed-batch reactor to a runaway that completely consumes the valuable product, i.e. 2-octanone. The reader might also notice that the revenues produced by the BSMBO&C in the current simulation are higher than those obtained in the perturbations-free situation. This is not surprising because it can also exploit perturbations as an advantage and this is probably what is happening here.

In conclusion, this first scenario certainly shows the capability of BSMBO&C and BSMBO&C-like methods (i.e. specific NMPC/DRTO-like methods) of ensuring elevated performances even when the controlled system is potentially subject to runaway. It also introduces the effectiveness of these strategies in the rejection of critical process disturbances, thus avoiding safety hazards. Therefore, a first but still partial practical achievement of the aims of this work has been shown (see the introduction).

4.4. The case of the cooling system temporary and permanent failure

This second and last scenario addresses the response of the 2-octanol oxidation reactor, equipped either with the BSMBO&C or with the PID-CS, to a temporary and permanent failure in the cooling fluid refrigerating cycle. Therefore, in this section four different simulations are performed, one for each type of failure and each type of control and/or optimization suite. Notice that a failure in the coolant refrigeration cycle is simulated by instantaneously increasing the $T_{coolant}^{IN}$ to the ambient temperature, i.e. 298 K. On the other hand, a reactivation of the coolant refrigeration cycle is mimed by restoring the original $T_{coolant}^{IN}$ value, i.e. 261 K. Thus each simulation is carried out basically in the same way, i.e. first $T_{coolant}^{IN}$ is set to 298 K starting from 3.025 h from the beginning of the batch cycle and then, only in two of the four simulations, the original value of the coolant inlet temperature is restored to 261 K after 1.1 h. The responses produced by the 2-octanol oxidation reactor are finally analyzed and compared on some aspects.

Once again, before describing the achieved results, some additional information on the four simulations are needed. In detail, the feeding policy for the fed-batch reactor and the selection of the

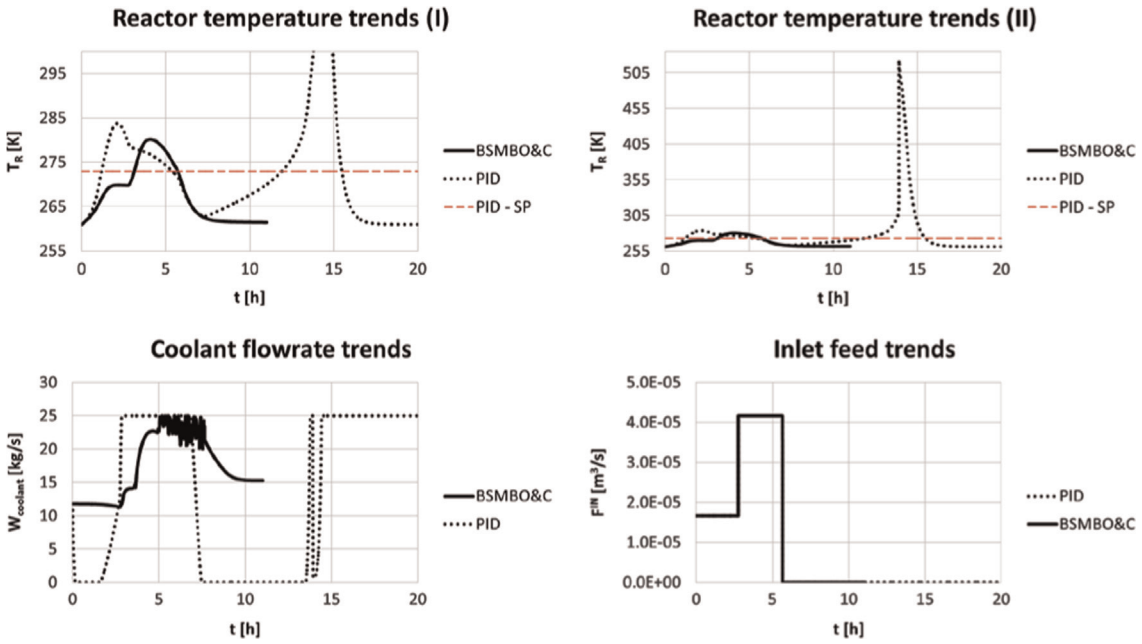

Fig. 4. Operation of the 2-octanol oxidation reactor, equipped with the BSMBO&C and the PID-CS, when a step-change on F^{IN} is observed (check Section 4.3 for further details on the F^{IN} profile).

Table 3
Economic data for the F^{IN} step-change simulation.

Yields, conversions and revenues relating to the ideal simulation without any perturbation						
	χ_A	η_C	η_X	Ern_{real}	Ern_{max}	$(Ern_{real})/(Ern_{max})$
BSMBO&C	99.99 [%]	85.01 [%]	12.14 [%]	421.15 [kg]	486.40 [kg]	86.59 [%]
PID-CS	100 [%]	76.40 [%]	19.93 [%]	379.40 [kg]		78.00 [%]
Yields, conversions and revenues relating to the F^{IN} step-change simulation						
	χ_A	η_C	η_X	Ern_{real}	Ern_{max}	$(Ern_{real})/(Ern_{max})$
BSMBO&C	99.27 [%]	88.55 [%]	8.30 [%]	438.23 [kg]	486.40 [kg]	90.10 [%]
PID-CS	100 [%]	0.00 [%]	89.17 [%]	8.81 [kg]		1.81 [%]

*Notice that the sum of η_C and η_X is not exactly 100% because of both the presence of other components in the reacting mixture and the structure of the oxidation process kinetic scheme (Eq. (5))

batch cycle time and reactor temperature set-point for the PID-CS must be conveyed. The batch cycle time and reactor temperature set-point selection is performed as in Section 4.3, thus the employed methodology is not repeated. Instead, the feeding policy is different. Indeed, here F^{IN} is kept at a constant value that equals $F^{IN,0}$ (see Section 4.3).

Coming now to the results presentation, the essential profiles, concerning the operation of the 2-octanol oxidation reactor when a permanent failure in the coolant cooling system occurs, are reported in Fig. 5. Instead, the corresponding assignments relating to a temporary failure are presented in Fig. 6. Observe that, once again, the control system representing the industrial state-of-the-art (PID-CS) takes the fed-batch reactor to a dangerous runaway. This applies to the occurrence of both the temporary and the permanent failure in the coolant refrigeration cycle. Instead, the BSMBO&C is able, once again, to pre-dict and automatically prevent the hazardous control loss. Indeed, it decides to abort the batch cycle immediately after the coolant refrig-erating system failure because it detects that there is no way to keep the fed-batch reactor under control. The only chance is to immediately stop the production cycle and unload the reactor content. Notice that most of the standard NMPC/DRTO-like methods, where the batch cycle time is fixed a-priori, would have failed in avoiding the control loss in this special circumstance. These remarks on the BSMBO&C apply for the occurrence of both the temporary and the permanent coolant cooling system failure. This indirectly suggests that the reac-tivation of the coolant refrigeration cycle after approximately one hour from the failure is not enough to make the fed-batch reactor man-ageable. A quicker intervention would be necessary.

In the end, this second scenario clearly shows that BSMBO&C and BSMBO&C-like methods (i.e. specific NMPC/DRTO-like methods) can be used to automatically detect and prevent runaways, even when the controlled system cannot be kept under control by simply adjusting its manipulated variables. As already mentioned in the paper, it is the choice of considering the batch cycle time as an independent variable that is the key for this runaway detection and prevention capability.

Finally, by merging the contents of this section and those of Section 4.3, it can be immediately understood that BSMBO&C and BSMBO&C-like methods can both provide a (fed-)batch controlled system with a profitable optimization/control policy and ensure the online detection and prevention of dangerous runaways. Therefore, the practical achievement of the aims of the paper is now complete.

4.5. The BSMBO&C computational effort

Even though the conceptual aims of the paper have already been reached, the numerical results of the current case study have to be supported with some data relating to the BSMBO&C computational effort. Indeed, it must be shown that, limited to the case study, the time that BSMBO&C requires to compute a single control action is negligible with regard to the characteristic time over which the single batch is carried out and a potential runaway phenomenon may occur. By looking at the results reported in Sections 4.3 and 4.4, the reader can immediately understand that the characteristic times to complete a single batch and for a runaway phenomenon to occur are in the order of magnitude of several hours and minutes, respectively. On the contrary, BSMBO&C requires only some seconds (from 5 s to 15 s typically) to compute a control action. Therefore, BSMBO&C computational effort is certainly negligible with respect to the characteristic time of the phenomena occurring into the oxidation fed-batch reactor.

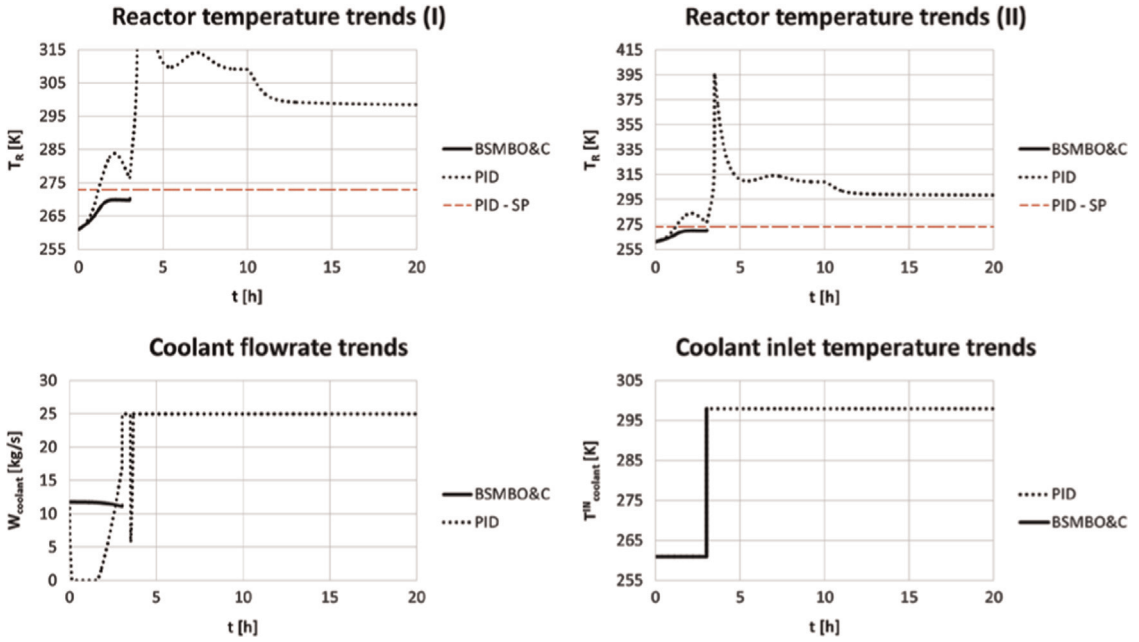

Fig. 5. Operation of the 2-octanol oxidation reactor, equipped with the BSMBO&C and the PID-CS, when a permanent failure in the coolant cooling cycle occurs.

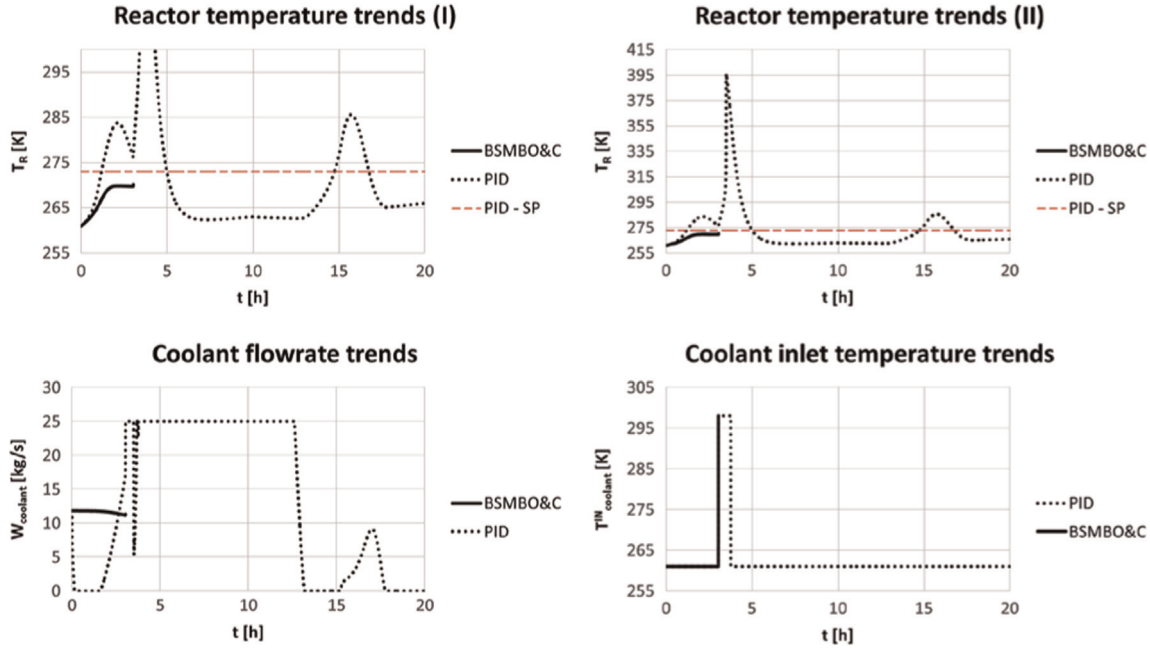

Fig. 6. Operation of the 2-octanol oxidation reactor, equipped with the BSMBO&C and the PID-CS, when a temporary failure in the coolant cooling cycle occurs.

This shows that the results reported in Sections 4.3 and 4.4 are really applicable in real life.

As a last remark, notice that if a specific runaway controlled system is found for which BSMBO&C is not fast enough in providing control actions in real-time (even though it seems very unlikely), then the entire conceptual framework described in the paper still holds. How-ever, there is the need for a more efficient algorithmic implementation of the overall strategy. Such a fast implementation can be developed based on literature references like (Zavala et al., 2008; Wolf et al., 2011).

5. Conclusions

In this paper, an advanced model-based strategy for the online optimization and/or optimal control of (fed-)batch systems, the BSMBO&C, is used to show that specific NMPC/DRTO-like methods can be used to both provide profitable optimization/control policies and predict and automatically prevent possible runaways. All this is shown both in conceptual and in practical terms, i.e. through a case study based on the oxidation process of 2-octanol with nitric acid in aqueous solution. The achieved results are very promising and open the way to the merging of the runaways prediction techniques with the dynamic optimization and optimal control algorithms, towards a new concept of online profitable and safe optimization/control of (fed-)batch processes. Even though the results reported in this work are obtained in the special case of negligible model mismatch, future works will be aimed at removing this assumption and deal with the detection and prevention of runaways under uncertainty. The final target is the formulation of a framework for the online profitable and safe optimization/control of batch/fed-batch processes under uncertainty.

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