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Combined Dynamic Optimization, Optimal Control and Online Runaway Detection & Prevention under Uncertainty

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This contribution investigates the extent to which dynamic optimization and optimal control can provide reliable prediction and insure prevention of runaways under uncertainty. We limit our analysis to batch systems because both the issue of model uncertainty and that of hazardous loss of control are widespread within this type of processes. The paper shows that, surprisingly, a specific class of deterministic dynamic optimization and optimal control algorithms allows us to easily identify and prevent runaways, even when no accurate process model is available. The production process of 2-butyl propanoate via acid-catalyzed esterification of 2-butanol serves as case study to substantiate our claims.

1. Introduction

Nowadays, many high value added chemical products (fine chemicals, APIs, etc.) continue to be synthesized batch-wise because of economic and technical considerations. Unfortunately, the production of many of these products involve highly exothermic chemical reactions, which might potentially trigger thermal runaways. Thus, the problem of finding efficient criteria to design and operate batch processes in safe and profitable fashion ("to design" means "to select the most suitable recipe" in this context) remains important and relevant to safe operation.

The traditional solution to this problem is to combine safety diagrams, which allow safe and profitable offline design, and conventional control systems, which should insure safe and profitable online operation. For the sake of clarity, let us briefly introduce the concept of safety map. Safety diagrams are charts showing design regions where, under nominal conditions, it is safe to carry out the batch process. The boundaries of such regions are often identified by critical values of dimensionless numbers measuring the interplay of heat generation and heat removal efficiency. In the past, several authors proposed their own safety diagrams (Zaldívar et al., 2003), which usually differ in both range of applicability and characteristics of the employed dimensionless numbers. On the other hand, recent research primarily focuses on finding novel methods to construct these safety maps, e.g. Copelli et al. (2013) propose to use topology tools while Milewska et al. (2005) suggest to rely on computational fluid dynamics. This said, it is important to point out that safety diagrams are still the state-of-the-art approach used to design batch processes, as recent contributions confirm (Casson et al., 2012).

This traditional approach to safe design and operation of batch processes is two-stage, i.e. we first take care of the design phase offline and then we seek the optimal and safe operating conditions associated with the resulting recipe in real-time (a control system handles this latter phase). However, especially for highly nonlinear batch processes, it is more effective to choose the recipe and define the optimal operation policy in both simultaneous fashion and real-time. This is why Rossi et al. (2015) recently proposed a framework for safe, online, simultaneous design and operation of batch processes, which relies on a specific class of dynamic optimization (DRTO) and optimal control (NMPC) algorithms. In particular, the NMPC/DRTO method used in (Rossi et al., 2015) is BSMBO&C (Rossi et al., 2014a), which is a tested methodology (Rossi et al.,

2014b) originating from the expertise of Prof. Manenti's research group in the development and application of DRTO/NMPC strategies (Viganò et al., 2010).
The strategy introduced by (Rossi et al., 2015), named BMBO&RP for the sake of brevity, shows to be reliable and effective but implies knowledge of an accurate model of the batch process. This is a challenge in many real settings because batch processes often involve multi-phase mixtures, complex chemical reactions, and so on. Therefore, this paper studies the extent to which BMBO&RP can still provide reliable prediction and insure prevention of runaways under uncertainty. Moreover, it also proposes simple qualitative modifications to BMBO&RP, which should allow improving its reliability under uncertainty. In order to accomplish this objective, we rely on a meaningful case study, i.e. the production of 2-butyl propanoate via acid-catalyzed esterification of 2-butanol.
The remaining portion of this article will report the principal features of BMBO&RP along with those of BSMBO&C, will analyze the impact of model uncertainty on BMBO&RP and suggest improvements to it, and will show the performance/reliability insured by BMBO&RP within the aforementioned case study.

2. Application of dynamic optimization and optimal control to runaway detection/prevention

NMPC/DRTO algorithms generate the optimal control policy for a given system via the system model. In particular, these methods use the model to predict the future operating conditions of the process as a function of the trajectories of its manipulated variables and calculate the trajectory (control policy), which insures the best system performance in the future. Consequently, it is evident that any NMPC/DRTO strategy for batch systems can predict runaways before they occur. However, the only NMPC/DRTO methods, which are able to automatically prevent runaways, are those which treat the batch cycle time as an additional optimization variable (BSMBO&C is one of the few methods having this feature). Such methods can automatically decide/suggest to stop a batch cycle whenever a critical event (critical process disturbance, equipment fault, etc.) occurs that would unavoidably cause a runaway in the future.
This said, BMBO&RP is an adaptation of BSMBO&C, where the user-supplied objective function $f_{Obj}^{BSMBO\&C}$ (a measure of the performance of the batch process) and the tuning coefficients are modified/selected according to specific rules. In particular, $f_{Obj}^{BSMBO\&C}$ is modified by adding an event-based penalty term that progressively increases as the system approaches runaway conditions. The specific definition of this penalty term is problem-dependent but, a very reasonable choice for batch reactors is to formulate it as shown in Eq(1) (this is the commonest case). If the batch unit, which may undergo runaway, is not a reactor, we need to reformulate the penalty term from case to case.

$$\textit{Penalty term} = \left[\textit{Binary on / off switch}\right] \frac{\int_0^{\left[\substack{\textit{Batch cycle}\\ \textit{time}}\right]} \left[\textit{Coolant flow}\right] dt}{\left[\textit{Scale coefficient}\right]} \tag{1}$$

The tuning coefficients are computed via ad-hoc formulas found in the article by Rossi et al. (2015). We do not report those formulas for brevity but encourage the reader to read the reference paper.
Since BMBO&RP strongly relies on BSMBO&C, we have to convey some additional information on this latter methodology before discussing the issue of model uncertainty.

2.1 The BSMBO&C framework

BSMBO&C is a strategy for the dynamic optimization and optimal control of batch systems (Rossi et al., 2014a). This approach allows us to manage a batch process by simultaneously adjusting both its manipulated variables and its batch cycle time. Moreover, this framework supports any user-defined objective function (even non-smooth ones), which has to measure the system profitability.
At run time, BSMBO&C first performs an initialization step and then iteratively executes a sequence of operations (BSMBO&C basic step) until a stopping condition is satisfied (Figure 1). The initialization serves to provide the algorithm with the user-defined inputs: the process model, the user-supplied objective function ($f_{Obj}^{BSMBO\&C}$), the upper/lower bounds on the system states and the manipulated variables, and the tuning parameters. The basic step is the core of the algorithm and consists of three phases: (I) an optimization step used to compute the next optimal control action; (II) the application of this control action to the batch process; and (III) the measurement of the system response and check of the stopping condition. Finally, the stopping condition allows the algorithm to identify whether the optimal cycle time is reached by the end of the current control action, thus deciding when to terminate the iterative execution of the basic step.

As a final remark, it is important to mention that BSMBO&C relies on the numerical routines of BzzMath library (Buzzi-Ferraris and Manenti, 2012), which are very efficient in handling strongly nonlinear problems. Therefore, BSMBO&C is particularly suitable for application to batch systems that may exhibit runaway/loss of control.

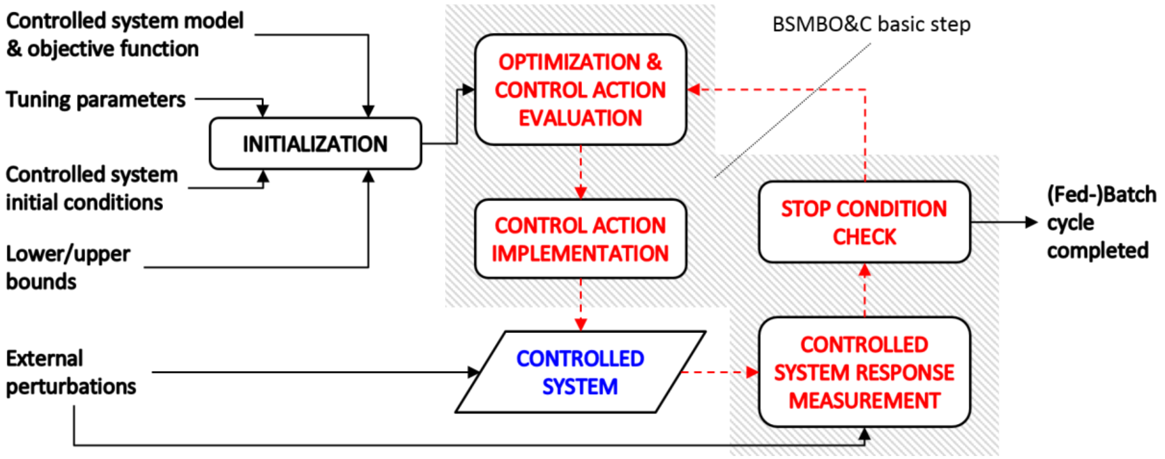

Figure 1: Simplified block diagram of the BSMBO&C framework.

2.2 The impact of model uncertainty

BMBO&RP has been designed under the assumption that a very accurate model of the batch process is available. Because it relies on a deterministic NMPC/DRTO framework, i.e. BSMBO&C, the presence of model uncertainty might potentially alter both its capability of predicting and preventing runaways and its ability of insuring high process performance. In fact, BMBO&RP fully relies on model predictions to identify future runaways and optimize the process performance, but such predictions are no longer reliable.
The most intuitive solution to this problem is to preserve the general architecture of BMBO&RP and replace BSMBO&C with a robust NMPC/DRTO framework, which retains all of its features (Rossi et al. (2016) have already developed this robust version of BSMBO&C and named it RBSMBO&C). The resulting robust version of BMBO&RP, named RBMBO&RP, would rely on RBSMBO&C, which is perfectly able to handle model uncertainty using stochastic programming. However, it is worth mentioning that this modification generates a downside, i.e. RBMBO&RP is much more computationally demanding than BMBO&RP.
A less computationally demanding solution is to alternate BMBO&RP and RBMBO&RP based on this rationale: (I) we use BMBO&RP whenever all the process states are sufficiently far away from their upper and lower bounds; and (II) we switch to RBMBO&RP whenever one or more states approach either their lower or their upper bounds. This alternative approach is reasonable only whether BMBO&RP can identify and prevent runaways even under uncertainty. This is sensible because the driving-force of a runaway is usually a huge process disturbance or a critical fault, which would cause loss of control according to the predictions of any realization of model uncertainty, i.e. any possible inaccurate model with which BMBO&RP is provided. Moreover, even if BMBO&RP were unable to detect a future runaway, RBMBO&RP would eventually predict it and prevent it before it can occur. Recall that RBMBO&RP would take over whenever one of the process states approaches one of its bounds and this is going to happen before the runaway can take place.
Both of the proposed solutions are reasonable and worth some further investigation. In this manuscript, we focus on the second. In particular, we use a case study to show that BMBO&RP can identify and prevent runaways under uncertainty in a reliable fashion.

3. Safe production of 2-butyl propanoate via acid-catalyzed esterification

The production of 2-butyl propanoate via acid-catalyzed esterification of 2-butanol is a typical example of process, which can exhibit thermal runaway. Since it represents an entire category of unstable chemical processes, it is a meaningful benchmark. We assume that it is carried out batch-wise using a fed-batch reactor, where 2-butanol is preloaded in the vessel along with a small amount of sulfuric acid, which acts as homogeneous catalyst, and propionic anhydride is slowly fed to the reaction environment over the entire batch cycle (Figure 2). Our final goal is to maximize the productivity of 2-butyl propanoate that corresponds to maximizing the conversion of 2-butanol, because no significant side reactions take place inside the process operating window. In order to perform this task, we can manipulate both the feed flow of propionic anhydride (F_{IN}) and the coolant flow (F_j).

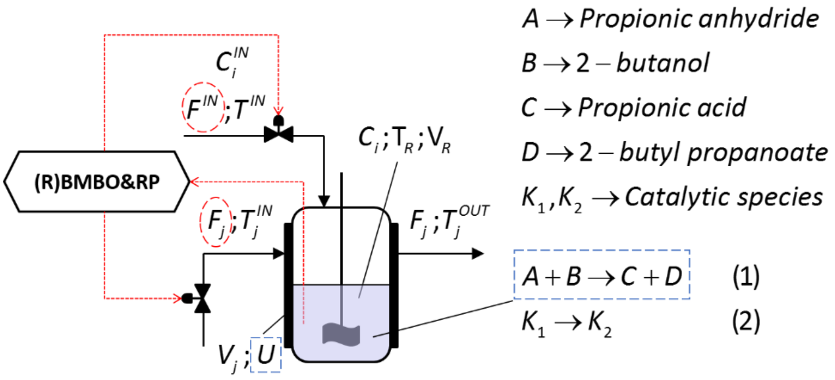

Figure 2: Simplified PFD of the production process of 2-butyl propanoate via acid-catalyzed esterification of 2-butanol (manipulated variables are enclosed in circles while uncertain parameters are enclosed in squares).

Since in this case study we focus on showing that BMBO&RP can identify and prevent runaways even under uncertainty, we assume that both the global heat transfer coefficient of the reactor U and the activation energy E_2, used to compute the kinetic constant k_2^0 of reaction (1) (see Figure 2), are uncertain parameters. In particular, we assume that U can vary up to $\pm$ 20% and E_2 up to $\pm$ 3% with regard to their nominal values. We also consider that the joint probability distribution of U and E_2 is a bivariate Gaussian distribution with diagonal variance-covariance matrix, i.e. the two uncertain parameters are uncorrelated.
Finally, the uncertain process model is derived under conventional assumptions such as perfect mixing, temperature-independent thermodynamic properties, and constant density of the reacting medium (this assumption has been verified). The resulting model is a system of 9 ODEs, including 7 mass balances and 2 energy balances, which are not reported for space limitations.

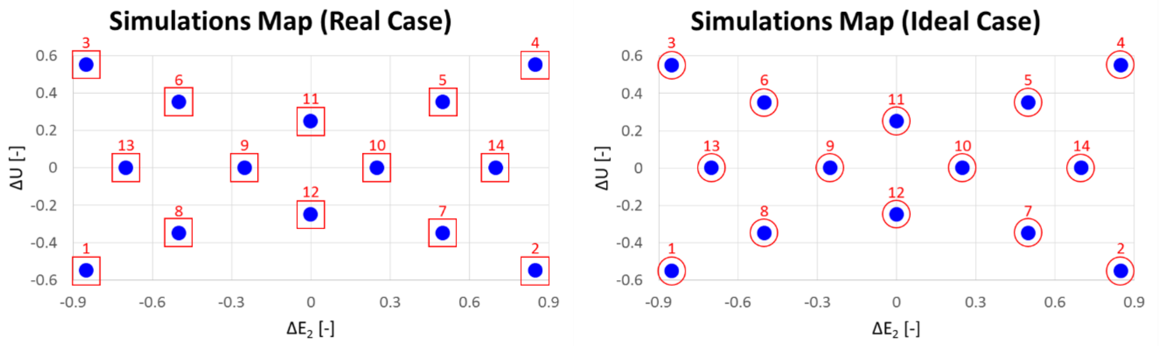

Figure 3: Simulations performed with BMBO&RP both in the presence and in the absence of model uncertainty, i.e. in both real and ideal conditions (dots surrounded by squares or circles represent the simulations where BMBO&RP can successfully identify and prevent a runaway).

Exploiting all the data reported so far, we have used BMBO&RP to run 14 simulations in ideal conditions, i.e. in the absence of model uncertainty, and as many simulations in real conditions, i.e. in the presence of model uncertainty. The pseudo-real processes used to run the two groups of simulations have been selected so as to cover the uncertainty space (bi-dimensional space of U and E_2) uniformly. Moreover, in all of the 28 simulations, we have assumed that a critical equipment fault occurs about 15 min after the beginning of the batch cycle. The fault selected is a leakage in the feed flow control valve, which causes an unwanted and uncontrollable amount of propionic anhydride to enter the reactor over time.
Figure 3 shows how the ideal and real simulations are laid out in the uncertainty space, represented in terms of two dimensionless parameters $\Delta\mathrm{U}$ and ΔE_2, which are proportional to U and E_2 according to Eq(2). This figure also shows that the equipment fault (feed valve uncontrolled leakage) triggers a runaway in every single

simulation and confirms that BMBO&RP is able to identify all those runaways both in the presence and in the absence of model uncertainty (all dots are surrounded by circles/squares).

$$
\begin{cases}
U = \left[Nominal\ value\ of\ U\right]\left(1+\dfrac{\Delta U}{\left[Scale\ coefficient\right]}\right) \\
E_2 = \left[Nominal\ value\ of\ E_2\right]\left(1+\dfrac{\Delta E_2}{\left[Scale\ coefficient\right]}\right)
\end{cases}
\tag{2}
$$

After observing that BMBO&RP can also identify runaways under uncertainty, we are interested in the control policy applied to the batch reactor before any cycle is aborted. This information is reported in Figure 4.

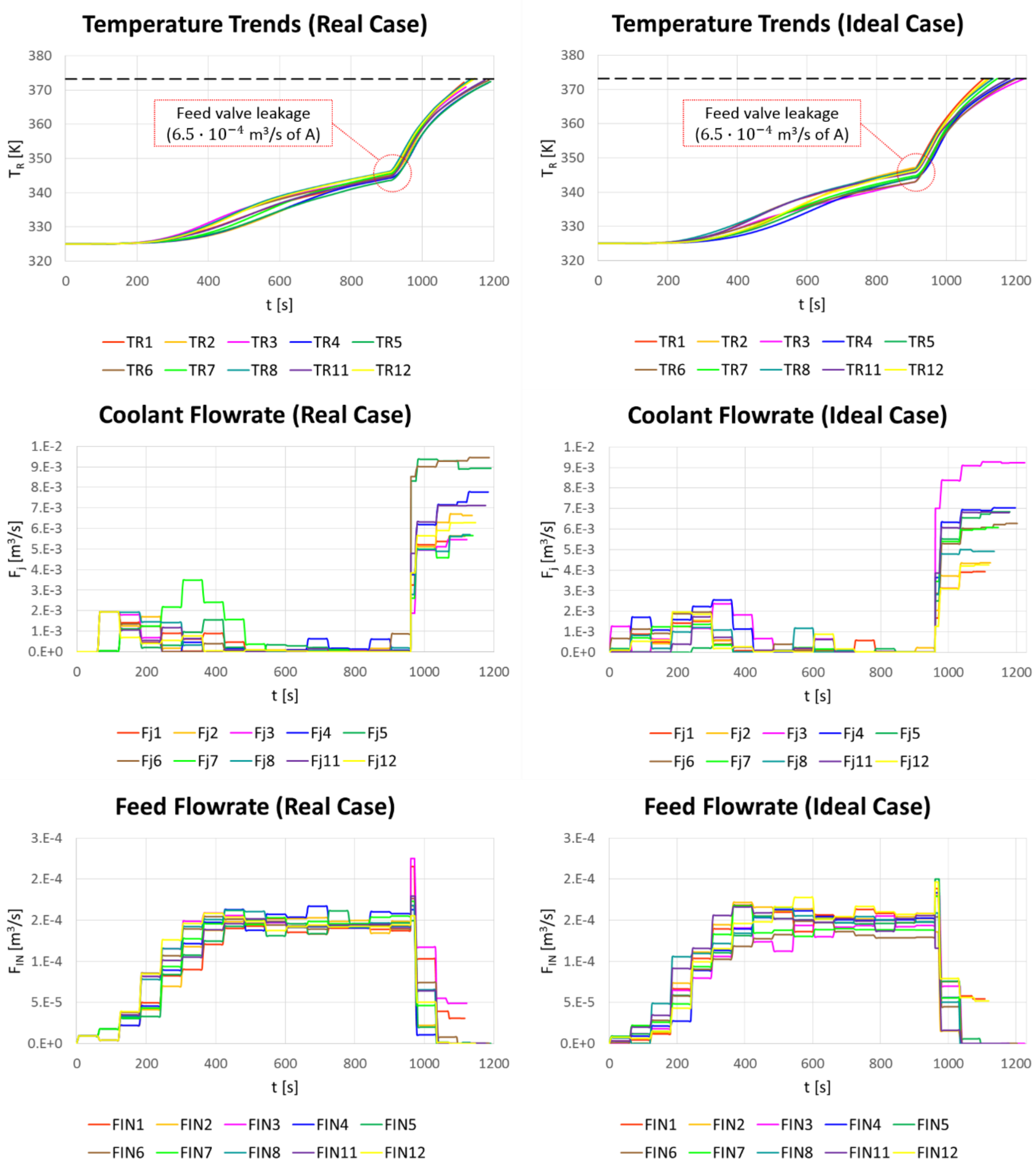

Figure 4: Control policy applied to 10 of the simulations showed in Figure 3 and resulting temperature profiles inside the reactor (F_{IN} is the actual feed flow reduced by the flow due to the leakage and represents the actual control policy suggested by BMBO&RP).

Note that, as soon as the equipment fault occurs, BMBO&RP tries to increase the coolant flowrate and reduce the feed flow (the valve is leaking but we can still try to close it at least to reduce the flow of propionic anhydride entering the reactor). However, it soon realizes that it is impossible to keep the reactor under control, thus it decides to terminate the cycle a few minutes later. It is important to notice that BMBO&RP lets the reactor temperature (T_R) almost reach the upper bound, i.e. 373.15 K, before stopping the batch cycle. At least in this specific case, this is not a serious concern because it is enough to introduce a small amount of sodium hydroxide in the reactor to neutralize the sulfuric acid and stop the reaction immediately. On the other hand, this temperature trend is compliant with our objective, i.e. the maximization of the conversion of 2-butanol. This latter observation suggests that BMBO&RP can not only predict and prevent runaways but also decide when to abort a batch cycle to minimize performance loss. In that, BMBO&RP is smarter than a regular control system coupled with a conventional alarm system.

4. Conclusions

In this contribution, we have discussed the extent to which dynamic optimization and optimal control algorithms for batch processes can identify and insure automatic prevention of runaways under uncertainty. The key concepts, which we have discussed, are: (I) the features that an NMPC/DRTO strategy must possess to be suitable for runaway prediction and prevention; (II) the usage of RBMBO&RP and the alternated use of both RBMBO&RP and BMBO&RP to handle the rigorous identification and prevention of runaways under uncertainty; and (III) the confirmation that specific classes of deterministic NMPC/DRTO frameworks can reliably identify and prevent runaways even under uncertainty (see the results of the case study).

The third observation is the most important finding of the paper. Specific classes of deterministic NMPC/DRTO frameworks can always identify and prevent runaways because runaway is an extreme phenomenon generated by a critical event, which is very likely to cause loss of control according to the predictions of any possible inaccurate model fed to the NMPC/DRTO strategy. We can say that NMPC/DRTO is somewhat intrinsically robust with regard to the identification and prevention of runaways.

In conclusion, it is important to say that specific types of deterministic NMPC/DRTO can predict and prevent runaways under uncertainty but cannot convey any information on how to shut down the batch unit safely (this usually implies introducing some inhibitor). As already pointed out, this is not a serious concern for the example reported in the manuscript, where the optimal shutdown policy is straightforward. However, in order to cope with this latter problem, we can only rely on RBMBO&RP. This is subject for future research work.

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