INTEGRATION OF CAMPAIGN SCHEDULING, DYNAMIC OPTIMIZATION AND OPTIMAL CONTROL IN MULTI-UNIT BATCH PROCESSES

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Abstract

This contribution proposes a two-phase framework for dealing with the integrated campaign scheduling, dynamic optimization and optimal control of batch processes (MUBSMBO&C). The strategy allows evaluation of the optimal campaign schedule of the batch process in real time as well as determination of the optimal control actions in order to achieve maximum profit and/or performance. As a result of the two-phase architecture, the algorithm does not require solution of a mixed-integer optimization problem in real-time and can support virtually any processing recipe including various types of material recycles. In order to show its potential, we demonstrate this methodology by applying it to the integrated campaign scheduling, dynamic optimization and optimal control of a nopol production campaign carried out in a dedicated batch production facility.

Keywords

Dynamic optimization, Model predictive control, Scheduling

Introduction

In the last few decades, optimization techniques have been widely applied to many problems of industrial relevance, e.g. supply-chain management and planning, scheduling, dynamic optimization and optimal regulatory control. The resulting benefits have been significant in terms of (economic) performance, environmental impact and safety. Therefore, there is continuing interest in developing more flexible and effective optimization strategies for any of the aforementioned classes of problems. This paper contributes to this area, by advancing a framework for integrating scheduling, dynamic optimization and optimal control for batch processes (MUBSMBO&C). Note that a number of strategies have been reported in the literature to tackle these three classes of problems both individually and simultaneously.

The first applications of dynamic optimization (DRTO) and optimal control (NMPC) to batch operations date back approximately to 1980. Thirty years later, we can find further studies showing how to take advantage of these strategies to both improve process performance and prevent safety hazards. In addition, various extensions and improvements continue to appear, comprising mostly of new algorithmic formulations (Rossi et al., 2014), novel implementation schemes or explicit incorporation of model uncertainty into the framework (Rossi et al., 2016).

The first application of scheduling algorithms to batch operations dates back approximately to 1990. Twenty-five years later, we can find several of these algorithms in the literature, which we can categorize mostly on the basis of how they perform task allocation decisions and what type of process models they use. Some illustrative examples

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include: (I) methods where the process models are simple recipes and the tasks allocation is solved via heuristic approaches (Chu et al., 2014) or combinatorial methods (Hegyháti and Friedler, 2011); (II) frameworks in which the process models are linearized or consist of simplified recipes and the tasks allocation is performed via mixed-integer linear programming (MILP) (Sundaramoorthy and Maravelias, 2011); and (III) strategies where the process models are non-linear and the tasks allocation is carried out via mixed-integer non-linear programming (MINLP) (Capón-García et al., 2013).

Finally, very recent contributions propose methods for solving the tasks allocation phase in real-time while simultaneously providing optimal control actions to all of the batch units (SCH-DRTO&C). These methods combine scheduling frameworks with NMPC/DRTO strategies and can be divided into approaches exploiting linearized or piecewise linear process models and those which employ complete non-linear process models (Nie et at., 2015).

Many of these existing SCH-DRTO&C strategies suffer from three principal limitations: (I) they cannot effectively handle mixed process recipe structures, i.e. recipes where some batch operations run in series and other run in parallel; (II) they are quite unsuitable for handling recycles between and within successive production batches; and (III) they require solution of MILPs/MINLPs online. Unfortunately, real batch processes often include material recycles and their associated models are usually strongly non-linear, thus solution of these MILPs/MINLPs online may be difficult (for example, see the nopol production process). Therefore, in this paper, we propose an alternative SCH-DRTO&C strategy that mitigates these three aforementioned limitations (MUBSMBO&C).

MUBSMBO&C involves an offline and an online phase. The first requires solution of a conventional campaign scheduling problem and serves to collect key information needed for the second phase. The latter relies on a modified NMPC/DRTO algorithm (Rossi et al., 2014), allows updating the offline campaign schedule in real time and provides the batch process with optimal control actions. Due to this particular two-phase architecture, MUBSMBO&C does not require solution of an MILP/MINLP online and can support virtually any process recipe structure, including various types of recycles. However, in its present form, it only supports single-product production campaigns or batch processes that can be decomposed into a sequence of independent single-product production campaigns (the pharmaceutical and fine chemicals sectors and other industrial productions usually rely on this type of campaign structure).

We next describe the concepts underlying MUBSMBO&C and present a case study in which we apply it to a nopol production campaign. We also solve the same case study with a simpler and more conventional method (ITBSMBO&C) to provide some basis for comparison and to draw preliminary conclusions about MUBSMBO&C efficiency and resilience.

Nopol Production Process

Nopol is an organic compound used in the formulation of detergents, nail polishes, perfumes, etc. for which several production pathways exist. However, one of the common ones simply involves three batch operations, i.e. reaction, filtration and vacuum distillation, which are executed sequentially but are interconnected with each other via three main recycle loops (Figure 1).

The batch reaction phase is isothermal, usually lasts up to 12 h and comprises reacting β-pinene with formaldehyde in the presence of a heterogeneous catalyst in a solvent (ethyl acetate) to produce the desired nopol. Upon reaching desired conversion, the unreacted formaldehyde is vented and sent for downstream treatment. The batch filtration phase is isobaric, serves to separate the heterogeneous catalyst from the mixture of β-pinene, nopol and ethyl acetate and is about 0.5 h in duration. The vacuum batch distillation phase is isobaric, separates nopol from the mixture of β-pinene and ethyl acetate and has a duration of between 4 and 10 h. Note that nopol is heat sensitive, thus is only recovered from the pot of the batch distillation column in order to minimize the temperature needed to meet its purity specification.

Finally, the three recycle loops consist of: (I) recycling the heterogeneous catalyst from one filtration phase to the following reaction phase; (II) reusing the β-pinene and ethyl acetate recovered in a distillation phase as input to the next reaction phase; and (III) recycling the residual volume of β-pinene, nopol and ethyl acetate left at the end of a distillation phase to the next distillation phase.

Before describing the logic of MUBSMBO&C, we call attention to two features of this example. First, the optimal schedule of a nopol production campaign can, on the basis of the recipe description, be represented as the repetition of a number of partially overlapping logical blocks (LBs) consisting of a reaction, a filtration and a vacuum distillation step in series. This modular and periodic feature is not only characteristic to this example but is common to batch production campaigns in general. The architecture of MUBSMBO&C relies on this modular nature. Second, this relatively simple batch process does involve two complicating features: multiple recycles and batch unit operations with strongly non-linear dynamics. These typical characteristics of batch productions, motivate the development of alternative SCH-DRTO&C strategies, e.g. MUBSMBO&C.

MUBSMBO&C Framework

MUBSMBO&C is a framework for addressing the integrated campaign scheduling, dynamic optimization and optimal control of single-product production campaigns in batch processes (multiple instances of the algorithm are needed for those batch processes where multiple single-product campaigns are performed in parallel).

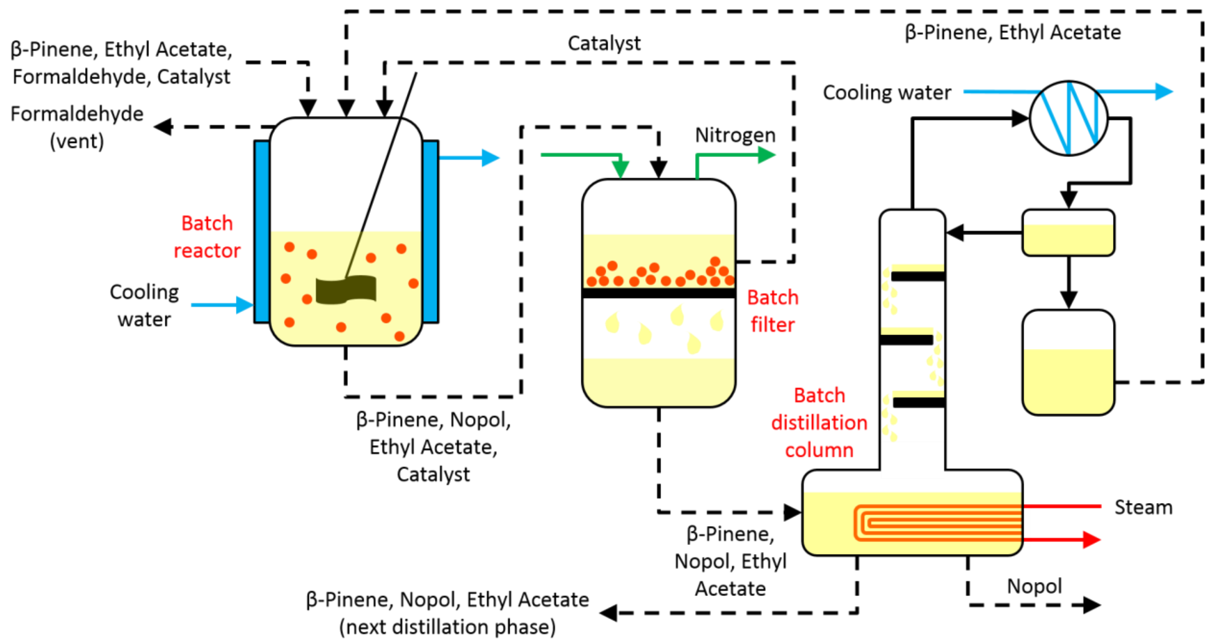

Figure 1. Flow diagram of the nopol production process

The algorithm is applicable under two reasonable assumptions: (I) the production campaign is assigned dedicated batch units; and (II) the supply of raw materials and/or utilities is not limiting for scheduling purposes. As previously outlined, the method is comprised of an offline phase (phase I) and an online phase (phase II), whose rationales are outlined below.

Phase I is performed only once before the production campaign is carried out and provides key parameters that are kept constant in phase II. It relies on conventional scheduling algorithms and involves three steps in series.

First, a regular campaign scheduling problem is solved where some additional constraints are imposed to force the resulting schedule to be periodic (step A). Next, a set of batch operations and/or fractions of batch operations, called an equivalent cycle (EC), is identified. This is done so that the entire campaign schedule can be described by an appropriate number of ECs which are executed sequentially (step B). Finally, on the basis of the EC structure, the recycles present in the recipe are classified as either internal recycles, which connect the operations within a given EC, or external recycles, which connect operations in different ECs (step C).

The key information generated in steps A, B, C and retained in phase II is the structure of the EC, i.e. the number/order of the operations in the EC and their starting/ending sequence, and the recycle classification.

As final remarks, note that although we have developed a procedure for addressing step B in general, we can not report it here due to space limitations. For illustrative purpose, the EC determined by applying step B to the nopol production campaign is shown in Figure 2. Note that the EC has the reaction operation split into two parts so as to accommodate the recycle of catalyst as an internal recycle and also defines the nature of the additional two external material recycle steps. This EC structure is treated as an integrated entity in phase II.

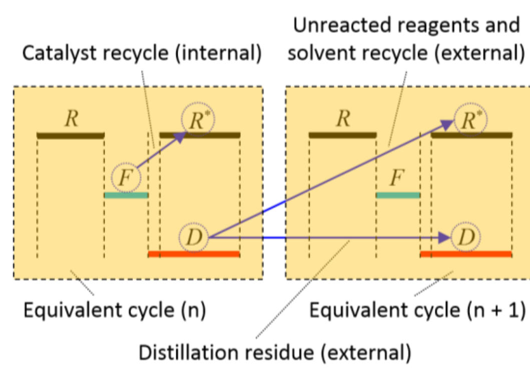

Figure 2. Structure of the equivalent cycle of the nopol production campaign and resulting recycle classification (R, R^* – Fractions of batch reaction operations, F – Batch filtration operation, D – Batch distillation operation)

Phase II is an adaptation of the NMPC/DRTO algorithm described in (Rossi et al., 2014). It serves to determine online the optimal residual number of ECs needed to complete the production campaign, to optimize some of the variables of the current EC in real time (its duration and the times of its constituent operations) and to provide the optimal control actions for each of its batch operations. It consists of an initialization step performed only once and three iterative steps executed in rolling horizon fashion until a certain stopping condition is met (Figure 3).

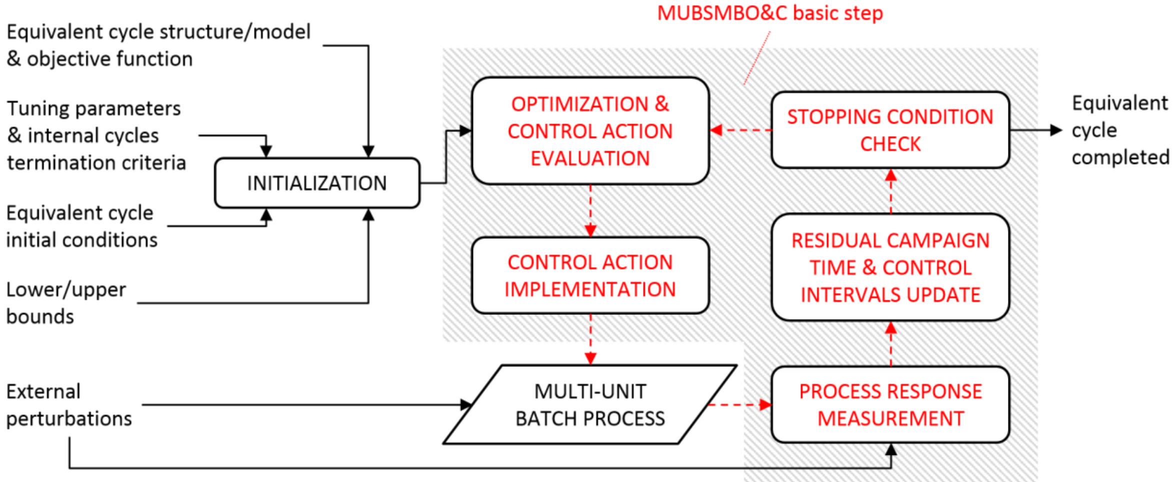

Figure 3. Architecture of phase II of MUBSMBO&C

The first iterative step serves to re-estimate several internal parameters of MUBSMBO&C, the most important of which is the residual time available to complete the production campaign (step D). The second iterative step implies solving a specific non-linear optimization problem (NLP), which determines the residual number of ECs, the dynamic properties of the current EC and the control policies for its batch operations. The objective function of this optimization problem measures the profitability and/or performance of the fraction of the production campaign yet to be completed (all recycle streams are included directly or indirectly in this function). This second iterative step also takes care of evaluating the current set of control actions from the optimization results (step E). Finally, the last iterative step comprises the application of the current set of control actions to the proper batch units and the measurement of their dynamic response (step F).

The aforementioned stopping condition serves to identify when the optimal time of the current EC has been reached and thus there is no need to perform another MUBSMBO&C basic step. In other words, it allows identifying when the current EC must terminate.

The last key aspect to mention about phase II is that it must be executed iteratively as well because we need to carry out a series of ECs to complete the whole production campaign (see the definition of EC previously provided). In particular, we need to execute new phase II calculations until the optimal residual number of ECs estimated at the end of the current online phase assumes the value of one. This occurs only when it is possible to satisfy all of the specifications of the production campaign (production volume, product purity, etc.) at the end of the current EC and there is no longer a need to perform further ECs.

As final remarks, note that we can not convey the mathematical details of the execution of steps D and E due to space limitations. However, the optimization problem solved in step E is an NLP, even though one of the optimization variables is conceptually integer (the residual number of ECs needed to complete the production campaign). This is possible due to the special way in which we compute this variable, i.e. by rounding a combination of continuous variables. Finally, we wish to call attention to the important features that MUBSMBO&C does not require solution of an MILP/MINLP online and that it supports any type of process recipe structure, including various types of material recycles between batch operations internal and external to the EC.

Online Scheduling, Dynamic Optimization and Control of the Nopol Production Process

We validate MUBSMBO&C by applying it to the problem of integrated campaign scheduling, dynamic optimization and optimal control of a nopol production campaign, which is performed in a dedicated production facility. We also perform the optimization with a simpler version of the integrated optimization strategy, ITBSMBO&C, which involves solving the integrated campaign scheduling, dynamic optimization and optimal control of every individual batch operation of the production campaign. This latter strategy requires first the definition of proper production campaigns for each of these batch operations according to the output of step A of phase I of MUBSMBO&C. Then, it involves applying a slightly modified version of phase II of MUBSMBO&C to the same single batch operations individually (the equivalent cycle comprises a single batch operation in every different application instance). The two most relevant differences between MUBSMBO&C and ITBSMBO&C are the following: (I) ITBSMBO&C does not support the dynamic update of the residual time available to complete the production campaign of every single batch operation; and (II) ITBSMBO&C only allows optimal management of a single batch operation at a time.

Table 1. Principal economic and process-related data associated with the nopol production campaign optimized/designed online (productivity target of nopol: 925 [kg], minimum molar purity of nopol: 0.975 [-])

Physical quantity	MUOpt – NoD	MUOpt – MD	SUOpt – NoD	SUOpt – MD
Number of LBs or ECs [-]	8	8	8	8
Productivity of nopol [kg]	925.0	925.0	925.0	921.6
Molar purity of nopol [-]	0.97501	0.97515	0.97514	0.97500
Net income [$]	2504	2521	2520	2505

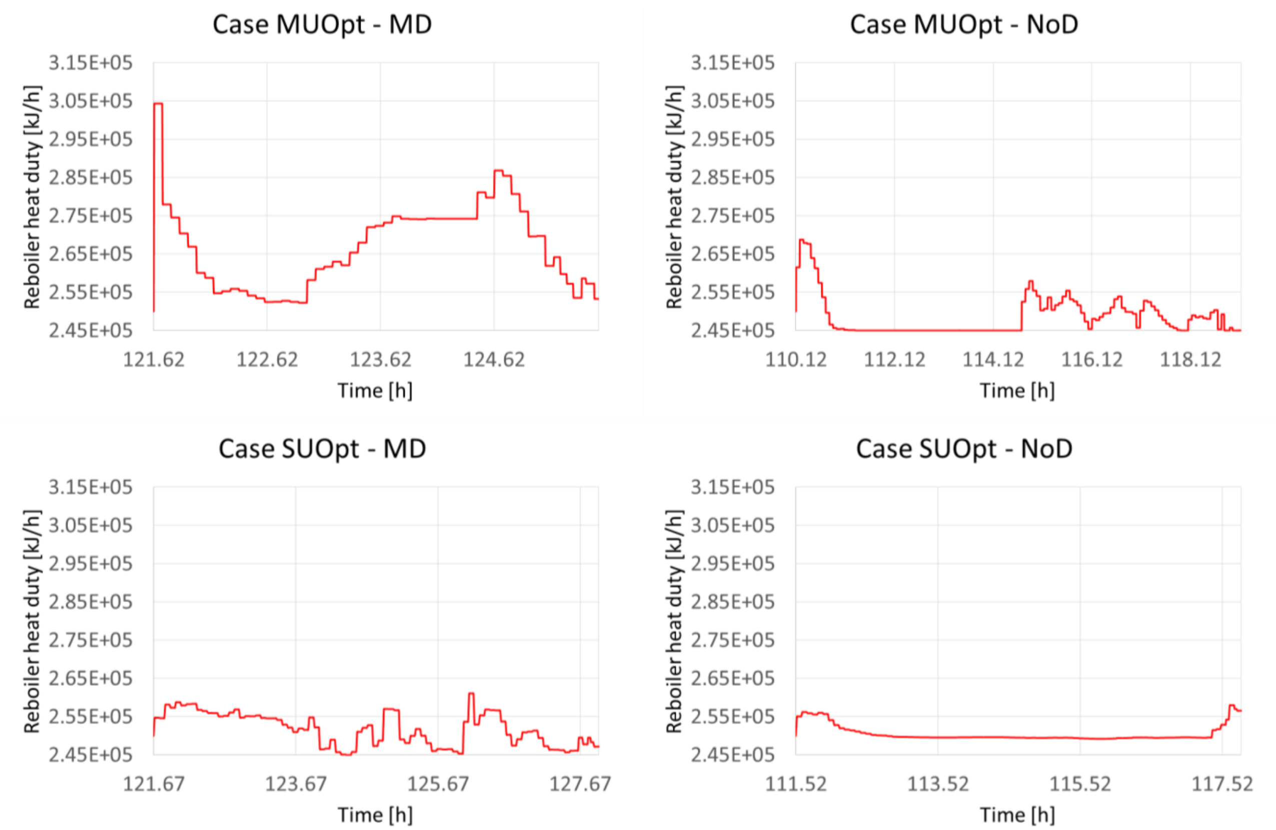

Figure 4. Trajectories of the reboiler heat duty related to the eighth batch distillation phase

We apply the two aforementioned frameworks to two different scenarios, namely one where process disturbances are present and the other where such disturbances are absent. The two MUBSMBO&C-based cases are named MUOpt – NoD and MUOpt – MD, where acronyms NoD and MD stand for the absence and presence of process disturbances, respectively. The two corresponding ITBSMBO&C-based cases are named SUOpt – NoD and SUOpt – MD. The set of process disturbances applied in cases MUOpt – MD and SUOpt – MD includes perturbations affecting the batch reaction and batch distillation phases. The most critical disturbance affects all batch reaction phases from the fifth onwards, i.e. all ECs and LBs from the fifth onwards, and consists of 20% loss in the mass of heterogeneous catalyst. The other disturbances affect the fifth, seventh and eighth distillation phases and comprise multiple variations in the operating pressure of the distillation column (+ 20 – 30 %) as well as the insurgence of a heat loss in the reboiler heat duty of the column (eighth distillation phase).

Illustrative dynamic profiles resulting from the MUBSMBO&C and ITBSMBO&C strategies are shown in Figure 4. This figure shows the optimal profiles of the reboiler heat duty associated with the eighth distillation phase and cases MUOpt – NoD, MUOpt – MD, SUOpt – NoD and SUOpt – MD (the same trends are observed in different distillation phases). This heat duty is probably the most important operational variable that MUBSMBO&C and ITBSMBO&C can dynamically adjust. It is clear that the two frameworks generate significantly different results both in the presence and in the absence of process disturbances. This is because they differ in the conceptual aspects mentioned at the beginning of this section.

According to Figure 4, we would also expect significant differences in both the economic performance and the resilience (capability of rejecting disturbances) of

MUBSMBO&C and ITBSMBO&C. However, the data summarized in Table 1 shows that no significant difference in economic performance arises between the two approaches. The net income achieved at the end of the nopol production campaign is essentially the same in cases MUOpt – NoD, MUOpt – MD, SUOpt – NoD and SUOpt – MD. This is mainly a consequence of the nature of the nopol production process, where the principal cost is due to raw materials and this cost is essentially the same as long as the same production target is achieved. On the other hand, Table 1 also suggests that MUBSMBO&C is more resilient than ITBSMBO&C because it always satisfies the purity and productivity specifications of the production campaign. ITBSMBO&C fails to satisfy the productivity specification in presence of process perturbations. This last aspect originates from the fact that ITBSMBO&C does not support the dynamic update of the residual time available to complete the production campaigns of the single batch operations. In fact, in the presence of process disturbances, the loss of heterogeneous catalyst, which occurs in the fifth reaction phase, causes the overall time needed to complete all of the reaction phases to increase. ITBSMBO&C cannot handle this situation because it cannot dynamically increase the residual time available to complete the production campaign of the batch reaction phase. Therefore, it must violate the productivity specification of the nopol production campaign. This type of issue clearly does not arise under the MUBSMBO&C approach.

Based on this case study, we suggest that MUBSMBO&C performs at least as well and is more resilient than ITBSMBO&C. Moreover, ITBSMBO&C can be expected to offer better and more resilient performance than typical hierarchical strategies for managing batch production campaigns in which the scheduling phase is solved at a higher level and dynamic optimization and control are applied at a lower level. We believe that MUBSMBO&C is more effective than these conventional approaches as well. These initial results suggest that the SCH-DRTO&C-like framework for batch processes that we have developed is a promising approach for achieving both good performance and resilience for (periodically operated) general batch operations.

Finally, we make some observations regarding the computational performance of the MUBSMBO&C strategy. The average time to evaluate a single set of control actions in any execution of phase II is about 1 min. This result is achieved on a conventional laptop computer with 8 GB of RAM and a dual core processor i7 – 451U 2.0 GHz. This level of computational efficiency is sufficient for online application for this particular case study but also in many other realistic situations. This level of performance is a direct consequence of a framework that does not require solution of MILPs/MINLPs online and suggests that MUBSMBO&C should have more favorable scalability than the existing SCH-DRTO&C-like methods, which tackle integrated scheduling, dynamic optimization and optimal control problems via direct mathematical programming approaches.

Conclusions

This contribution proposes a framework, MUBSMBO&C, which tackles the problem of integrated campaign scheduling, dynamic optimization and optimal control of single-product production campaigns involving batch operations. The two principal advantages of the methodology lie in its applicability to batch processes with arbitrary recipe patterns, including recycles, as well as in its avoidance of the need for online solution of MILPs/MINLPs. The MUBSMBO&C framework is validated via the integrated campaign scheduling, dynamic optimization and optimal control of a nopol production campaign. Additionally a simpler strategy, ITBSMBO&C, is also used to solve the same problem for purposes of comparison. The results achieved in the test case suggest that MUBSMBO&C performs at least as well and is more resilient than ITBSMBO&C. Moreover, the results suggest, but of course do not prove, that it is superior to many conventional hierarchical strategies for managing batch production campaigns. Finally, MUBSMBO&C seems to offer good computational efficiency and appears to be more scalable than SCH-DRTO&C-like methods that require online solution of MILPs/MINLPs.

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