A Reactive Optimization Strategy for the Simultaneous Planning, Scheduling and Control of Short-Period Continuous Reactors

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Abstract

The efficient and economic operation of processing systems is normally addressed within a planning, scheduling and control framework. Due to its complexity, these activities are commonly approached in a decoupled rather than in a simultaneous manner. Although the decoupled approach leads to a computationally tractable problem, the solution of such a problem can result in a suboptimal solution because interaction among planning, scheduling and control activities are neglected. Even when the optimal simultaneous solution of this problem can result in large scale optimization problems, such a solution can represent economical advantages making feasible its computation using optimization decomposition and/or few operating scenarios. After reducing the complexity of the optimal simultaneous deterministic solution, it becomes feasible to take into account the effect of model and process uncertainties on the quality of the solution. In this work we will consider that changes in plant product demands hit the process once the process is already under continuous operation. Therefore, a reactive strategy is proposed to meet the new product demands. Based on an optimization formulation for handling the simultaneous planning, scheduling, and control problem of continuous reactors, we propose a heuristic strategy for dealing with unexpected events that may appear during operation of a plant. Such strategy consists of the rescheduling of the products that remain to be manufactured after the given disturbance hits the process. Such reactive strategy for dealing with planning, scheduling and control problems under unforeseen events is tested using two continuous chemical reaction systems.

1 Introduction

Planning, Scheduling and Control (PSC) are activities closely related to the global and efficient operation of processing industries. They are normally practiced in a hierarchical manner from top to bottom (see Figure 1(a)). Planning decisions are normally taken first and involve settings plans or strategies which can span over weeks or even months. In a second step, based on these strategies, the main components of the processing systems are scheduled such that target product demands are met in the best possible manner. Finally, the third step involves computing lower level control actions to operate the processing systems around the target processing conditions leading to manufacturing the set of plant products. Due to the inherent complexity of PSC activities they are normally approached in a sequential rather than in a simultaneous manner (see Figure 1(b)). However, decoupling PSC actives can lead to take decisions which can result in suboptimal operation simply because natural interactions among PSC actives are not fully exploited. On the other hand, a clear disadvantage of the simultaneous approach for handling the solution of PSC problems lies in the fact that the optimal solution of such problems tend to be computationally demanding. However, the deployment of advanced decomposition optimization techniques [1], [2], [3] can make computationally tractable the optimal solution of such large and complex optimization problems. The optimal simultaneous solution of SC (scheduling and control) [4] and lately of PSC problems has been previously addressed [5]. However, there are some related issues in PSC problems which remain to be addressed. To begin with most of the published works only address PS (planning and scheduling) or SC problems. Very few strategies have been proposed for dealing with the optimal solutions of integrated PSC problems [5], [6], [7]. Additionally, PSC strategies need to be developed to cope with unexpected or unforeseen situations. In the present context unexpected or unforeseen situations refer to any event which takes the process away from the nominal operating conditions for which the PSC problem was originally solved. Most of the time such events can result in changes in the demand of certain plant products, but they can also involve some other variables such as change in the value of plant products or even a kind of process upset hitting the system (although this last type of event is normally handled using a proper control system). Under these conditions it turns out that the optimal PSC strategies computed under nominal (i.e. fixed) processing conditions are not longer valid and they should be some way corrected to reflect the new processing environment. Such strategies are normally named reactive strategies since they update the processing conditions (i.e. production schedule, flowrates , temperatures, etc.) such that the process can met the new processing scenarios [8]. Most of proposed reactive strategies have been formulated in the context of planning and scheduling problems [9]. It is clear that if uncertainties are known to happen in advance, then stochastic optimization techniques [10] can be used to cope with such issues. However, in face of unforeseen events reactive optimization strategies can be a better alternative to deal with on-line production environments. Moreover, when PSC strategies also include a closed-loop control system to track product transitions, then both process upsets and process modelling errors can also be rejected and taken into account, respectively, to enhance the quality of the optimal PSC solutions.

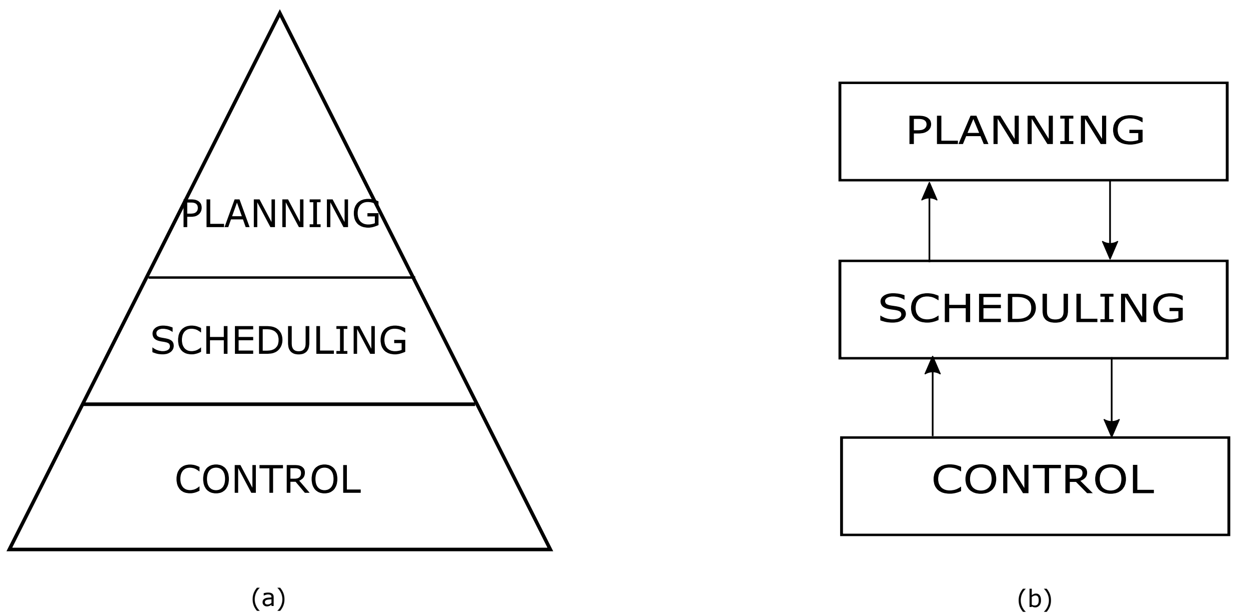

Figure 1: (a) Sequential and (b) Simultaneous approaches for dealing with Planning, Scheduling and Control problems.

In this work we propose a heuristic reactive strategy for addressing the simultaneous optimization of PSC systems in the face of unforeseen events. The present work is an extension of previous work where we have proposed an integrated approach for dealing with PSC problems featuring short-term production periods [5]. The work reported in [5] included an extended horizon production policy and a nonlinear model predictive control for tracking the transition trajectories between target products.

Because continuous and binary decision variables were involved and since process dynamics was also required to model dynamic system behaviour, the underlying optimization problem turned out to be complex Mixed-Integer Dynamic Optimization (MIDO) problem. Details about the solution of the MIDO problems can be found elsewhere [11]. Specifically in the present work, we deal with processing scenarios where the demand of some plant products is modified. Due to: (1) the complexity of the underlying MIDO problem and (2) because no optimization decomposition techniques are deployed, only short-period processing systems are taken into account. Initially, the simultaneous PSC problem is solved considering nominal demands and processing conditions. Once the nominal PSC problem has been solved, new demands are enforced over certain plant products at specific processing times. It is clear that under the new unforeseen conditions, the nominal PSC solution will not necessarily remain optimal. Therefore, new optimal PSC solutions ought to be computed such that the new products demand is fully met.

2 Literature review

Following, we review some of the most representative works concerning the use of robust optimization strategies for dealing with unexpected or unforeseen events when addressing mainly PS or SC problems. A new approach for efficient rescheduling of multiproduct batch plants was introduced in [12]. The authors propose a two-stage strategy for robust scheduling (RS). In the first step a deterministic approach is used for batch scheduling. In a second step a set of constraints are introduced into the deterministic formulation for addressing two practical cases: machine breakdown and rush order arrival. The idea of the approach consists in finding new scheduling solutions such that the difference between the original and the modified scheduling formulation be minimum through the introduction of a new set of constraints which are applied starting from the time the disturbance hits the system. The authors also proposed a methodology for addressing several disturbances being the main idea to repeat the above mentioned steps for one of the disturbances in the first step whereas considering the remaining disturbance in the second step. In [13] the authors present a methodology to take into account two types of unforeseen events when approaching the scheduling a process: unit shutdowns and the arrival of new or modified production orders. In a first step a nominal schedule is obtained. When a reactive event takes place, binary variables associated with past production results are fixed and a new reschedule task is carried out. For the two types of unforeseen events, the optimization formulation needs to be properly modified to reflect the type of unexpected event. They applied this strategy to long production horizons by spliting such horizon into a set of short-term production horizons for which efficient scheduling formulations are well known. The formulation can also be extended to handle several unforseen events. In [14] the authors propose a reactive scheduling strategy based on the use of Multiparametric Programming as a way to reduce the computational load associated with on-line scheduling strategies during the presence of unforeseen events. The idea is to use a state-space linear representation of the system to be scheduled and then to deploy multi-parametric programming for finding new scheduling solutions under uncertain conditions which are off-line computed. Finally, the computed off-line solutions can be on-line implemented. The authors apply this methodology to a system of combined heat and power units. Although the advantages of reduced computational load, one of the main issues with this strategy lies in the fact that a linear representation of the scheduling system is required. Whether or not this represents a disadvantage fully depends upon the specific application. Sun and Xue [15] propose what they call a dynamic reactive production scheduling mechanism for modifying the originally created schedules when these schedules cannot be completed due to changes in production orders and manufacturing resources. Changes in orders include cancellation of previously scheduled orders and insertion of urgent orders. The authors developed a RS method to minimize the scheduling changes for improving the efficiency of RS, while maintaining the quality of RS. Van den Heever and Grossmann [16] propose a strategy for the integration of production planning and RS. They propose two integrated multiperiod MINLP models for planning and RS and a strategy for the integrated solution; a Lagrangian decomposition-based heuristic to deal with large size problems at the planning level is also deployed. Uncertainty in the forecasted demand is partly dealt with allowing changes in operation when demands are different from their predicted values. Li and Ierapetritou [17] review the methodologies that have been developed to address the problem of uncertainty in production scheduling environments. Verderame et. al. [18] review the planning and scheduling problem under uncertain scenarios focusing on several production sectors. They suggest that deterministic optimization algorithms can provide a rigorous assertion of solution optimality especially when system variables are continuous in nature and better solutions can be obtained if uncertainties were explicitly considered in the model formulation. The authors list a number of techniques to explicitly take into account parameter uncertainty within a mathematical programming framework. Schultz and Diaz [19] propose optimal scheduling and process optimization formulations considering uncertainty in demands while avoiding overproduction. They use a two stage stochastic model which is transformed into a deterministic mixed integer non linear programming equivalent problem. Li and Ierapetritou [20] claim that the preventive scheduling based on robust counterpart optimization avoids increasing problem size when the number of parameters increases and scenario-based optimization methodologies are used. Price, processing times, and demands are three parameters subjected to uncertainty in their examples. They studied three robust counterpart optimization formulations and compared their performance under uncertain scheduling scenarios. Yisu, et. al. [21] propose an MINLP model for the optimal reactive scheduling of a mixed batch/continuous process. Arguing that the conventional Resource Task Network (RTN) model is generally unsuitable for reactive scheduling as it does not track the history of tasks nor incorporate disturbance terms, they employ the state space form of the RTN model to overcome the limitation and carry out reactive scheduling tasks, working in conjunction with a rolling horizon scheme. They conclude that their formulation is able to address different scenarios as it successfully obtains reasonably good schedules within short computation time limits. You and Grossmann [22] propose an integrated approach in order to consider simultaneously supply chain network design, production planning and scheduling, demand uncertainty and inventory management to resolve the trade-offs between economics and responsiveness in an optimal manner. They propose a multi-period MINLP formulation which predicts the detailed design decisions, production and inventory profiles, and schedules of the process supply chain network (PSCN) with different specifications of the expected lead time. Wang and Rong [23] propose a two-stage robust model that can deal with uncertain parameters with both continuous and discrete probability distributions within a finite number of scenarios. They use their model to address the crude oil Scheduling problem under two uncertain conditions, ship arrival times and crude distillation units (CDU) charging demands. Tang, et. al. [24] develop an MPC based rolling horizon strategy to address the problem of dynamic scheduling. They present a mixed integer nonlinear programming model for the scheduling (rescheduling) problem. Lagrangian relaxation is deployed to solve the model corresponding to each rolling window in their work.

3 Planning, Scheduling and Control under unforeseen events

In a previous work [5] we have presented a MINLP optimization formulation for the integrated planning, scheduling and control of short-period processing units using a non-linear model predictive control (NLMPC) strategy for on-line set-point tracking. Such a strategy permits to take care of certain specific types of uncertainties: model uncertainty and uncertainties related to variations in the feed stream conditions. However, there may be some other types of unforeseen events for which this strategy will not be able to cope with them. Two types of these unexpected events are related to processing equipment breakdown and modification of the amount to be produced for each product [12]. Before the emergence of the unforeseen events, a *nominal* planning, scheduling and control optimization solution would normally be available. However, when the unexpected events affects the system, the nominal optimal solution would be either suboptimal or infeasible making necessary to correct the nominal optimal solution to take care of such unforeseen events. Regarding the best way of correcting the nominal optimal solution no general agreement exists as the past reactive scheduling literature review clearly indicates.

Broadly speaking, a set of heuristics have been used for addressing the effect of unforeseen events on previously computed nominal optimal solutions. In this work we have also used a set of heuristics for assessing the effect of a specific type of unexpected event on the planning, scheduling and control of short-period processing units. The type of disturbance or unexpected event to be considered has to do with the modification of the amount to be produced of a set of given products. We will assume that after a *nominal* planning, scheduling and control problem has been obtained, so a set of target conditions (i.e. production demands) are met, for a given set of production periods then an under/over demand of certain products is enforced. Therefore, there is not any guarantee that under the presence of unforeseen events, the remaining schedule sequence and processing conditions are either optimal or even feasible meaning that the nominal solution could not be able to meet the production demands under the new scenario. To cope with this situation we propose a simple reactive planning, scheduling and control strategy: (a) If the unexpected event hits the process when the production of product i is under way, then wait until the production demand of product i is met, (b) Solve again a planning, scheduling and control problem under the new production demand scenario so all the target demands are met. The optimization problem to be solved in part (b) ought to consider products $i+1...n$ where n is the total number of products. Therefore, products $1, ..., i-1$ are discarded in part (b). It is clear that this reactive heuristic strategy only makes sense assuming that rush orders involve products that have not been manufactured yet when the unexpected event hits the process. If the rush order involves an over demand of a product that has been manufactured, then a different heuristic should be considered (i.e. running again the planning, scheduling and control problem taking into account such a product together with the remaining products that were not manufactured yet). Of course, we do not claim that this is the best way of addressing the effect of unforeseen events on planning, scheduling and control problems since a comparison with other potential reactive strategies was not undertaken. We should stress that, with few exceptions, in most of the published works only the effect of unforeseen events on the scheduling of processing systems has been considered. Up to our best knowledge, no reactive strategies have been analysed for addressing the integrated planning, scheduling and control of processing systems as recent reviews indicate [6], [7] .

4 Problem statement

The problem to be addressed in this work can be stated as follows:

"Taking as starting point the results of the *nominal* simultaneous planning, scheduling, and control problem (PSC/NMPC) of a multi-product plant consisting of the optimal sequence of production (scheduling), during various periods of production (planning), subject to a nonlinear model predicted control scheme (control), a set of unexpected product demand operating scenarios hit the process. A reactive optimization strategy is then applied to overcome the effect of the disturbances introduced into the production planning, scheduling and control of the process. The problem consists in the determination of a new optimal production sequence and processing conditions for each remaining period of production by solving the integrated planning, scheduling, and control problem such that process profit is maximized".

5 Reactive Planning, Scheduling and Control formulation

In this work we will use the same planning, scheduling and control optimization formulation proposed in [5], Equations (1)-(35), to address both the calculation of the *nominal* optimal solution and the new reactive optimal solution under the presence of the unforeseen events detailed in the past item. For doing so, we will use two examples dealing with continuous stirred tanks reactors and a set of hypothetical product demand unexpected scenarios will be assumed. It should be stressed that in the present work, because a decomposition optimization strategy [1], [2], [3] has not been used to cope with long processing periods problems, only systems involving short-period scenarios will be considered. Another potential option to cope with large-scale planning, scheduling and control problems could be to consider reduced or approximated dynamic models [25] to represent the fundamental dynamic behaviour of the assessed system. Of course, the combination of decomposition optimization methods and reduced dynamic models can be also a way to cope with large-scale planning, scheduling and control problems.

6 Examples

In this section two examples with different degree of nonlinearity are presented. The problems involve continuous stirred tank reactors featuring in the first case relatively simple kinetic rate expressions, whereas the second example features complex polymerization kinetic relationships. In both problems we have used 20 finite elements and 2 internal collocation points within each finite element for dealing with the optimization of the underlying dynamic models [11].

Case Study 1. CSTR with a Simple Irreversible Reaction

The following third-order reaction takes place in an isothermal continuous stirred tank reactor:

$$3R \xrightarrow{k} P, \qquad -\Re_R = kC_R^3 \tag{1}$$

The dynamic composition model is given by

$$\frac{dC_R}{dt} = \frac{Q}{V}(C_0 - C_R) + \Re_R \tag{2}$$

where C_R is the reactant concentration, C_0 denotes the feed stream composition, V is the reactor volume, k is the reaction rate, and Q is the feed stream volumetric flow rate which is also used as the manipulated variable. Using the following values of design and kinetic parameters: C_0= 1 mol/L, V=5000 L, k= 2 L^2/mol^2-h, and under the processing conditions shown in Table 1, the reactor can manufacture a series of products denoted by **A, B, C, D** and **E** depending upon the value of Q. The different costs concerning the objective function are shown in Table 2. The planning horizon is composed of two production periods lasting each one of them one week. Hence, the total planning horizon spans two weeks.

Table 1: Operating Conditions for Manufacturing Products for Case Study 1.

Product	Q, L/hr	C_R, mol/L	Product cost, $/mol
A	10	0.0967	200
B	100	0.2	150
C	400	0.3032	130
D	1000	0.393	125
E	2500	0.5	120

Table 2: Operating and Transition Costs (C^{oper}, C^{tran}) for Case Study 1.

Product	C^{oper}, \$/mol		C^{tran}, \$					
	Period 1	Period 2		**A**	**B**	**C**	**D**	**E**
A	0.13	0.13	**A**	0	10	6	12	15
B	0.22	0.22	**B**	15	0	5	8	10
C	0.35	0.35	**C**	20	15	0	10	15
D	0.29	0.29	**D**	9	10	12	0	10
E	0.25	0.25	**E**	15	14	10	15	0
Inventory costs: 0.0000306								

When solving the *nominal* integrated planning, scheduling, and control problem (PSC/NMPC) the optimal production sequence turns out to be the following one: (a) First period: **ABCDE**, (b) Second period: **EBDAC**. Additional results are shown in Table 3. Following, different production demands scenarios will be assumed and the new planning, scheduling and control optimal solution will be obtained for each one of the different scenarios.

Table 3: Nominal Planning, Scheduling, and Control results for Case study 1.

	Period 1				
Slot	Product	Demand (kmol/week)	Processing Time (h)	Total Production (kmol)	Transition Time (h)
1	**A**	200	22.22	200.73	5
2	**B**	3000	37.5	3000.0	4.7
3	**C**	7000	25.12	7000.5	2.8
4	**D**	15000	24.7	15000.0	1.5
5	**E**	35000	38.45	48062.0	-
	Period 2				
1	**E**	31000	37.5	46924.0	5
2	**B**	3600	45.0	3600.0	3
3	**D**	11000	18.1	11000.0	5
4	**A**	200	22.22	200.73	4.7
5	**C**	7000	25.12	7000.5	-
Profit:	\$17,499,815				
CPU Time:	65.5 min				

Scenario 1. A product **D** over demand (20%) at the end of the first period is enforced. The modification of the demand for product **D** occurs while product **B** is being manufactured.

Strategy. A decision is taken to continue producing product **B** until meting the target demand level. In the meantime a rescheduling for the production of the remaining products (**C, D**, and **E**) of the first period and those of the second period (**A, B, C, D**, and **E**) is carried out. A summary of the obtained results is presented in Table 4. The results of applying the proposed reactive strategy show that the optimal production sequence turns out to be the same than the nominal one after the unforeseen event hits the system. However, it should be noted that the new results involve a decrease in the objective function value with respect to the nominal solution. This should be considered a normal situation and a correct response from the solution of the optimization formulation since product **D** is the second product with less value, and its overproduction (3000 kmoles) is done at the cost of reducing the production of product **E** in 6178 kmoles after the reactive strategy is applied.

Scenario 2. It is required to satisfy an over demand of product **A** (50%) at the end of the first period. Products **A, B**, and **C** had already been produced in the first period according to the nominal planning.

Strategy. A reactive planning, scheduling and control strategy for the production of the **A, D**, and **E** products of the first period and those of the second period (**A, B, C, D**, and **E**) is carry out. A summary of the results is shown in Table 4. The results show that the over production demand is fully met. However, in this case the optimal production sequence of the second production period is modified by the reactive strategy. It should be stressed that product **D** is not longer manufactured in the new processing sequence concerning period two. Anyway, the target demands for product **D** are completely satisfied for the two periods since the 26000 kmoles (15000 + 11000) required by the two periods have been manufactured in the first period. Finally, the profit is increased since the production of products **A** and **E** is increased from 200 to 300 kmoles and from 94986 to 115124 kmoles, respectively.

Scenario 3. A product **A** over demand (50%) at the end of the second period is enforced.

Strategy. It has been decided to run the production sequence concerning the first period until completion. In the meantime a rescheduling for the production sequence of the second period is

Table 4: Operating and Transition Costs for the three scenarios of the first case study. Prod. rate stands for production rate [kmol] and Proc. Time stands for processing time [hr]. SEQ denotes a given sequence and CPU is the execution time [min]. The numerical value after the name of each scenario represents the process profit. Finally, P-1, P-2 and P-3 denote the first, second and third periods, respectively.

	Scenario 1 ($17,134,155)				Scenario 2 ($ 19,891,302)				Scenario 3 ($ 15,856,678)			
	Prod. rate		Proc. Time		Prod. rate		Proc. Time		Prod. rate		Proc. Time	
Prod	P-1	P-2	P-1	P-2	P-1	P-2	P-1	P-2	P-1	P-2	P-1	P-2
A		200.7		22.22	**300.4**	200.7	22.22+11.11	22.22		**301.1**		22.22+11.11
B		3600		45	3000	3600		25.18		3600		45
C	7000	7000	25.18	25.18	7000.5	700.5		45		7000		25.18
D	**18000**	11000	29.66	18.13	**26000**	0	42.83	0		11000		18.13
E	**41883.9**	48061.8	33.51	37.54	**39298.3**	75826.4	31.44	60.66		33035.2		26.43
SEQ	**-CDE**	**EBDAC**			**-DEA**	**ABBEC**				**ABCDE**		
CPU	11:05				9:11				4:06			

carry out. A summary of the results is shown in Table 4. The results indicate that the new demand for product **A** is met. However, the total production concerning product **E** has decreased. This explains why a decrease in the process profit is observed. We also observe that the optimal production sequence is modified with respect to the original one.

Case Study 2. polymerization of Methyl-Methacrylate (MMA)

The second case study used to demonstrate the advantages of the reactive planning, scheduling and control strategy deals with a continuous isothermal free-radical dynamic model of bulk-mass polymerization of Methyl-Methacrylate (MMA) [26]. The dynamic mathematical model reads as follows:

$$\begin{aligned}
\frac{dC_m}{dt} &= -(k_p + k_{tm})C_m P_0 + \frac{F(C_{m_{in}} - C_m)}{V} && (3)\\
\frac{dC_I}{dt} &= -k_I C_I + \frac{F_I(C_{I_{in}} - FC_I)}{V} && (4)\\
\frac{D_0}{dt} &= (0.5k_{tc} + k_{td})P_0^2 + k_{fm}C_m P_0 - \frac{FD_0}{V} && (5)\\
\frac{D_1}{dt} &= M_m(k_p + k_{fm})C_m P_0 - \frac{FD_1}{V} && (6)\\
y &= \frac{D_1}{D_0} && (7)
\end{aligned}$$

where

$$P_0 = \sqrt{\frac{2f^* k_I C_I}{k_{td} + k_{tc}}} \qquad (8)$$

In the above model C_m is the monomer concentration, C_I is the initiator concentration, D_0 and D_1 are the zero and first moment of the molecular weight distribution, respectively, F is the monomer volumetric flow rate, F_I is the volumetric flow rate of the initiator, V is the reactor volume, f^* is the efficiency of the initiator. Similarly, k_i, $i = p, I, tc, td, tf, fm$ are constant rates for the different polymerization reaction steps, M_m is the molecular weight of monomer, and P_0 is defined as total concentration (or moment zero) of live polymer. The subscript *in* denotes information regarding feed stream conditions. All the kinetic and design information is provided in Table 5, whereas Table 6 shows information regarding the value of the states and the manipulated variable (the initiator flow rate F_I) for 3 different grades defined in terms of the number average molecular weight (y).

$k_{\tau c}$	1.3281x10^{10}	m^3/kmol-h
$k_{\tau d}$	1.0930x10^{11}	m^3/kmol-h
k_I	1.0225x10^{-1}	1/h
k_p	1.4952x10^6	m^3/kmol-h
k_{fm}	2.4522x10^3	m^3/kmol-h
f^*	0.58	
F	30	m^3/h
V	5	m^3
$C_{I,in}$	8.0	kmol/m^3
$C_{m,in}$	6.0	kmol/m^3
M_m	100.12	kg/kmol

Table 5: Kinetic Parameters for MMA production

$y = D_1/D_0$	15000 (**A**)	25000 (**B**)	45000 (**C**)	[=]
$x_1 = C_m$	4.816	5.252	5.645	kmol/m^3
$x_2 = C_I$	0.361	0.121	0.024	kmol/m^3
$x_3 = D_0$	0.008	0.003	0.00079	kmol/m^3
$x_4 = D_1$	118.547	74.871	35.56	kg/m^3
$u = F_I$	1.375	0.461	0.90	m^3/h
X_M	0.1973	0.125	0.0591	

Table 6: Parameter values leading to the Manufacture of the **A,** **B**, and **C** Grades of MMA

Such values of y are typical for this kind of bulk-mass polymerization system where high values of y cannot be achieved since the gel-effect was not taken into account. Moreover, the transition costs are assumed to be the same for all the transitions and set to \$ 3; similarly the inventory costs are set to \$ 0.0013 and the cost of the products are \$ 0.13, \$ 0.22 and \$ 0.35 for products A, B and C, respectively. For the present case study we will assume two scenarios and within them three production periods lasting each one of them one week. Hence, the short-term planning period is extended to three weeks. The nominal optimal solution of the integrated planning, scheduling, and control problem (PSC/NMPC) establishes the optimal production sequences as: **BCA**, **ACB**, and **BCA** for the first, second and third production periods, respectively. In table 7 the nominal optimal results are shown.

Scenario 1. A product **A** over demand (20%) at the end of the first and second periods is enforced.

Table 7: Nominal Results for case study 2.

		Period 1		
Slot	Grade	Demand (Kmol)	Total Production (Kmol)	Process Time (h)
1	**B**	5.0	4.993	55.6
2	**C**	1.0	1.322	55.8
3	**A**	12.0	12.004	50.6
		Period 2		
Slot	Grade	Demand (Kmol)	Total Production (Kmol)	Process Time (h)
1	**A**	13.0	13.005	54.8
2	**C**	1.0	1.222	51.6
3	**B**	5.0	4.993	55.6
		Period 3		
Slot	Grade	Demand (Kmol)	Total Production (Kmol)	Process Time (h)
1	**B**	5.0	4.993	55.6
2	**C**	1.0	0.417	17.6
3	**A**	14.0	21.064	88.9

The modification of the demand for product **A** takes place while product **B** in the first period is being manufactured.

Strategy. In this case we have decided to continue producing **B**, until the desired target level is reached. In the meantime a new reactive planning, scheduling and control strategy for the production of the remaining products (**C** and **A**) of the first period and those of the second and third periods (**A, B**, and **C**) is run to adapt to the presence of the unforeseen demand. A summary of the results obtained using the PSC reactive strategy is presented in Table 8. From Table 8 we can see that the new demands are met with a small increase in the process profit, and that the rescheduling strategy has altered the nominal order of the production sequence. Interestingly, there is also an overproduction of product **A** at the end of the third production period.

Scenario 2. A product **A** over demand (20%) at the end of the second period and an over demand of product **B** (20%) at the end of the third period are simultaneously enforced. Such demand modi-

Table 8: Operating and Transition Costs for the two scenarios of the second case study. Prod. rate stands for production rate [kmol] and Proc. Time stands for processing time [hr]. SEQ denotes a given sequence and CPU is the execution time [min]. The numerical value after the name of each scenario represents the process profit. Finally, P-1, P-2 and P-3 denote the first, second and third periods, respectively.

	Scenario 1 ($1,122,761)						Scenario 2 ($ 1,105,783)					
	Prod. rate			Proc. Time			Prod. rate			Proc. Time		
Prod	P-1	P-2	P-3	P-1	P-2	P-3	P-1	P-2	P-3	P-1	P-2	P-3
A	**14.405**	**15.61**	16.1	60.759	65.823	65.751	12.004	**15.61**	15.85		65.823	66.767
B		4.993	4.993	55.552	55.556	55.556	4.993	4.993	**5.993**		55.556	66.667
C	1.083	0.963	0.917	45.685	40.622	38.693	1.322	0.963	0.677		40.622	28.567
SEQ	**-CA**	**ABC**	**CBA**					**BAC**	**CAB**			
CPU	14:46						6:00					

fications take place while product A at the first period is being produced.

Strategy. It has been decided to continue the whole production of the first period until completion. In the meantime a new optimal planning, scheduling and control solution for the production of the second and third periods is carry out. A summary of the results is presented in Table 8. Again, from the results in Table 8 we can see immediately that new demands are met featuring a decrease in the process profit. We also note that the optimal production sequence after the rescheduling process takes place is different with respect to the nominal one. We should note that in this case the model has lead to a cyclic variation of the optimal production sequence.

7 Conclusions

In this work a reactive heuristic strategy was proposed and tested to cope with the simultaneous optimization of short-term PSC problems under the presence of unexpected or unforeseen events. When these events hit a system the *nominal* optimal solution of the original PSC problem can give rise to a suboptimal or even infeasible solution under the new operation scenario. Therefore, the nominal optimal solution ought to be someway updated to take into account the presence of such events. In this work we have considered that the main unforeseen event deals with unexpected modifications in the production demands of some plant products while the nominal optimal PSC solution was running. The results indicate that the proposed reactive heuristic strategy takes care of the new processing scenarios leading to an updated optimal PSC solution which meets the new production demands. However, one of the main disadvantages of the present reactive heuristic strategy for handling the integrated solution of PSC problems under unforeseen events has to do with the computational burden when using detailed first principles dynamic models. This issue is particularly relevant for on-line applications of the simultaneous solution of PSC problems. There are at least to ways of handling this kind of problems. The first one refers to the use of reduced order or simplified dynamic models [25]. The second one involves the deployment of decomposition techniques for addressing the optimal solution of large scale MIDO problems [1], [2], [3]. Both strategies for the reactive optimization of PSC problems will be explored in future work. Finally, if a priori knowledge of some kind of process uncertainties is available then stochastic optimization techniques [10] can be used for addressing the solution of uncertain PSC problems.

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