Simultaneous Cyclic Scheduling and Control of Tubular Reactors: Parallel Production Lines

Antonio Flores-Tlacuahuac*

Departamento de Ingeniería y Ciencias Químicas, Universidad Iberoamericana
Prolongación Paseo de la Reforma 880, México D.F., 01210, México

Ignacio E. Grossmann

Department of Chemical Engineering, Carnegie-Mellon University
5000 Forbes Av., Pittsburgh 15213, PA

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*Author to whom correspondence should be addressed. E-mail: antonio.flores@uia.mx, phone/fax: +52(55)59504074, <http://200.13.98.241/~antonio>

Abstract

In this work we propose a simultaneous scheduling and control optimization formulation to address both optimal steady-state production and dynamic product transitions in multiproduct tubular reactors working in several parallel production lines. Because the problem involves integer and continuous variables and the dynamic behavior of the underlying system the resulting optimization problem is cast as a Mixed-Integer Dynamic Optimization (MIDO) problem. Moreover, because spatial and temporal variations are considered when modeling the addressed systems, the dynamic systems give rise to a system of one-dimensional partial differential equations. For solving the MIDO problems we transform them into a mixed-integer nonlinear programs (MINLP). We use the method of lines for spatial discretization, whereas orthogonal collocation on finite elements was used for temporal discretization. The proposed simultaneous scheduling and control formulation is tested using three multiproduct continuous tubular reactors featuring complex nonlinear behavior.

1 Introduction

We present an extension of previous work reported on the simultaneous scheduling and control (SC) of tubular reactors in a single production line [1] to the case of parallel production lines. We refer to the reader to previous publications of our research group [2] and others [3, 4] for a detailed description of SC problems as well as for a recent literature review on this research topic.

Scheduling and control problems are examples of highly integrated production systems where improved optimal solutions can be found by simultaneously solving SC problems in comparison to the case when both problems are solved sequentially. However, the simultaneous solution of SC problems demands significant computational effort. As the complexity of the addressed production system grows, so does the solution of the underlying optimization problem. In previous works [2, 5] we have addressed the efficient solution of SC problems by casting as Mixed-Integer Dynamic Optimization (MIDO) problem that upon proper transformation can be transformed into Mixed-Integer Non-Linear Programs (MINLP).

In this work we use a previous SC formulation [1] aimed at tubular reactors in a single production line and extend it to deal with tubular reactors in several parallel production lines. We have taken a SC optimization formulation for several production lines in lumped systems [6] and extended it to distributed parameters systems. We would like to highlight that the aforementioned extension is not trivial since it involves a larger number of integer and continuous decision variables. Moreover, the nonlinear behavior embedded in the mathematical models of the addressed systems are explicitly taken into account giving rise to more complex and demanding MINLP problems whose solution demands the use of a decomposition scheme for initialization as proposed in this work. The SC optimization formulation for tubular reactors in parallel lines is illustrated through the solution of three tubular reactors examples of increasing complexity.

2 Problem definition

Given are a number of products that are to be manufactured in a series of PFRs in a parallel production lines arrangement. Steady-state operating conditions for manufacturing each product are also computed,

as well as the demand rate and price of each product and the inventory and raw materials costs. The problem consists of the simultaneous determination of the optimal production wheel (i.e. cyclic time and the sequence in which the products will be manufactured) as well as the transition times, production rates, length of processing times, amounts manufactured of each product, leading to the maximization of the economic profit and subject to meet a series of constraints representing scheduling and dynamic transition decisions.

Similarly to work reported previously [2], in the following simultaneous scheduling and control (SSC) formulation for parallel production plants, we assume that (1) each production line is composed of a single plug flow tubular reactor (PFR), where desired products are manufactured, and (2) the products follow a production wheel, meaning that all the required products are manufactured in an optimal cyclic sequence (see Sahinidis and Grossmann [7] for a discussion on parallel line scheduling formulation). As shown in Figure 1a, each production line is divided into a set of slots. We stress that the number of slots is unknown since we do not know ahead of time how many products will be assigned in each production line. We recall that two operations happen inside each slot: a transition period between the products that are to be manufactured and a continuous production period. Figure 1b displays these two dynamic generic responses conceptually. When the optimizer decides to switch to a new product, the optimization formulation will try to develop the best dynamic transition policy featuring the minimum transition. After the system reaches the processing conditions leading to the desired product, the system remains there until the production specifications are met. In this work, we assume that, after a production wheel is completed, new identical cycles are executed indefinitely. The detailed formulation of the MIDO involved is given in the appendix.

3 MIDO solution strategy

The efficient solution of MIDO problem is a complex task. Presently, we can solve MIDO problems mainly for small or medium size problems. However, as the number of binary variables tends to grow so does the computational time. Moreover, the problem becomes more difficult to converge due to the

Figure 1: (a) The process consists of l parallel production lines. At each line l the cyclic time is divided into N_s slots. (b) When a change in the set-point of the system occurs there is a transition period followed by a continuous production period.

presence of nonlinear behavior such as multiple steady states, parametric sensitivity, oscillatory behavior, etc. The optimization of distributed parameter systems (DPS) will only add complexity to the already complex solution of MIDO problems because of the infinite dimensional nature of such systems. Presently the MIDO solution of complex and large scale problems seems to be feasible only if special optimization decomposition procedures are used [8], [9], [10], [11], [12]. In fact, the solution of MIDO problems normally demands efficient initialization and solution procedures. Without them sometimes it is almost impossible to compute an optimal solution.

In this work we take advantage of the structure embedded in scheduling and control problems such that a

solution strategy can be developed and that will allow us to compute optimal solutions of the addressed MIDO problems. This means that the MIDO problem was decomposed into simpler parts. The solution of the simpler parts was used to provide initial guesses to more complex versions of the MIDO problem until the original problem to be solved was obtained. The decomposition and MIDO solution strategy involves the following steps:

1. Solve the parallel lines scheduling problem to obtain an initial scheduling solution using guesses of the transition times and production rates.
2. Compute steady-state processing conditions of the desired products.
3. Solve the dynamic optimization problem to obtain initial optimal transition times and production rates.
4. Solve the entire MIDO problem for the simultaneous scheduling and control problem.

We have used the aforementioned solution strategy for computing MIDO optimal solutions with a reasonable computational effort for all the problems addressed in the present work. We found that if a direct solution approach is used (meaning the solution of the entire MIDO problem approached in a single step) in most of the case studies it was impossible to compute an optimal solution. Even when a solution could be found, an increase around 2-3 orders of magnitude in computation time was required. This is so because very good initial values of the decision variables are normally required for the efficient solution of dynamic optimization problems using the simultaneous approach as described in [13]. In all cases the optimal solutions using either approach were the same with the computational load being the main difference between both solution methods. For any solution method (decomposition or direct) only local solutions were sought. The computation of global optimal solutions for the addressed MINLP problems requires large computational times and was not addressed in the present work. Accordingly, all the simultaneous scheduling and control problems were solved using the above solution strategy. For the numerical solution of the MINLP problem arising from the discretization of the original MIDO problem, the **SBB** MINLP solver in **gams** [14] was used.

Discretization of distributed parameter systems using finite difference techniques demands some care regarding the selection of both the number of discretization points and the kind of discretization equations. For instance, it is well known that distributed parameter systems featuring convection and diffusion terms require different discretization strategies for each one these terms [15]. Regarding the number of points for discretization purposes we normally set this number after comparing results using different number of discrete points. As a rule of thumb we keep reducing the number of points until from one iteration to another the results are practically the same. Of course, at first sight, we can be tempted to use a large number of discrete points aiming to get a small approximation errors. However, by increasing the number of discrete points we also include the stiffness of the system. Therefore, a trade-off between approximation error and stiffness ought to be observed. Hence, we came to the conclusion after some trials that 11 equal sized points were enough for spatial discretization, whereas 20 finite elements and 3 internal collocation points sufficed for time discretization. Moreover, all the problems were solved using 2 Ghz, 4 Gb computer.

4 Case studies

In this section several simultaneous scheduling and control problems taking place in tubular reactors are addressed using the optimization formulation shown in the appendix. The examples were selected to feature different degrees of steady-state and dynamic nonlinear behavior, such that the complexity of solving scheduling and control problems is highlighted. We also did so hoping to justify the use of advanced decomposition optimization techniques such as Lagrangian decomposition [8] to address the scheduling and control of more complex reaction system such as polymerization reaction systems. We stress that for all the case studies all the parallel lines are equipped with identical PFRs. Moreover, when discussing results we define a *productivity* term for each product in a given production line as the ratio of the amount manufactured of such product in the production line divided by the corresponding cyclic time of the production line.

Isothermal tubular reactor

To test the proposed SSC optimization formulation we have selected as the first case study a problem that is relatively easy to optimize but that will allow us to tackle more complex systems. The system in question consists of an isothermal plug flow reactor with both convective and diffusive mass transfer and where the $2X \rightarrow Y$ second order reaction takes place. The distributed model is given as follows:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} - KC^2 \quad (1)$$

subject to the following initial,

$$C(x, 0) = C_f \quad (2)$$

and boundary conditions,

$$@ x = 0 \quad C = C_f + \frac{D}{v} \frac{\partial C}{\partial x} \quad (3)$$

$$@ x = L \quad \frac{\partial C}{\partial x} = 0 \quad (4)$$

where C stands for the concentration of the X component, x is the longitudinal coordinate, t is the time, D is the mass diffusivity and v is the linear velocity, K is the reaction constant, C_f is the feed stream composition of reactant X and L is the reactor length. To improve the chances of finding an optimal solution the model is scaled as follows:

$$C' = \frac{C}{C_f}, \quad x' = \frac{x}{L}, \quad \theta = \frac{tv}{L}$$

Hence, in terms of the dimensionless variables, the scaled model reads as follows,

$$\frac{\partial C'}{\partial \theta} = \frac{1}{Pe_M} \frac{\partial^2 C'}{\partial x'^2} - \frac{\partial C'}{\partial x'} - \frac{\alpha}{Pe_M} C'^2 \quad (5)$$

Product	C [kmol/m ³]	Q_f [m ³ /h]	Demand rate [Kg/h]	Product cost [\$/kg]	Inventory cost [\$/kg]
A	50	1.169	280	620	1.5
B	40	0.62	360	730	1
C	30	0.302	480	750	2
D	20	0.1	320	770	3
E	10	0.02	400	790	2.5

Table 1: Process data for the isothermal tubular reactor case study. A, B, C, D and E stand for the five products to be manufactured.

subject to the following initial,

$$C'(x', 0) = 1 \quad (6)$$

and dimensionless boundary conditions,

$$@ x = 0 \quad \frac{\partial C'}{\partial x'} = Pe_M(C' - 1) \quad (7)$$

$$@ x = 1 \quad \frac{\partial C'}{\partial x'} = 0 \quad (8)$$

where $Pe_M = \frac{Lv}{D}$ is the mass transfer Peclet number and $\alpha = \frac{L^2 K C_f}{D}$. Using $L = 20$ m, $D = 10$ m²/s, $C_f = 100$ kmol/m³, $r = 0.5$ m and $K = 1 \times 10^{-3}$ m³/kmol-h, lead to the production of five products A, B, C, D and E which are defined in Table 1. In addition, Table 1 contains information regarding the cost of the products, demand rate, inventory cost, and production rate of each one of the hypothetical products. In this case the control variables used for the the computation of the optimal product transitions is the feed stream volumetric flow rate (Q_f). Because the parallel lines optimization scheduling formulation was taken from Sahinidis and Grossmann [7] all the production, transition and inventory costs were computed as described in section 5.3 of that paper; we also used an objective function similar to the one deployed there.

In Table 1 the design information is shown. In this problem we have specified 5 slots and 2 production lines. Table 2 contains the optimal scheduling and control results. In this case, the first production line turns out to be completely dedicated to the production of product E , whereas in the second production line the optimal sequence is given by the $E \rightarrow C \rightarrow A \rightarrow B \rightarrow D$ production wheel. Because there are not product transitions in the first production line only dynamic product transitions for the second line

Line 1					Line 2				
Slot	Prod	Amount Prod.[kg]	Productivity [kg/h]	Process Time [h]	Slot	Prod	Amount Prod. [kg]	Productivity [kg/h]	Process Time [h]
1-5	E	2040	156.9	13	1	E	177286	494.64	265.72
					2	C	172041	480	26.5
					3	A	100357	280	9.5
					4	B	129031	360	14.08
					5	D	114694	320	42.63

Table 2: Simultaneous scheduling and control results for the isothermal tubular reactor case study. The total cyclic time in the first line is 13 h, whereas the cyclic time in the second line is 358.42 h. The objective function value is 1723253.

are displayed as shown in Figure 2. Problem statistics are as follows. The number of constraints is 29553, the number of continuous decision variables is 30443, the number of integer variables is 50, the number of branch and bounds nodes is 85, the solution gap is 0.099134 and the CPU time is 2.23 h.

It should be stressed that the transition order is partially a function (as seen from the objective function defined in Equation 18) of several factors such as transition cost, inventory cost and production cost. On the other hand, the transition order is also function of the deviation (from their steady-state desired values) of the controlled and manipulated variables. Hence, it should not be expected that the optimal transition order between products to be given by just the progressive conversion increase between them. Moreover, we would like to remark that the simultaneous scheduling and control problem is actually a multi-objective optimization problem. In fact, as noticed from Equation 18, in the present optimization formulation we merge cost terms with other terms related to process operation (such as deviation of the control variables). This way of addressing the solution of scheduling and control problems can give rise to optimal solutions that are actually not Pareto-optimal. Improved optimal solutions can be obtained by solving the scheduling and control problem by true multi-objective problems.

Regarding the results of the two production lines we would like to remark that both lines are independent and that only the production from them needs to be merged such that product demand is met. The first line features 13 h whereas the second line features 358.42 h as cyclic times. This means that the first line repeats over and over after 13 h without caring about the status of the second production line. At first sight it may seem obvious just to use the second production line since productivity looks rather small for

Figure 2: Isothermal tubular reactor case study. In the second production line the optimal schedule is given by the $E \rightarrow C \rightarrow A \rightarrow B \rightarrow D$ sequence, the total cyclic time is 358.42 h.

the first production line. However, this is not the case. In fact, when the second production line completes a production cycle the first production line manufactures 56178 kg of product B which is around the third part of product E manufactured by the second production line.

Although this problem is simple (in terms of number of equations and embedded nonlinear behaviour) the optimal scheduling and control solution is not obvious and is rather a complex task to compute it. In fact, the optimal solution was found in around 2 h of CPU time. Therefore, we cannot state a priori an expected optimal solution that involves transition sequence and optimal production rates among other

decision variables. Because of the size and complexity in dealing with the optimal solution of MINLPs only local optimal solutions were sought.

Non-isothermal adiabatic tubular reactor

The second example refers to an irreversible first order reaction $X \rightarrow Y$ that takes place in an non-isothermal plug flow reactor whose one-dimensional dynamic model reads as follows [16]:

$$\frac{\partial C}{\partial t} = -\frac{\partial C}{\partial z} + \mathcal{R}(C, T) \quad (9)$$

$$\frac{\partial T}{\partial t} = -\frac{\partial T}{\partial z} - \mathcal{R}(C, T) - U(T_w - T) \quad (10)$$

$$\mathcal{R}(C, T) = -10^{11} C e^{-75/T} \quad (11)$$

subject to the following initial,

$$C(z, 0) = C_f \quad (12)$$

$$T(z, 0) = T_f \quad (13)$$

and boundary conditions,

$$@z = 0 \quad C = C_f + \frac{\partial C}{\partial z} \quad (14)$$

$$@z = 0 \quad T = T_f + \frac{\partial T}{\partial z} \quad (15)$$

where C stands for the dimensionless concentration of component X , T is the dimensionless temperature, z is the dimensionless axial coordinate, U is the dimensionless heat transfer coefficient and T_w is the dimensionless reactor wall temperature. Moreover, $C_f = 0.85$ is the dimensionless feed stream concentration of reactant X and $T_f = 2.713$ is the dimensionless feed stream temperature. For modeling this system we have assumed that mass and heat transport occur only along the axial reactor direction and that the diffusive effects can be neglected.

Figure 3: Steady-state diagrams of the second example using the dimensionless feed stream temperature (T_f) as the continuation parameter. The required products A, B, C are manufactured around a highly parametric sensitive region. All the operating points correspond to open-loop stable steady-states.

Product	C	T	T_f	Demand rate [Kg/h]	Product cost [\$/kg]	Inventory cost
A	0.425	3.175	2.75	100	6	1.5
B	0.255	3.351	2.756	90	7	1
C	0.085	3.525	2.76	120	8	2

Table 3: Process data for the non-isothermal adiabatic tubular reactor case study. A , B and C stand for the three products to be manufactured.

Line 1					Line 2				
Slot	Prod	Amount Prod.[kg]	Productivity [kg/h]	Process Time [h]	Slot	Prod	Amount Prod. [kg]	Productivity [kg/h]	Process Time [h]
1-3	C	600000	100	6000	1	A	495	100	2.382
					2	B	445.5	90	1.568
					3	C	99	20	1

Table 4: Simultaneous scheduling and control results for the non-isothermal adiabatic tubular reactor case study. The total cyclic time in the first line is 6000 h, whereas the cyclic time in the second line is 4.95 h. The objective function value is 363.14

Using as continuation parameter the dimensionless feed stream temperature (T_f) in Figure 3, the steady-state diagrams are depicted. From this Figure we can see that the three required products are manufactured around a highly sensitive parametric region. As a matter of fact very small variations in the continuation parameter give rise to large variations in the system states represented by the concentration (C) and reactor temperature (T). In other words, the reaction system operates in a highly nonlinear region and this normally translates into difficulties in computing a MIDO solution to the simultaneous scheduling and control problem although no multiple steady-states were detected. As can be seen from Figure 3 the operating region embeds only open-loop stable steady-states. This fact has more relevance for closed-loop control purposes because our MIDO strategy works equally well no matter what the stability of the system is.

Table 3 shows the design parameters. In this problem we have specified 3 slots and 2 production lines. Table 4 contains the optimal scheduling and control results. In this case the first production line is completely dedicated to manufacture product C , whereas in the second production line the optimal sequence is given by the $A \rightarrow B \rightarrow C$ production wheel. As shown in Table 4 the optimal solution consists of splitting the production requirements in the two available production lines. Most of the processing time in both

production lines is dedicated to manufacture product C . Because the cost of the inventories is relatively low, the optimal solution consists in manufacturing as much as possible of each one of the products. In fact, the demand rate for each product is completely fulfilled and no product is overproduced. The objective function value is \$ 363.14. Regarding the optimal dynamic transition responses, because only one product (C) is manufactured in the first line actually no product transitions take place in this line and so no dynamic transitions are shown. However, optimal dynamic transitions occur for the second line and they are shown in Figure 4. It is worth to mention that when changing the value of the controlled variable in a step-like form between any couple of the products, the open-loop transition times turn out to be extremely small. This is so because, as seen in Figure 3, the distributed parameter system operates around a highly sensitivity region: very small changes in the value of T_f cause a transition from an initial to a final product. In practical terms, we can consider that the tubular reactor operates in a quasi steady-state pattern. This explains the shape of the optimal dynamic response displayed in Figure 4. Hence, we expected, as it was the case, short optimal transition times between the steady-state processing conditions. Therefore, when preparing Figure 4 the abscissa coordinate (i.e. processing time) was divided by the maximum observed transition time among all optimal transition curves. A similar procedure was deployed to scale the processing time of the third case study. From Figures 3(a) and 3(b) it is clear that the same kind of process sensitivity is exhibited either in terms of concentration or temperature. For this reason we decided not to include the reactor temperature response curves. As a matter of fact, the reactor temperature curves are very similar (in shape) to the reactor concentration response curves (see top part of Figure 4): the optimal response curve features fast transitions from one steady-state to another. Problem statistics are as follows. The number of constraints is 50928, the number of continuous decision variables is 51468, the number of integer variables is 18 and the CPU time is 2.50 min using GAMS/SBB.

Figure 4: Non-isothermal adiabatic tubular reactor case study. The second line optimal production sequence is $A \rightarrow B \rightarrow C$. The cyclic time is 4.95 h.

Non-isothermal adiabatic tubular reactor with recycle and mixing tank

The third example is a variation of the second case study where no recycle was allowed [16]. As depicted in Figure 5, the modification consists in introducing a recycle stream and in mixing the main feed stream with the recycle stream, the resulting stream is fed to the tubular reactor.

The dynamic mathematical model describing this case study is the same represented by Equations 9-15. However, the concentration (C_o) and temperature (T_o) of the main feed stream are described by the

Figure 5: Nonisothermal, adiabatic plug flow tubular reactor with recycle stream and mixing tank.

following set of algebraic equations:

$$C_o = (1 - R)C_f + RC_e \quad (16)$$

$$T_o = (1 - R)T_f + RT_e \quad (17)$$

where $R = 0.5$ is the recycle fraction, C_e, T_e are the outlet dimensionless concentration and temperature, respectively. Moreover, in this case study the values of the dimensionless feed stream concentration C_f and temperature T_f are 1 and 2.3, respectively.

Figure 6 depicts the steady-state multiplicity diagram of the addressed system using the dimensionless feed stream temperature (T_f) as continuation parameter. As noted, the three required products A, B, C are manufactured around an open-loop steady-state unstable operating region where up to three steady-states were found. The presence of multiple steady-state solutions might represent a computational difficulty for computing a MIDO solution to the present case study. However, we do not expect additional computational problems because of the unstable nature of the steady-states. This desired feature of our MIDO approach has to do with using the simultaneous approach for solving dynamic optimization problems [13].

Figure 6: Steady-state multiplicity diagrams of the third example using the dimensionless feed stream temperature (T_f) as the continuation parameter. The continuous line denotes open-loop stable steady-states, whereas the dashed line stands for open-loop unstable steady-states. The required products A, B, C are manufactured around an unstable steady-state multiplicity region.

Product	C	T	T_f	Demand rate [Kg/h]	Product cost [\$/kg]	Inventory cost [\$/kg]
A	0.5	3	2.501	280	3	1.5
B	0.3	3.131	2.431	360	5	1
C	0.1	3.267	2.367	480	8	2

Table 5: Process data for the non-isothermal, adiabatic tubular reactor with recycle and mixing tank case study. A , B and C stand for the three products to be manufactured.

Line 1					Line 2				
Slot	Prod	Amount Prod.[kg]	Productivity [kg/h]	Process Time [h]	Slot	Prod	Amount Prod. [kg]	Productivity [kg/h]	Process Time [h]
1	B	557.015	180.91	1	1	C	600.101	118.83	1
2	A	641.435	208.33	1.079	2	A	361.975	71.678	1
3	B	551.445	179.1	1	3	C	1823.899	361.17	3.05

Table 6: Simultaneous scheduling and control results for the non-isothermal adiabatic tubular reactor case study. The total cyclic time in the first line is 3.079 h, whereas the cyclic time in the second line is 5.05 h. The objective function value is 6503.

Table 5 shows the design information for this example. In this case study we have specified two production lines and 3 slots within each line. Table 6 contains part of the results of the SSC problem. As seen, in the first production line the optimal production schedule is given by the sequence $B \rightarrow A \rightarrow B$, whereas in the second production line the $C \rightarrow A \rightarrow C$ schedule turns out to be the optimal sequence. From the results shown in Table 6 we note that the total processing times for any product are similar and that product A is the only common product between both lines. It should also be stressed that the requested demands are met without overproducing any product. Regarding the dynamic transition behavior between each one of the products depicted in Figures 7 and 8, we again observe fast transition times. The reason of the fast transition times is related to the nonlinear operating region around which the three products from this reactors are manufactured (see Figure 6). From this Figure we clearly note that very small variations in the value of the manipulated variable are responsible for relatively large variations in the controlled variables. Moreover, the closed-loop transitions turn out to be fast. Because the system operated around open-loop unstable regions no estimate of this type of transition times is possible. Problem statistics are as follows. The number of constraints is 50952, the number of continuous decision variables is 51480, the number of integer variables is 18 and the CPU time is 4.20 min using GAMS/SBB.

Figure 7: Non-isothermal adiabatic tubular reactor with recycle and mixing tank case study. The first line optimal production sequence is $B \rightarrow A \rightarrow B$. The cyclic time is 3.079 h.

Figure 8: Non-isothermal adiabatic tubular reactor with recycle and mixing tank case study. The second line optimal production sequence is $C \rightarrow A \rightarrow C$. The cyclic time is 5.05 h.

5 Conclusions

In this paper we have extended previous work [2] to include the simultaneous scheduling and optimal control optimization during product transitions featuring distributed parameter systems. Although the optimization formulation shown in [2] is similar to the one used in the present work, there are some important differences that deserve comment. First the SSC formulation presented in [2] is restricted to the optimization of single production lines and in this work several parallel production lines are considered.

Second, such an optimization formulation assumes that the system dynamics is represented in terms of lumped parameters systems. We have taken the scheduling optimization formulation from Sahinidis and Grossmann [7]. However, we found that it is a no trivial task to merge it with an optimal control formulation to get the SSC formulation. Regarding the system dynamics, in the present work we have addressed the optimal control of distributed parameters systems. Intuitively, one would expect that the optimization of distributed parameters systems to be harder than the corresponding optimization of lumped parameters systems. This is so because discretized distributed parameters system give rise to a set of lumped systems. As the dimensionality of the distributed system increases so does the complexity of solving these kind of optimization problems. The dynamic and static optimization of distributed systems is presently a challenging research area. Moreover, as far as we know the SSC optimization of distributed parameters systems has not been reported in the open literature. In summary, the proposed SSC optimization formulation for distributed systems operating in parallel lines has allowed us to tackle some practical problems and compute local optimal solutions in reasonable computational time.

Appendix

Simultaneous Scheduling and Control Parallel Lines Optimization Formulation

This section contains the formulation for the simultaneous scheduling and control parallel lines optimization previously published in reference [2]. It has been included in the present work only for completeness. A complete description of the meaning of the objective function and constraints can be found elsewhere [2], whereas model discretization can be found in [1]. All the indices, decision variables, and system parameters used in the SSC MIDO problem formulation are as follows.

1. Indices

Products	$i, p = 1, \dots N_p$
Slots	$k = 1, \dots N_s$
Lines	$l = 1, \dots N_l$
Finite elements	$f = 1, \dots N_{fe}$
Collocation points	$c, l = 1, \dots N_{cp}$
System states	$n = 1, \dots N_x$
Manipulated variables	$m = 1, \dots N_u$

2. Decision variables

y_{ik}	Binary variable to denote if product i is assigned to slot k
y'_{ik}	Binary auxiliary variable
z_{ipk}	Binary variable to denote if product i is followed by product p in slot k
p_k	Processing time at slot k
t_k^e	Final time at slot k
t_k^s	Start time at slot k
t_{fck}	Time value inside each finite element k and for each internal collocation point c
G_i	Production rate
T_c	Total production wheel time [h]
x_{fck}^n	N-th system state in finite element f and collocation point c of slot k
u_{fck}^m	M-th manipulated variable in finite element f and collocation point c of slot k
W_i	Amount produced of each product [kg]
θ_{ik}	Processing time of product i in slot k
θ_k^t	Transition time at slot k
Θ_i	Total processing time of product i
$x_{o,fk}^n$	n -th state value at the beginning of the finite element f of slot k
$\bar{x}_k^n$	Desired value of the n -th state at the end of slot k
$\bar{u}_k^m$	Desired value of the m -th manipulated variable at the end of slot k
$x_{in,k}^n$	n -th state value at the beginning of slot k
$u_{in,k}^m$	m -th manipulated variable value at the beginning of slot k
X_i	Conversion

3. Parameters

N_p	Number of products
N_s	Number of slots
N_l	Number of lines
N_{fe}	Number of finite elements
N_{cp}	Number of collocation points
N_x	Number of system states
N_u	Number of manipulated variables
D_i	Demand rate [kg/h]
C_i^p	Price of products [\$/kg]
C_i^s	Cost of inventory [€]
C^r	Cost of raw material [€]
h_{fk}	Length of finite element f in slot k
$\Omega_{N_{cp}, N_{cp}}$	Matrix of Radau quadrature weights
θ^{max}	Upper bound on processing time
t_{ip}^t	Estimated value of the transition time between product i and p
$x_{ss,i}^n$	n -th state steady value of product i
$u_{ss,i}^m$	m -th manipulated variable value of product i
F^o	Feed stream volumetric flow rate
X_i	Conversion degree
x_{min}^n, x_{max}^n	Minimum and maximum value of the state x^n
u_{min}^m, u_{max}^m	Minimum and maximum value of the manipulated variable u^m
$\gamma_{N_{cp}}$	Roots of the Lagrange orthogonal polynomial

Objective Function

$$\begin{aligned}
\min \phi = & \sum_i \sum_k \sum_l c_{il}^p \frac{t'_{ikl}}{T_{cl}} + \sum_i \sum_j \sum_k \sum_l c_{ijl}^t \frac{Z_{ijkl}}{T_{cl}} + \sum_i \sum_k \sum_l c_{il}^i W_{ikl} \\
& + \omega \sum_i \delta_i + \alpha_x \int_0^{t_f} (\mathbf{x} - \mathbf{x}^s)^2 dt + \alpha_u \int_0^{t_f} (\mathbf{u} - \mathbf{u}^s)^2 dt
\end{aligned} \tag{18}$$

1. Scheduling

(a) Only one product should be manufactured in each slot

$$\sum_i Y_{ikl} = 1, \quad \forall k, \forall l \quad (19)$$

(b) Transition from product j to product i at slot k and line l

$$\sum_i Z_{ijkl} = Y_{jkl}, \quad \forall j, \forall k, \forall l \quad (20)$$

$$\sum_j Z_{ijkl} = Y_{i,k-1,l}, \quad \forall i, \forall k, \forall l \quad (21)$$

(c) Each product should be manufactured at least once.

$$\sum_l \sum_k Y_{ikl} \geq 1, \quad \forall i \quad (22)$$

(d) Upper and lower bounds for production times

$$t'_{ikl} \leq U_{il} Y_{ikl}, \quad \forall i, \forall k, \forall l \quad (23)$$

$$\sum_i t'_{ikl} \geq L_{il} Y_{ikl}, \quad \forall k, \forall l \quad (24)$$

(e) Production time for each line

$$T_{cl} = \sum_i \sum_k t'_{ikl}, \quad \forall l \quad (25)$$

(f) Amount manufactured of each product

$$W_{ikl} = r_{il} \left[t'_{ikl} - \sum_{j \neq i} \tau_{jil} Z_{jikl} \right], \quad \forall i, \forall k, \forall l \quad (26)$$

(g) Production demand

$$\sum_l \sum_k \frac{W_{ikl}}{T_{cl}} + \delta_i \geq d_i, \quad \forall i \quad (27)$$

2. Optimal Control

a) Dynamic mathematical model discretization

$$x_{fckl}^n = x_{o,fkl}^n + \theta_{k,l}^t h_{fkl} \sum_{m=1}^{N_{cp}} \Omega_{mc} \dot{x}_{fckl}^n, \quad \forall n, f, c, k, l \quad (28)$$

b) Continuity constraint between finite elements

$$x_{o,fkl}^n = x_{o,f-1,kl}^n + \theta_{kl}^t h_{f-1,kl} \sum_{m=1}^{N_{cp}} \Omega_{m,N_{cp}} \dot{x}_{f-1,mkl}^n, \quad \forall n, f \geq 2, k, l \quad (29)$$

c) Model behavior at each collocation point

$$\dot{x}_{fckl}^n = f^n(x_{fckl}^1, \dots, x_{fckl}^n, u_{fckl}^1, \dots, u_{fckl}^m), \quad \forall n, f, c, k, l \quad (30)$$

d) Initial and final controlled and manipulated variable values at each slot

$$x_{in,1l}^n = \sum_{i=1}^{N_p} x_{ss,il}^n y_{i,N_s,l}, \quad \forall n, l \quad (31)$$

$$x_{in,kl}^n = \sum_{i=1}^{N_p} x_{ss,il}^n y_{i,k-1,l}, \quad \forall n, k \neq 1, l \quad (32)$$

$$\bar{x}_{kl}^n = \sum_{i=1}^{N_p} x_{ss,il}^n y_{i,kl}, \quad \forall n, k, l \quad (33)$$

$$u_{in,1l}^m = \sum_{i=1}^{N_p} u_{ss,il}^m y_{i,N_s,l}, \quad \forall m, l \quad (34)$$

$$u_{in,kl}^m = \sum_{i=1}^{N_p} u_{ss,il}^m y_{i,k-1,l}, \quad \forall m, k \neq 1, l \quad (35)$$

$$\bar{u}_{kl}^m = \sum_{i=1}^{N_p} u_{ss,il}^m y_{i,kl}, \quad \forall m, k, l \quad (36)$$

$$u_{1,1,kl}^m = u_{in,kl}^m, \quad \forall m, k, l \quad (37)$$

$$u_{N_{fe},N_{cp},kl}^m = \bar{u}_{in,kl}^m, \quad \forall m, k, l \quad (38)$$

$$x_{o,1,kl}^n = x_{in,kl}^n, \quad \forall n, k, l \quad (39)$$

e) Lower and upper bounds of the decision variables

$$x_{min}^n \leq x_{fckl}^n \leq x_{max}^n, \forall n, f, c, k, l \quad (40a)$$

$$u_{min}^m \leq u_{fckl}^m \leq u_{max}^m, \forall m, f, c, k, l \quad (40b)$$

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