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A LAGRANGEAN DECOMPOSITION HEURISTIC FOR THE SIMULTANEOUS SCHEDULING AND OPTIMAL CONTROL OF MULTI-GRADE POLYMERIZATION REACTORS

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Abstract:
In this work we present the simultaneous scheduling and optimal control of polymerization reactors using a previously proposed MINLP formulation. The problem is then solved in two ways: first by directly using an Outer Approximation technique, and second, by applying a Lagrangean decomposition scheme that allows the independent solution of the scheduling and optimal control problems. However, both subproblems are linked by a set of Lagrangean Multipliers that evolve during an iterative solution process using a subgradient method. During this process the decomposition approach yields an upper bound to the original problem while a lower bound is obtained heuristically based on the solution of the decomposed problem. The methodology is tested on two polymerization processes and compared vs. the solution obtained when the problem is solved directly. In both cases optimal solutions are almost identical while solution times for the larger problem were reduced significantly when using the decomposition approach.

1. INTRODUCTION

The importance of industrial production scheduling and control is broadly recognized. An interest for addressing simultaneous scheduling and control (SSC) problems has appeared recently. (Mahadevan *et al.*, 2002),(Feather *et al.*, 2004),(Nystrom *et al.*, 2005). Because scheduling and control problems have strong interactions it looks reasonable to consider them in a simultaneous and integrated framework. Traditionally, scheduling and control problems were approached independently. As a matter of fact, scheduling problems commonly assume constant transition times and almost any aspect related to process dynamics. On the other hand, process control problems normally assume fixed produc-

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tion sequences. The close relationship between scheduling and control problems and the importance of a simultaneous solution is currently recognized (Mahadevan *et al.*, 2002),(Feather *et al.*, 2004),(Nystrom *et al.*, 2005). Moreover, a recent publication (Mishra *et al.*, 2005) concluded that not including process dynamics in scheduling problem formulations leads, in many cases, to obtaining suboptimal solutions. The rigorous inclusion of process dynamics for optimal grade transitions in a scheduling formulation results in a Mixed Integer Dynamic Optimization (MIDO) problem. Our research group has proposed a formulation for solving simultaneous scheduling and control problems (Flores-Tlacuahuac and Grossmann, 2006).

An important area of application for a simultaneous scheduling and control (SSC) approach is the polymer industry. It is now common for polymerization plants to operate in a continuous manner while several product grades are produced using the same equipment. Two recent works (Nystrom *et al.*, 2005; Prata *et al.*, n.d.) addressed scheduling and grade transition for polymerization systems. In these works the MIDO problem was transformed into a MINLP by a suitable discretization of the transition time, and then solved using a commercially available MINLP solver or coupling an NLP and a MIP solver through an iterative process.

The objective of this work is to solve the Simultaneous Scheduling and Control problem based on our proposed formulation (Flores-Tlacuahuac and Grossmann, 2006) by exploiting its decomposable nature through a Lagrangean Decomposition technique (Guignard and Kim, 1987).

2. PROBLEM DEFINITION

In polymerization plants a certain number of polymer grades are specified in terms of their conversion and/or molecular weight distribution (MWD). These grades are to be formed using a single CSTR operating in an isothermal manner. Each grade is obtained from the same raw material but using different operating conditions. Since the reactor operates continuously, the switch from a certain grade to another involves a dynamic transition which is carried out by manipulating the monomer feed flow rate or the initiator feed flow rate. The transition is accomplished once the conversion and/or MWD are within a certain tolerance of their desired steady state value.
In terms of the scheduling problem lower bounds for the demands rates are specified for all different polymer grades. In order to satisfy these demands all grades must be manufactured once during a production cycle whose cyclic time is to be determined. The manufacturing operation involves inventory holding costs and transition costs. Inventory holding costs, raw material costs and product prices of each grade are known, as well as steady state and upper and lower bounds for all variable.
Given the above stated problem the objective of the present work is to find the optimal manufacturing cycle in order to meet all grades demands while maximizing profit. The optimal cycle is described by the following decision variables. (1) Grade manufacturing sequence. (2) Optimal dynamic transitions. (3) Optimal cycle duration. (4) Amounts manufactured of each grade. For a complete description of the proposed MINLP formulation used to directly solve the simultaneous problem, the reader is kindly refereed to reference (Flores-Tlacuahuac and Grossmann, 2006)

3. SOLUTION METHODOLOGY

The nature of the problem at hand suggests the use of a decomposition technique in which the dynamic optimization problem and the scheduling problem are solved separately. The Lagrangean Decomposition technique (Guignard and Kim, 1987) is the base of the solution methodology presented in this paper. The scheduling and control formulation share the binary variables associated with a production schedule, the variables of transitions durations, and the variable of cycle duration. These variables are substituted by equivalent copies in either the scheduling or the control problem, and a new set of constraints makes the copies equal to the original variables. This new set of constraints is relaxed and added to the objective function using a lagrangean multiplier (Fisher, 1981). This modified SSC formulation is separable into a scheduling subproblem and a control subproblem where the sum of the objective functions of the two subproblems represents an upper bound to the objective function of the SSC original problem. A previous work that deals with the application of Lagrangean Decomposition (van den Heever *et al.*, 2001) proposes a heuristic in which the binary variables in the original formulation are fixed so that a lower bound is obtain by solving the resulting NLP. In this paper the binary variables obtained in the scheduling subproblem are fixed in the original SSC formulation to obtain an NLP that yields a lower bound in each iteration of the heuristic decomposition algorithm. Once an upper bound and a lower bound are obtained one Lagrangian iteration is completed, after which the lagrangian multipliers are updated. This heuristic algorithm stops once the upper and lower bound converge within a defined tolerance or once the maximum number of iterations is exceeded. Since the algorithm is heuristic, the maximum number

of iterations can be determined using different criteria. Generally this number will be set so that it is evident that the algorithm is not making any significant progress, but it can also be determined by the point in which bounds begin to degenerate or subproblems become infeasible. Due to space limitations, the SSC formulation and it's decomposition are not included in this paper, and the reader is referred to the following works for more details (Flores-Tlacuahuac and Grossmann, 2006; Terrazas-Moreno *et al.*, 2006; Terrazas-Moreno *et al.*, 2007). A formal mathematical description of the decomposition technique follows.

3.1 Lagrangean Decomposition

Guignard and Kim (Guignard and Kim, 1987) present Lagrangean Decomposition technique in which certain variables are duplicated and set equal by new constraints. These new constraints are then relaxed through Lagrangean Relaxation (Fisher, 1981; Geoffrion, 1974) yielding a decomposable model over two or more subsets of constraints. Consider the following mathematical programming problem:

$$(P) \quad \max\{fx | Ax \leqslant b, Cx \leqslant d, x \in X\}$$

It is equivalent to:

$$(P^{'}) \max\{fx | Ay \leqslant b, Cx \leqslant d, x \in X, y = x, y \in Y\}$$

A Lagrangean relaxation is obtained for $P^{'}$ by relaxing the constraint $y = x$. This procedure yields a decomposable problem, thus the name "Lagrangean Decomposition":

$$\begin{aligned}
&(LDu)\\
&\max\{fx + u(y - x) | Cx \leqslant d, x \in X,\\
&Ay \leqslant b, y \in Y\}\\
&= \max\{(f - u)\, x | Cx \leqslant d, x \in X\}\\
&+ \max\{uy | Ay \leqslant b, y \in Y\}
\end{aligned}$$

If the constraints are convex then LDu is an upper bound for P for any given u (Fisher, 1981).
Then if all of the constraints are convex and all of the variables are continuous, the tightest upper bound of LDu is equal to the optimal for P:

$$P = \min_{u} LDu$$

In the presence of integer variables and other nonconvexities a duality gap may exits (Guignard, 1995), (Bazaraa and Goode, 1979). Since this is the case of the current formulation the search for an optimum will be performed using an heuristic approach (van den Heever *et al.*, 2001). In such an approach upper bounds of the original problem are generated by solving a problem of the type LDu and lower bounds are generated by using a heuristic technique to produce feasible solutions to the original problem P. The multipliers used to solve the subproblems are updated iteratively using a formula proven to work well in practice (Fisher, 1985):

$$\begin{aligned}
&u^{k+1} = u^k + t^k(y^k - x^k)\\
&and\\
&t^{k+1} = \frac{\alpha_k(LD(u^k) - P^*)}{\| y^k - x^k \|^2}
\end{aligned}$$

Where t^k is a scalar step size and α is a scalar usually set between 0 and 2 and then decreased when LDu fails to improve in a fixed number of iterations.

3.2 Langrangean Decomp. in integer programming

Michelon and Maculan (Michelon and Maculan, 1991) present the extension of Lagrangean Decomposition for integer nonlinear programming with linear constraints. Polymerization reaction systems usually do not present only linear constraints, but the handling of integer variables during the decomposition can still be applied. Using again the example of problem (P), but in the context of integer programming, we have the following:

$$(P) \quad \max\{fx | Ax \leqslant b, Cx \leqslant d, x \in X\}$$

Where X is a set for which the integrality constraints are defined, e.g. $X = \{0, 1\}$. The feasible domain of (P) remains unchanged (Michelon and Maculan, 1991) if we add the constrains:

$$\begin{aligned}
&y = x\\
&Ay \leqslant b, \quad Cx \leqslant d \quad \text{and } y \in CO(X)\\
&where\ CO(X)\ represents\ the\ Convex\ Hull\\
&of\ set\ X
\end{aligned}$$

A lagrangean relaxation is obtained for (P) by relaxing the constraint $y = x$. The same procedure described under the Lagrangean Decomposition section of this paper can be followed afterwards.
The important fact to take notice of, is that the copy (y) of the original binary variable (x) is continuous, since the domain of the new variable is the convex hull of X, denoted as $CO(X)$. As mentioned above the set $X = \{0, 1\}$, and its convex hull includes all real numbers between 0 and 1. This allows the confinement of true

binary variables to the scheduling subproblem, while their continuous copies are used in the significantly more nonlinear control subproblem.

4. CASE STUDIES

In order to analyze the performance of the decomposition technique, applied to simultaneous scheduling and optimal control, it was tested on two polymerization processes. In the following sections the processes are described and the results using a direct method and a decomposition scheme are compared and discussed.

High Impact Polystyrene (HIPS)

The isothermal free radical bulk polymerization of styrene was carried out in a CSTR. The single CSTR model has been used in previous works (Flores-Tlacuahuac *et al.*, 2000; Flores-Tlacuahuac *et al.*, 2005) to describe this process. Five different HIPS grades were defined as desired products for the production cycle, corresponding to 15, 25, 35, 40 and 45 percent monomer conversion. Due to gel effect, normally higher conversions are not obtained in a single reactor. Instead, a sequence of CSTRs is used for that purpose. Monomer flow rate (Q_m)was chosen as the manipulated variable during grade transitions.The simultaneous scheduling and control formulation cast as a MIDO problem was transformed into a MINLP using the SDO technique with 20 finite elements and three collocation points. In a first step the problem was solved directly in GAMS using DICOPT, a MINLP solver that uses the outer approximation algorithm.

Methyl-Methacrylate Polymerization (MMA)

The isothermal free radical bulk polymerization of Methyl-Methacrylate was carried out in a CSTR. The system has already been presented by (Congalidis *et al.*, 1989) to address grade transition problems from a control point of view. Four polymer grades (A, B, C, D) were defined which correspond to molecular weight distributions of 15000, 25000, 35000 and 45000. The initiator flow rate (Q_i) was selected as the manipulated variable to achieve grade transition. The exact same solution procedure followed in the HIPS example was used for the MMA production system.

4.1 Results Isothermal HIPS

4.1.1. Transition times calculated through an iterative process. In this section the simultaneous scheduling and optimal control formulation used corresponds to that previously presented by our research group (Flores-Tlacuahuac and Grossmann, 2006). A precise description of this method is found in (Flores-Tlacuahuac and Grossmann, 2006). All calculations were performed using a 1.6 GHz processor. The comparison between the direct and decomposed approach is found in table 1 and the evolution of the Lagrangean solution is presented in table 2.

Table 1. Optimal solution and solution time for direct and decomposed methods when transition times are calculated iteratively for the HIPS example.

	Direct Method	Decomposition
Optimum	102 738	102 729
Sol. Time	5126 cpu s	4172

Table 2. Upper and lower bounds progression during solution process when transition times are calculated iteratively for the HIPS example.

Iteration	Lower Bound	Upper bound
1	96562	2.2e8
2	96559	3.1e9
3	78003	3.1e9
4	78002	3.1e9
5	NA	102781
6	102111	102772
7	102729	102772
8	102705	102779

Table 3. Optimal solution and solution time for direct and decomposed methods when transition times are calculated as decision variables for the HIPS example.

	Direct Method	Decomposition
Optimum	545.99	545.88
Sol. Time	7640 cpu s	3126

4.1.2. Transition times calculated as decision variables. A modification to the original formulation (Flores-Tlacuahuac and Grossmann, 2006) for the MINLP was carried out and the problem was solved using both the direct and the decomposed approaches. The modification consisted on including the duration of the transition stages as direct decision variables. The cost of transition is now expressed as the cost of raw materials consumed during transition rather than the squared difference of each state in each collocation point vs. a desired value. The modified approach is also detailed in another work (Terrazas-Moreno *et al.*, 2006). The comparison between the direct and decomposed approach for this modified formulation is found in table 3 and the evolution of the Lagrangean solution is presented in table 4.

Table 4. Upper and lower bounds progression during solution process when transition times are calculated as decision variables for the HIPS example.

Iteration	Lower Bound	Upper bound
1	330.50	737.60
2	545.88	813.08
3	545.88	737.61
4	330.50	737.61
5	545.88	813.09

Table 5. Optimal solution and solution time for direct and decomposed methods when transition times are calculated iteratively for the MMA example.

	Direct Method	Decomposition
Optimum	55.02	55.02
Sol. Time	40.27 cpu s	120 cpu s

Table 6. Upper and lower bounds progression during solution process when transition times are calculated iteratively for the MMA example.

Iteration	Lower Bound	Upper bound
1	55.02	81.61
2	55.02	81.67
3	55.02	81.74
4	55.02	81.81
5	55.01	55.04
6	55.01	55.03
7	55.01	55.03
8	55.01	55.04

4.2 Results isothermal MMA

All results for the isothermal MMA CSTR are equivalent to those presented for the HIPS example.

4.2.1. Transition times calculated through an iterative process. The comparison between the direct and decomposed approach is found in table 5 and the evolution of the Lagrangean solution is presented in table 6.

4.2.2. Transition times calculated as decision variables. The comparison between the direct and decomposed approach for this modified formulation is found in table 7 and the evolution of the Lagrangean solution is presented in table 8.

4.3 Discussion

An analysis of the optimal solutions is found in (Terrazas-Moreno *et al.*, 2006). The discussion section of this work is therefore based on the performance of the described decomposition heuristic when compared to the direct solution method.

Table 7. Optimal solution and solution time for direct and decomposed methods when transition times are calculated as decision variables for the MMA example.

	Direct Method	Decomposition
Optimum	32.60	32.81
Sol. Time	71.71 cpu s	240 cpu s

Table 8. Upper and lower bounds progression during solution process when transition times are calculated as decision variables for the MMA example.

Iteration	Lower Bound	Upper bound
1	31.75	86.92
2	31.75	86.92
3	32.43	87.64
4	32.43	87.64
5	31.54	86.78
6	32.50	87.64
7	32.60	87.15
8	32.60	86.54
9	32.81	87.82
10	31.75	86.92

The differences between the optimal solutions found by the direct and decomposed methods is not significant for any of the previous examples. For the MMA system with time determined as a decision variable, the optimal solution obtained with the decomposition heuristic is slightly better than that found with the direct method. This can be explained by the fact that the system is nonlinear and nonconvex and all solvers used for obtaining the presented results can only guarantee local solutions. The Lagrangean decomposition heuristic worked particularly well for both systems when transition times were determined through an iterative process and not as direct decision variables. This remark is based on the fact that the upper and lower bounding of the problem converged to the optimal solution after a certain number of iterations. When time is introduced as a decision variable lower bounds generate the optimal solution rather quickly but upper bounding remains loose throughout the iterative process. The difference between upper and lower bounding is 26% for the HIPS example and 62% for the MMA example. This was also reported by (van den Heever *et al.*, 2001) and it is not surprising given the nonlinearity and nonconvexity of the systems. The fact that the solution method with and without transition times as degrees of freedom behaved differently is explained by the nonconvexities introduces when transition times are included as decision variables. The solution times for the HIPS system were considerably lower when the decomposition approach was used. This was not the case for the MMA system, although both the direct method and the

decomposed method present solution times in the order of a few minutes. The higher solution times for the MMA example using the decomposition technique are well justified since a slightly better optimum was found.

5. CONCLUSIONS

A decomposition that exploits the nature of the simultaneous scheduling and control problem was presented. The resulting formulation casts the scheduling problem and the dynamic optimization as separate subproblems linked by a set of Lagrangean multipliers. A solution methodology was applied in which an upper bound for the original maximization problem is set by the decomposition scheme and a lower bound was obtained heuristically. This method has been previously applied to a different kind of problem (van den Heever *et al.*, 2001), and in this work it has been proven to be effective for simultaneous scheduling and control problems. Moreover, the method becomes more effective as problems grow larger and more complex. More complicated examples, not included in this paper, are being solved by our team (Terrazas-Moreno *et al.*, 2007), and it is our experience that the benefits of using the decomposition become more evident as the problems grow in size and complexity. This explains the differences in performance of the method for the MMA example and the HIPS example in this paper, since the former is significantly smaller and less nonlinear than the latter.

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