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Efficient Decomposition Method for Integrating Production Sequencing and Dynamic Optimization for a Multi-Product CSTR

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Integration of scheduling and control can improve the overall performance of a manufacturing process. However, the integration leads to a mixed-integer dynamic optimization problem (MIDO), which could be challenging to solve. We propose a novel algorithm based on the generalized Bender decomposition method that takes advantage of the special structure of the integrated problem. It decomposes the binary variables from the dynamic optimization. The resulting master problem is a mixed integer linear program (MILP) while the primal problem is a coupled dynamic optimization. Compared with the conventional simultaneous method, the proposed decomposition algorithm can reduce the computational time by over one order of magnitude in a case study.

1. Introduction

Scheduling and dynamic optimization are two important decision levels in process engineering (Zamarripaa et al., 2013). Traditionally, the two problems are solved separately (Engell and Harjunkoski, 2012). The dynamic optimization problem is solved to determine the operational conditions, which provide the recipe data for the scheduling problem (Brasielloa , 2013). These recipe data are treated as fixed parameters when the production schedule is optimized (Chu and You, 2014a). However, it has been recently demonstrated that a collaborative optimization approach which solves the integrated scheduling and dynamic optimization problem simultaneously can significantly improve the overall performance of the entire process system because the operational conditions can be optimized along with the production sequence and assignments (Flores-Tlacuahuac and Grossmann, 2006).

The integrated scheduling and dynamic optimization problem is generally formulated as a mixed integer dynamic optimization (MIDO) problem (Barton et al., 1998). A common solution strategy for the integrated MIDO problem is the simultaneous method (Chu and You, 2012). This method discretizes the differential equations by the collocation method (Cuthrell and Biegler, 1987). After the discretization procedure, the MIDO problem is reformulated as a mixed-integer nonlinear programming (MINLP) problem. A general-purpose MINLP solver can be used to solve the MINLP for the integrated problem. Though the simultaneous method is straightforward, the reformulated MINLP problem can be very challenging to solve (Kheawhom and Bumroongsri, 2013). Considering that multiple products are manufactured in a process, the integrated problem typically includes a number of dynamic models describing different operational modes for the products. Therefore, a large-scale MINLP problem is frequently reformulated after the discretization procedure (Chu and You, 2013a).

The objective of this work is to develop a fast optimization algorithm to solve the integrated scheduling and dynamic optimization problem. It has been demonstrated that an efficient solution strategy is a critical issue to implement the integrated method online for handling disturbances and process uncertainties (Chu and You, 2013b). In this work, we present a systematic decomposition method based on the framework of the generalized Benders decomposition - GBD (Geoffrion, 1972). This method is applied to solve the integrated scheduling and dynamic optimization problem for continuous processes in a CSTR, where multiple products are manufactured in a cyclic manner (Chu and You, 2013c).

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The decomposition method separates the binary decision variables from the dynamic optimization. The resulting master problem is a simple mixed integer linear programming (MILP) problem. The primal problem is a coupled dynamic optimization problem where all dynamic models are optimized simultaneously.
The decomposition method is demonstrated in a methyl methacrylate polymerization process. Compared with the popular simultaneous method which solves the integrated problem directly by discretizing the differential equations describing the dynamic models, the proposed decomposition method can reduce the computational time by more than one order of magnitude.

2. Model formulation

An illustrative diagram of the cyclic production in a CSTR is displayed in Figure 1. Multiple products A, B, C, D are produced one by one in a cyclic manner. Each product is only produced once in a cycle. After a production cycle finishes, another cycle begins with the same production sequence. The main decision in a cyclic scheduling problem is to determine the production sequence so that the total cost can be minimized.

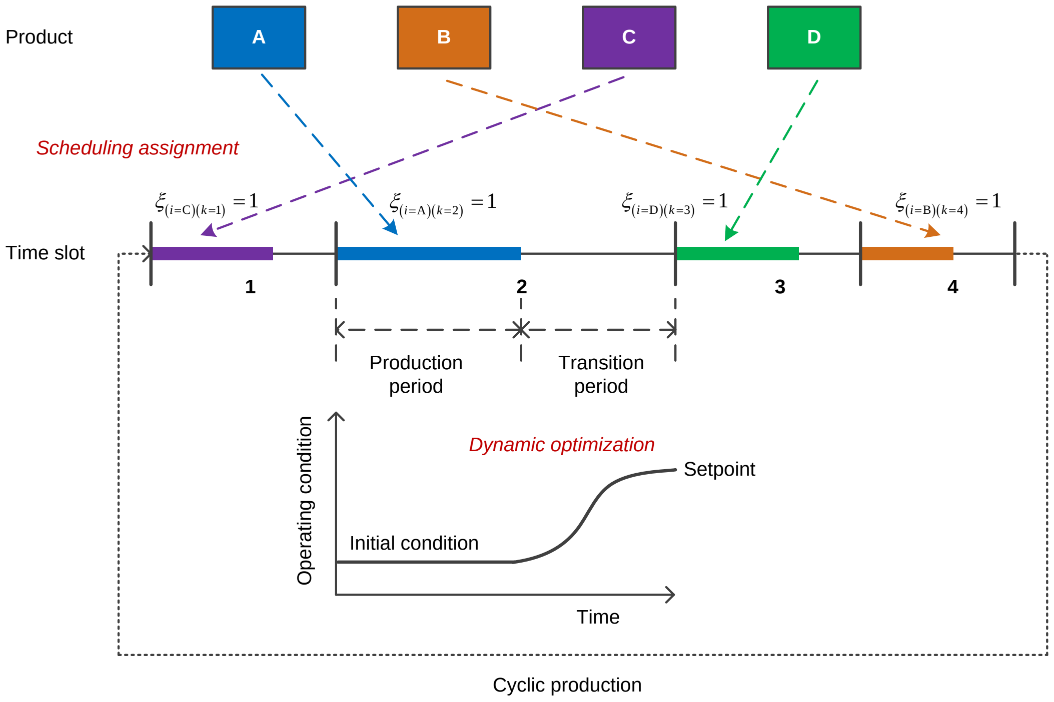

Figure 1: Illustrative example of the cyclic scheduling problem

In a traditional scheduling problem, we assume the transition from a product to another has a fixed cost. They are fixed parameters when the scheduling problem is solved. However, the transition costs are actually variables in practice. We can change them by manipulating the inputs of the dynamic system governing the transition. However, the transition cost is coupled with the transition time which also determines other components of the total cost, e.g. the inventory cost. Therefore, we cannot optimize the dynamic system in each transition period independently (Chu and You, 2014b). It requires simultaneous optimization of all dynamic systems and the scheduling decisions that leads to the integrated problem.
The integrated problem, denoted as (Integration_TS), is formulated as follows (Chu and You, 2013c):

$$\min \ a_1 \sum_{k=1}^{n_P} \Theta_k + a_2 \left(\sum_{k=1}^{n_P} \Delta_k \Big/ \sum_{k=1}^{n_P} \Theta_k \right) \tag{1}$$

$$\text{s.t.} \quad \xi_{ik} \in \{0,1\}, \ \forall i, \ k \tag{2}$$

$$\zeta_{ik} = \xi_{ik}, \ \forall i, \ k \tag{3}$$

$$\zeta_{ik} \in [0,1], \ \forall i, \ k \tag{4}$$

$$\sum\nolimits_{k=1}^{n_p} \zeta_{ik} = 1, \ \forall i \tag{5}$$

$$\sum_{i=1}^{n_p} \zeta_{ik} = 1, \ \forall k \tag{6}$$

$$\frac{dX_k(t)}{dt} = F\left(X_k(t), U_k(t)\right), \ \forall k \tag{7}$$

$$Y_k(t) = G\left(X_k(t), U_k(t)\right), \ \forall k \tag{8}$$

$$H\left(X_k(t), U_k(t), Y_k(t)\right) \le 0, \ \forall k \tag{9}$$

$$X_k(0) = X_k^0, \ \forall k \tag{10}$$

$$Y_k(t) = Y_k^{sp}, \ \forall t \ge \Psi_k, \ \forall k \tag{11}$$

$$\Delta_k = \phi_k\left(X_k(\Psi_k), U_k(\Psi_k), Y_k(\Psi_k)\right), \ \forall k \tag{12}$$

$$X_k^0 = \sum_{i=1}^{n_p} \zeta_{ik} x_i^0, \ \forall k \tag{13}$$

$$Y_k^{sp} = \sum_{i=1}^{n_p} \zeta_{ik++1} y_i^{sp}, \ \forall k \tag{14}$$

The objective is to minimize the total cost which is the sum of the inventory cost and the transition cost. Θ_k and Δ_k respectively denote the transition time and the transition cost in time slot k. a_2 and a_2 are parameters. The main scheduling decision is to assign the time slots to the products. The assignment is determined by a set of binary variables $\xi_{ik} \in \{0,1\}$. If $\xi_{ik} = 1$, then time slot k is assigned to product i. To facilitate the subsequent decomposition method, we introduce a copy of the binary variables, denoted by ζ_{ik}. They are continuous variables ranging from zero to one. However, they can only have the binary value according to the equality constraint (3). Because one product is manufactured only once in a time slot and a time slot is used to produce only one product, we have the constraints (5) and (6).

The dynamic models in time slots are formulated as constraints (7)-(12). The dynamic models are indexed by k and there are n_p dynamic models we need to consider. In each dynamic model, the state variables are represented by $X_k(t)$, the inputs by $U_k(t)$, and the outputs by $Y_k(t)$. To have a compact expression, we use the vector notation. Each state, input, or output vector can include multiple elements. The vector notation is applied to the equations as well. The differential equation (7) represents the systems equation and the equation (8) determines the outputs. Inequality (9) imposes path constraints on the states, inputs and outputs. The initial condition is specified in Eq(10) and the setpoint value is given in Eq(11). The transition time Θ_k is defined as the length of the time interval from the starting point of the transition to the ending point after which the output stays at the setpoint value. Eq(12) gives the definition of the transition cost Δ_k. For different processes, we have different expressions of the transition cost.

The dynamic models are coupled with the binary scheduling variables through Eq(13) and (14). These equations define the interface between the scheduling model and the dynamic models. The assignment variable is used to determine the initial condition and the setpoint value of each dynamic system. The steady state value x_i^0 and the setpoint value y_i^{sp} for a product are given parameters. However, the initial condtion X_k^0 and the setpoint value Y_k^{sp} in a time slot are variables depending on the assignment decisions. Because the production is carried out cyclically, the cyclic addition k ++ 1 is used in Eq(14), which is a shortcut notation for

$$\xi_{ik++1} = \begin{cases} \xi_{ik+1}, & 1 \le k \le n_p - 1 \\ \xi_{i1}, & k = n_p \end{cases}, \ \forall i \tag{15}$$

Due to the linking equations and the consensus equality between ζ_{ik} and ξ_{ik}, the assignment variable ξ_{ik} has an strong effect on the dynamic system. When ξ_{ik} varies, the initial condition and the setpoint are changed and in turn all variables regarding the dynamic models are changed.

3. Generalized Benders decomposition method

Direct solution to the complicated MIDO problem which integrates the scheduling model with the dynamic models can be computationally expensive. A decomposition method is helpful to reduce the computational time (Chu and You, 2013d). Generally, GBD consists of several main steps (Geoffrion, 1972):

(1) Identify the complicating variables. The presence of these variables makes the optimization problem difficult to solve. However, when they are temporarily fixed, the optimization problem with the remaining variables turns out to be much easier to solve.
(2) Project the optimization problem, including the objective function and the constraints, onto the space of the complicating variables. The GBD methods typically express the projected objective function by its Lagrangean relaxation. In the same way, the projected feasible range can be expressed.
(3) Decompose the optimization problem into a primal problem and a master problem. The primal problem is solved when the complicating variables are fixed. Then the master problem is solved to update the complicating variables based on the dual information returned by the primal problem.
(4) Solve the original problem by iterating between the primal and the master problems. The iteration stops when the gap between the lower bound and the upper bound is less than a specified threshold value.

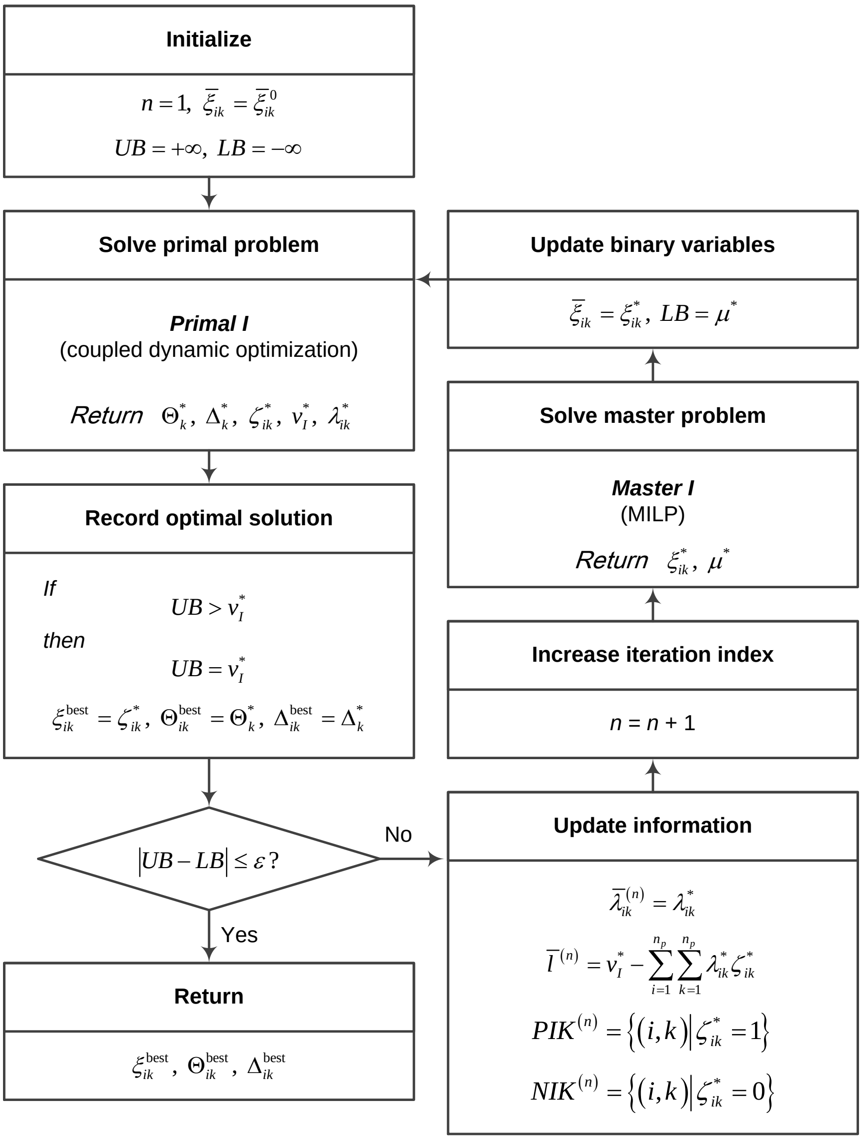

Figure 2: Procedure of the decomposition method

The detailed procedure of the decomposition method is displayed in Figure 2. The iteration is initialized by fixing the binary variables at $\bar{\xi}_{ik}^{0}$. Then the primal problem is solved with the fixed binary variables. The optimal solution, objective function value, and dual variables are returned. The upper bound is updated according to the optimal function value. The best solution, which is found till the current iteration, is recorded. If the gap between the lower bound and the upper bound falls in the tolerance range specified by a given value ε, then the iteration stops and the best solution is returned. Otherwise, the dual information is

used to generate a new Benders' cut constraint in the master problem. Then the master problem is solved to update the binary variables and the lower bound of the optimal solution. When solving the master problem, we don't need to search over the values at which the binary variables have once been fixed. We can add integer cuts to eliminate these values from the search procedure. The primal problem is
(***Primal I***)

$$v_I\left(\left\{\bar{\xi}_{ik}\right\}\right) = \min\ a_1 \sum_{k=1}^{n_p} \Theta_k + a_2 \left(\sum_{k=1}^{n_P} \Delta_k \Big/ \sum_{k=1}^{n_P} \Theta_k \right) \tag{16}$$

s.t. Constraints (4)-(14)

$$\zeta_{ik} = \bar{\xi}_{ik},\ \forall i,\ k \tag{17}$$

The projected problem is the integrated problem with the assignment variables ζ_{ik} fixed at $\bar{\xi}_{ik}$. The projected objective function is represented by $v_I(\cdot)$ which is dependent on the fixed value $\bar{\xi}_{ik}$. In this work, we use the bar to denote a fixed value of the corresponding variable. For the short notation, we use the curly bracket around the variable to denote the set of the variables, e.g. $\left\{\bar{\xi}_{ik}\right\}$ denotes all $\bar{\xi}_{ik}$ for $\forall i,\ k$.

The master problem is denoted as (Master I) and give below:

$$\min\ \mu \tag{18}$$

$$\text{s.t.}\ \sum\nolimits_{i=1}^{n_p} \zeta_{ik} = 1,\ \forall k \tag{19}$$

$$\sum\nolimits_{k=1}^{n_p} \zeta_{ik} = 1,\ \forall i \tag{20}$$

$$\mu \geq \bar{l}^{(m)} + \sum_{i=1}^{n_p} \sum_{k=1}^{n_p} \bar{\lambda}_{ik}^{(m)} \xi_{ik},\ 1 \leq m \leq n-1 \tag{21}$$

$$\sum_{(i,k)\in PIK^{(m)}} \xi_{ik} - \sum_{(i,k)\in NIK^{(m)}} \xi_{ik} \leq \left|PIK^{(m)}\right| - 1,\ 1 \leq m \leq n-1 \tag{22}$$

4. Case study

The case study is a methyl methacrylate (MMA) polymerization process. The dynamic model under consideration is a nonlinear free radical polymerization with azobisisobutyronitrile as initiator and toluene as the solvent. The detailed reactor dynamic model is given in our previous work (Chu and You, 2013c).

Table 1: Model and solution statistics of the solution methods

Method		Decomposition	Simultaneous
Number of Iterations		20	–
Total CPU (s)		172.8	2,141.3
Objective (m.u/h)		212.49	212.49
Optimal sequence		A→B→C→D→E→F→G	A→B→C→D→E→F→G
Gap (%)		1.0	1.0
Primal problem	Equations	28,669	–
	Variables	28,130	–
	CPU (s)	171.0	–
Master problem / Integrated problem	Type	MIP	MINLP
	Equations	54	28,620
	Variables	50 (all) 48 (binary)	28,130 (all) 48 (binary)
	Solver	CPLEX	SBB
	CPU (s)	1.8	2,141.3
	Gap (%)	0	1.0

We initialize the problem with the production sequence A→G→F→E→C→B→D. The variables of dynamic models are initialized by the steady state values according to the production sequence. The results of the decomposition method and the simultaneous method are shown in Table 1. The decomposition method converges to the optimal solution identical to the one found by the simultaneous method. However, the computational time considerably reduces from 2,141.3 s to 172.8 s. The optimal sequence returned is A→B→C→D→E→F→G.

5. Conclusions

Integrated scheduling and dynamic optimization coordinates the two decision layers. As a result, the integrated method can achieve a better performance in optimizing the entire production system than the conventional method which solve the scheduling problem and the dynamic optimization problem one after the other. However, the integrated problem is a complicated MIDO problem, which is much more challenging to solve than the subproblems. To simplify the computational complexity, we proposed a decomposition method based on the GBD framework. It decomposed the binary scheduling variables from the dynamic optimization. The primal problem was a coupled dynamic optimization problem. The decomposition is demonstrated by a case study. Compared with the simultaneous method, the decomposition method returned the same optimal solution while it reduced the computational time by more than one order of magnitude. The computational efficiency enables the proposed method to solve large-scale industrial problems which the direct solution method fails to solve.

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