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A multicut generalized benders decomposition approach for the integration of process operations and dynamic optimization for continuous systems

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ABSTRACT

The integration of process operations and dynamic optimization leads to large scale optimization problems whose monolithic solution is challenging. In this paper we propose a new formulation of the integrated planning, scheduling, and dynamic optimization problem for continuous single stage systems. We analyze the structure of the problem using Stochastic Blockmodeling and we show that the estimated structure can be used as the basis for a multicut Generalized Benders decomposition (GBD) algorithm, which can solve the problem in reduced computational time. Furthermore, we propose an accelerated hybrid multicut algorithm which can lead to further reduction in computational time. Through case studies, we analyze the computational performance of the proposed formulation and decomposition based solution algorithms.

1. Introduction

The optimal operation of process systems depends on the solution of a wide class of optimization problems which are typically considered independently. However, fast changing economic environments render this approach suboptimal and motivate the integration of different decision levels (Grossmann, 2005; Daoutidis et al., 2018). A typical example is the integration of process operations, i.e. production planning and scheduling, with dynamic optimization (Baldea and Harjunkoski, 2014; Chu and You, 2015; Dias and Ierapetritou, 2017). In these problems, production decisions such as execution of a task and allocation of resources are made simultaneously with optimal control decisions leading to increased profitability.

In order to achieve this integration two solution approaches have been proposed in the literature (Baldea and Harjunkoski, 2014). In the "top-down" approach, the dynamic behavior of the system is incorporated in the planning/scheduling problem, the problem is solved once and the results provide the production sequence which is the set point for the control level (Flores-Tlacuahuac and Grossmann, 2006; Nie et al., 2012; Gutiérrez-Limón et al., 2014). In the "bottom up" approach the integrated problem is solved in a rolling horizon manner resulting in a closed loop implementation (Zhuge and Ierapetritou, 2012; Pattison et al., 2017; Chu and You, 2014b; Risbeck et al., 2019; Caspari et al., 2020).

We can argue that the main limitation in both approaches is the solution of the resulting optimization problem. The main challenges arise due to the inherently nonlinear behavior of most process systems, which in conjunction with the multiple time scales of the different decision making problems lead to large scale Mixed Integer Nonlinear Programs (MINLP). The monolithic solution of such problems is challenging due to the presence of continuous and discrete variables which are coupled through nonlinear constraints (Belotti et al., 2013). In order to improve the tractability of these problems two paths can be followed. In the first, the optimization problem is simplified using surrogate models, typically approximating the nonlinear dynamic behavior of the system (Pattison et al., 2016; Zhuge and Ierapetritou, 2014; Burnak et al., 2018; Chu and You, 2014a; Shi et al., 2015; Charitopoulos et al., 2017). The alternative approach is to use decomposition based solution algorithms and exploit the structure of the full optimization problem. Typical examples of this approach include the application of Lagrangean (Terrazas-Moreno et al., 2008; Mora-Mariano et al., 2020) and Benders (Nie et al., 2015; Chu and You, 2013a; 2013b) decomposition. Although these algorithms can potentially reduce the computational time, their application is challenging too. First, a decomposition of the optimization problem itself is necessary. Its structure however, as it relates to the requisite solution algorithm, is not always evident. In recent research in our group we have proposed the application of Stochastic Blockmodeling (SBM)

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and Bayesian inference as a tool to learn the underlying structure of the problem (Mitrai et al., 2021; Mitrai and Daoutidis, 2021). In this approach the optimization problem is represented as a graph, and application of statistical inference allows learning the structure of the problem which can guide us towards the selection of the most appropriate decomposition based solution algorithm.

The second issue is related to the convergence of decomposition based solution algorithms which depends strongly on the problem formulation. For the integration of planning, scheduling, and dynamic optimization for continuous systems, two problem formulations have been proposed: one based on slots (Gutiérrez-Limón et al., 2014) and another one based on the Traveling Salesman Problem (Charitopoulos et al., 2017). In this work we will focus on the slot based formulation, where the planning horizon is discretized into periods, and each period is discretized into slots. The values of the state and manipulated variables for each slot and period depend on the production sequence and the transition time. We have recently shown that application of *nested* SBM (Mitrai and Daoutidis, 2021) can reveal the underlying structure of such a problem and can be used as the basis for the application of Generalized Benders Decomposition (GBD) (Mitrai and Daoutidis, 2021; Geoffrion, 1972). However, global optimality can not be guaranteed due to the nonconvexity of the dynamic optimization problems that consider the dynamic transition of the system between the different products.

In this work, we propose a new formulation of the integrated problem for single stage continuous processes. Specifically, motivated by the formulation of the integrated scheduling and dynamic optimization problem for batch systems (Chu and You, 2013a), we consider all the transitions between the products for all the slots and periods simultaneously. We analyze the structure of the problem using SBM and Bayesian inference. Based on the inference results, we find that the planning/scheduling and dynamic optimization constraints are coupled only through the transition times. Therefore, the cost associated with the dynamic optimization problem for each transition, slot, and period depends only on the transition time and can be replaced by its value function in the objective function. This structure lends itself to the application of multicut Generalized Benders decomposition, which solves the problem in reduced computational time compared to other formulations of the problem and decomposition based solution algorithms (Gutiérrez-Limón et al., 2014; Mitrai and Daoutidis, 2021). In order to reduce further the computational time we propose a hybrid multicut Generalized Benders decomposition algorithm where the cut associated with one transition in one slot and period is added for all slots and periods. We show that this approach leads to further reduction in computational time without affecting the solution quality. The rest of the document is organized as follows: In Section 2 we present the integrated optimization problem, in Section 3 we analyze the structure of the integrated problem and in Section 4 we present the decomposition based solution algorithms. Finally in Sections 5,6 we analyze the performance of the proposed algorithms.

2. Problem formulation

2.1. Production planning and scheduling

In this section we will present the planning and scheduling model for a single stage single line continuous process proposed in Dogan and Grossmann (2006). We assume that N_p $(i=\{1,\dots,N_p\})$ products must be produced over a planning horizon which is discretized into N_{pr} $(p=\{1,\dots,N_{pr}\})$ periods, which are further discretized into N_s $(k=\{1,\dots,N_s\})$ slots. First we define a binary variable W_{ikp} which is equal to 1 if product i is produced at slot k in period p and zero otherwise. We also define the variable $Z_{ijkp}\in\{0,1\}$ which is equal to 1 if a product i is followed by product j in slot k in period p, and the variable Zp_{ijp} which is equal to one if transition occurs between product i and j between time periods. At each time slot only one product can be produced, which is enforced with the following constraints:

$$\sum_i W_{ikp}=1 \ \forall k,p. \tag{1}$$

Based on the sequence of the products at the end of each slot, either a transition occurs from product i to j or the same product is produced in the next slot. The transition between products for every slot and period is modeled though the following equations:

$$\begin{aligned} Z_{ijkp} &\geq W_{ikp}+W_{j,k+1,p}-1 \ \forall i,j,k\neq N_s,p \\ Zp_{ijkp} &\geq W_{iN_sp}+W_{j,1,p+1}-1 \ \forall i,j,p, \end{aligned} \tag{2}$$

where the first constraint considers the transitions between the slots in a period, and the second constraint considers the transitions between the periods. Due to the possible transitions, each slot is composed of a production and a transition regime. The production time of product i in slot k in period p is Θ_{ikp} and the transition time in slot k in period p is $\check{\theta}^t_{kp}$. The timing constraints are the following:

$$\begin{aligned} T^s_{1,1} &= 0 \\ T^e_{k,p} &= T^s_{k,p}+\sum_i \Theta_{ikp}+\check{\theta}^t_{kp} \quad \forall k,p \\ T^s_{k+1,p} &= T^e_{k,p} \quad \forall k\neq N_s,p \\ T^s_{1,p+1} &= T^e_{N_s,p} \quad \forall k,p\neq N_{per} \\ \Theta_{ikp} &\leq W_{ikp}H_p \quad \forall i,k,p \\ \hat{\Theta}_{ip} &= \sum_k \Theta_{ikp} \quad \forall i,p \\ T^e_{k,p} &\leq pH_p \quad \forall k,p, \end{aligned} \tag{3}$$

where T^s_{kp} is the starting tine of slot k in period p, T^e_{kp} is the ending time in slot k and period p, H_p is the duration of period p and $\hat{\Theta}_{ip}$ is the production time of product i in period p. We assume that the demand of product i in period p (d_{ip}) must be satisfied in the end of the period. The production rate of product i is r_i, the amount of product i produced in slot k at period p is $\hat{q}_{ikp}$ and the amount of product i produced in period p is q_{ip}. The production and inventory constraints are:

$$\begin{aligned} \hat{q}_{ikp} &= r_i\Theta_{ikp} \quad \forall i,k,p \\ q_{ip} &= \sum_k \hat{q}_{ikp} \quad \forall i,p \\ I_{ip} &= I_{ip-1}+q_{ip}-S_{ip} \quad \forall i,p \\ A_{ip} &= H_p(I_{ip-1}-S_{ip-1})+q_{ip}H_p \quad \forall i,p \\ S_{ip} &\geq d_{ip} \quad \forall i,p, \end{aligned} \tag{4}$$

where I_{ip} is the inventory of product i in period p, A_{ip} is the linear overestimation of the integral of inventory, S_{ip} is the amount of product i sold in period p. Finally, the following symmetry breaking constraints are included:

$$\begin{aligned} Y_{ip} &\geq W_{ikp} \quad \forall i,k,p \\ Y_{ip} &\leq N_{ip}\leq \bar{N}Y_{ip} \quad \forall i,p \\ N_{ip} &\geq N-\left(\sum_i Y_{ip}-1\right)-M(1-W_{i1p}) \quad \forall i,p \\ N_{ip} &\leq N-\left(\sum_i Y_{ip}-1\right)+M(1-W_{i1p}) \quad \forall i,p \\ N_{ip} &= \sum_k W_{ikp} \quad \forall i,p \end{aligned} \tag{5}$$

where $Y_{ip} \in \{0, 1\}$ is equal to 1 if product i is assigned in period p and zero otherwise, $\bar{N}$ is the number of slots, M is a parameter, and N_{ip} is equal to the number of slots that product i is manufactured in period p. The first constraint (in Eq. (5)) ensures that every product is assigned to at least one slot every period, the second constraint guarantees that if a product is manufactured in a period then at least one slot must be used, and the last constraint enforces that a product is manufactured in consecutive slots if necessary. We refer the reader to Dogan and Grossmann (2006) for a detailed explanation of these constraints.

2.2. Dynamic model

We assume that the dynamic behavior of the system is described by a system of ordinary differential equations

$$\dot{x}(t) = F(x, u), \tag{6}$$

where $x \in \mathbb{R}^n$ are the states of the system, $u \in \mathbb{R}^m$ are the manipulated variables and $F : \mathbb{R}^{n+m} \to \mathbb{R}^n$ are vector functions. The differential equations are discretized using the method of orthogonal collocation on finite elements using N_{fe} $(f = \{1, \ldots, N_{fe}\})$ finite elements and N_c $(c = \{1, \ldots, N_c\})$ collocation points. In this work, we will consider simultaneously all the possible transitions and will define the variables x^n_{ijfckp} and u^m_{ijfckp} as the values of the nth state and mth manipulated variable for a transition from product i to product j at finite element f, collocation point c, slot k and period p. We will also define θ_{ijkp} as the transition time for the transition from product i to j in slot k and period p. The discretized differential equations are:

$$\begin{aligned}
x^n_{ijfckp} &= x0^n_{ijfkp} + h^{fe}_{kp} \sum_{m=1}^{N_{cp}} \Omega_{mc} \dot{x}^n_{ijfmkp} \quad \forall n, i, j, f, c, k, p \\
h^{fe}_{ijkp} &= \frac{\theta_{ijkp}}{N_{fe}} \quad \forall i, j, k, p \\
x0^n_{ijfkp} &= x0^n_{ij,f-1kp} + h^{fe}_{ijkp} \sum_{m=1}^{N_{cp}} \Omega_{mc} \dot{x}^n_{ij,f-1,mkp} \quad \forall n, i, j, f \geq 2, c, k, p \\
\dot{x}^n_{ijfckp} &= F(x^n_{ijfckp}, u^m_{ijfckp}) \quad \forall n, i, j, f, c, k, p \\
t^d_{ijfckp} &= h^{fe}_{ijkp}(f - 1 + \gamma_c) \quad \forall i, j, f, c, k, p \\
x0_{ij1kp} &= x^{ss}_i \quad \forall i, j, k, p \\
x_{ijN_{fe}N_{cp}kp} &= x^{ss}_j \quad \forall i, j, k, p \\
u_{ij11kp} &= u^{ss}_i \quad \forall i, j, k, p \\
u_{ijN_{fe}N_{cp}kp} &= u^{ss}_j \quad \forall i, j, k, p,
\end{aligned} \tag{7}$$

where x^{ss}_i, u^{ss}_i are the steady state values of the state and manipulated variables for product i, Ω is the collocation matrix, and γ are the Radau roots. We note that in this formulation, the values of the state and manipulated variables at the beginning and end of each slot and period do not depend on the binary variables W_{ikp} or Z_{ijkp}. This is different from Gutiérrez-Limón et al. (2014), Charitopoulos et al. (2017) where the values of the states/manipulated variables at the beginning and end of each slot and period depend on the values of the binary variables.

2.3. Integrated problem

The objective function of the integrated optimization problem is:

$$\begin{aligned}
\Phi = &\sum_{i,p} \left(P_{ip} S_{ip} - C^{oper}_{ip} q_{ip} - C^{inv} A_{ip} \right) \\
&- \sum_{i,j,k,p} C^{trans}_{ij} Z_{ijkp} - \sum_{i,j,p} C^{trans}_{ij} Zp_{ijp} \\
&- \sum_{i,j,p,k} Z_{ijkp} \left(\alpha_u \sum_{f,c} N^{-1}_{fe} t^d_{ijfckp} \Omega_{c,N_{cp}} (u_{ijfckp} - u^{ss}_j)^2 \right) \\
&- \sum_{i,j,p} Zp_{ijkp} \left(\alpha_u \sum_{f,c} N^{-1}_{fe} t^d_{ijfcN_sp} \Omega_{c,N_{cp}} (u_{ijfcN_sp} - u^{ss}_j)^2 \right),
\end{aligned} \tag{8}$$

where P_{ip} is the price of product i in period p, C^{oper}_{ip} is the operating cost of product i in period p, C^{inv} is the inventory cost, C^{trans}_{ij} is the transition cost from product i to j, and a_u is a weight coefficient. The first term represents the sales, the second and third terms are related to the operating and inventory costs, and the fourth and fifth terms represent the fixed transition cost between the slots and periods. The last two terms represent the transition cost. In these terms, the cost of a transition from product i to j in slot k and period p is multiplied by Z_{ijkp} (and by Zp_{ijp} if we consider the transition between the time periods). Therefore, if a transition does not occur, i.e. $Z_{ijkp} = 0$ or $Zp_{ijp} = 0$, then the cost does not contribute to the objective. Finally, the transition time for each slot and period depends on the transitions that occur and the following equations are added:

$$\begin{aligned}
\breve{\theta}^t_{kp} &= \sum_{i=1}^{N_p} \sum_{i=1}^{N_p} \theta_{ijkp} Z_{ijkp} \ \forall k, k \neq N_s, p \\
\breve{\theta}^t_{N_sp} &= \sum_{i=1}^{N_p} \sum_{i=1}^{N_p} \theta_{ijN_sp} Zp_{ijp} \ \forall p, p \neq N_{per} \\
\theta_{ijkp} &\geq \theta^{min}_{ij} \ \forall i, j, k, p,
\end{aligned} \tag{9}$$

where $\theta^{\min}_{ij}$ is the minimum transition time for a transition between product i and j. The integrated optimization problem is:

$$\begin{aligned}
&\text{maximize} \quad \Phi \\
&\text{subject to} \quad \text{Eq. } (1), (2), (3), (4), (5), (7), (9)
\end{aligned} \tag{10}$$

This is the general problem formulation for the integration of planning, scheduling, and dynamic optimization for a single stage single unit system. In this formulation, each slot is composed of a production and a transition regime. Therefore, if the number of slots is equal to the number of products, in the last slot of the last period no transition occurs. Hence the variables and constraints associated with all the transitions for this slot can be removed from the optimization problem.

3. Problem decomposition

In this section we will analyze the structure of the integrated problem using SBM and Bayesian inference. We refer the reader to the Supplementary material for an introduction to SBM and to Mitrai et al. (2021), Mitrai and Daoutidis (2021) for a detailed explanation on the application of this approach to optimization problems. For illustration, we consider an isothermal continuous stirred tank reactor where an irreversible reaction occurs ($A \to 3B$). The dynamic behavior of the system is described by the following equation (Gutiérrez-Limón et al., 2014):

$$\frac{dc(t)}{dt} = \frac{Q(t)}{V}(c_{feed} - c(t)) - kc(t)^3, \tag{11}$$

where c is the concentration of the reactant, Q is the inlet flowrate (manipulated variable) and $V = 5000$ $L, c_{feed} = 1$ $mol/L, k = 2$ $L^2/(hr\ mol^2)$ are the reactor volume, inlet concentration and reaction rate constant, respectively. In order to keep the graph simple, we will assume that two products must be produced in three planning periods and the dynamic model is discretized using 20 finite elements with 3 collocation points. We apply degree corrected SBM in the constraint graph of the problem using graph-tool (Peixoto, 2014). In this graph, the nodes are the constraints of

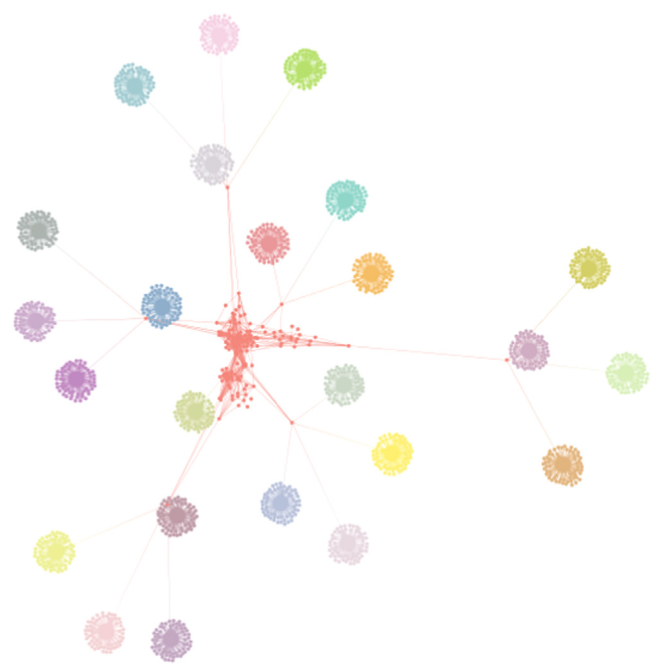

Fig. 1. Inference results on the constraint graph of the integrated optimization problem.

the problem and the edges are the variables that couple two constraints. Based on the inference results (Fig. 1), twenty five blocks are identified. The planning/scheduling constraints are assigned in one block (nodes in the middle of the graph), and the constraints that are associated with the dynamic behavior of the system for each transition, slot, and period are assigned into different blocks. These blocks are connected with the block in the center of the graph through one edge, the coupling variables. In this case the coupling variables are the transition times θ_{ijkp}. This *hybrid core community structure* in the graph is also manifested in the L shape of the ω (block density) matrix inferred for the SBM:

$$\omega = \begin{bmatrix} 1392 & 1 & 1 & \dots & 1 \\ 1 & 6794 & 0 & \dots & 0 \\ 1 & 0 & 6794 & \dots & 0 \\ \vdots & \vdots & & \ddots & \vdots \\ 1 & 0 & \dots & \dots & 6794 \end{bmatrix} \in \mathbb{R}^{25\times 25},$$

where the ω_{ij} entry of this matrix is equal to the number of edges between the nodes in block i and the nodes in block j. The planning/scheduling constraints form the core, which is connected with all the communities, i.e. the constraints of the dynamic optimization problems, through the variables θ_{ijkp}.

We note that although the structure of this problem is the same as the one identified using nested SBM in our previous work (Mitrai and Daoutidis, 2021) based on the problem formulation proposed in Gutiérrez-Limón et al. (2014), the coupling variables differ. In Mitrai and Daoutidis (2021) the coupling variables are the transition time, initial and final states, and manipulated variables. In this case the coupling variables are only the transition times θ_{ijkp}. This coupling of the variables/constraints can be attributed to the modeling of the transitions. The state and manipulated variables depend on the transition times through the discretization of the differential equations.

4. Decomposition based solution algorithm

4.1. Problem reformulation based on the identified structure from SBM

Given the structure of the problem the variables can be decomposed into three sets. The first contains the variables that are associated with planning and scheduling decisions, the second set contains the variables that are associated with transitions between products, and the last set contains the coupling variables (transition times) that couple the planning/scheduling decisions with the dynamic optimization decisions. Given this partition of the variables, if we fix the planning/scheduling and the coupling variables, then the dynamic optimization problems for the transitions are independent and depend only on the transition time θ_{ijk}. The dynamic optimization problem for a transition from product i to j in slot k and period p is:

$$\begin{aligned} \text{maximize} \quad & -\alpha_u \textstyle\sum_{f=1}^{N_{fe}} \sum_{c=1}^{N_{cp}} N_{fe}^{-1} t^d_{ijfckp} \Omega_{c,N_{cp}} \left(u_{ijfckp} - u_j^{ss}\right)^2 \\ \text{subject to} \quad & x^n_{ijfckp} = x0^n_{ijfkp} + h^{fe}_{kp} \textstyle\sum_{m=1}^{N_{cp}} \Omega_{mc} \dot{x}^n_{ijfmkp} \quad \forall n, f, c \\ & h^{fe}_{ijkp} = \frac{\hat{\theta}_{ijkp}}{N_{fe}} \\ & x0^n_{ijfkp} = x0^n_{ij,f-1kp} + h^{fe}_{ijkp} \textstyle\sum_{m=1}^{N_{cp}} \Omega_{mc} \dot{x}^n_{ij,f-1,mkp} \quad \forall n, f \geq 2, c \\ & \dot{x}^n_{ijfckp} = f\left(x^n_{ijfckp}, u^m_{ijfckp}\right) \quad \forall n, f, c \\ & t^d_{ijfckp} = h^{fe}_{ijkp}(f - 1 + \gamma_c) \quad \forall f, c \\ & x0_{ij1kp} = x_i^{ss} \\ & x_{ijN_{fe}N_{cp}kp} = x_j^{ss} \\ & u_{ij11kp} = u_i^{ss} \\ & u_{ijN_{fe}N_{cp}kp} = u_j^{ss} \\ & \hat{\theta}_{ijkp} = \theta_{ijkp}. \end{aligned} \tag{12}$$

We will write this problem as:

$$\begin{aligned} \text{maximize} \quad & -f^{dyn}_{ijkp} \\ \text{subject to} \quad & g^{dyn}_{ijkp} \leq 0 \\ & \hat{\theta}_{ijkp} = \theta_{ijkp} \end{aligned} \tag{13}$$

which is equivalent to minimizing f^{dyn}_{ijkp} subject to $g^{dyn}_{ijkp} \leq 0$ and $\hat{\theta}_{ijkp} = \theta_{ijkp}$. The solution of this problem depends on the value of the transition time θ_{ijkp}. We define as ϕ_{ijkp} the value function of a transition from product i to j in slot k and period p, which is equal to the optimal value of the objective function of the following optimization problem:

$$\begin{aligned} \text{minimize} \quad & f^{dyn}_{ijkp} \\ \text{subject to} \quad & g^{dyn}_{ijkp} \leq 0 \\ & \hat{\theta}_{ijkp} = \theta_{ijkp} \quad : \lambda_{ijkp} \end{aligned} \tag{14}$$

where λ_{ijkp} is the Lagrange multiplier for the equality constraint $\hat{\theta}_{ijkp} = \theta_{ijkp}$. The value function depends only on the transition time, i.e. the coupling variable.

The objective function of the integrated problem can be decomposed into two parts. The first contains the cost associated with the planning/ scheduling variables (Φ_1) and the second part considers the transition costs (Φ_2):

$$\Phi_1 = \sum_{i,p}\left(P_{ip}S_{ip} - C^{oper}_{ip} q_{ip} - C^{inv}A_{ip}\right) - \sum_{i,j,k,p} C^{trans}_{ij} Z_{ijkp} - \sum_{i,j,p} C^{trans}_{ij} Zp_{ijp}$$

$$\Phi_2 = \sum_{i,j,k,p} Z_{ijkp}\left(\alpha_u \sum_{f,c} N^{-1}_{fe} t^{d}_{ijfckp} \Omega_{c,N_{cp}} (u_{ijfckp} - u^{ss}_j)^2\right) + \sum_{i,j,p} Zp_{ijkp}\left(\alpha_u \sum_{f,c} N^{-1}_{fe} t^{d}_{ijfcN_sp} \Omega_{c,N_{cp}} (u_{ijfcN_sp} - u^{ss}_j)^2\right).$$

Based on the value function of the dynamic optimization problem, the integrated problem is written as follows:

$$\begin{aligned} &\text{maximize} \quad \Phi_1 - \sum_{ijkp} Z_{ijkp}\phi_{ijkp}(\theta_{ijkp}) - \sum_{ijp} Zp_{ijp}\phi_{ijN_sp}(\theta_{ijN_sp}) \\ &\text{subject to} \quad \text{Eqs. (1), (2), (3), (4), (5), (9).} \end{aligned} \tag{15}$$

This problem is equivalent to the original integrated problem (Eq. (10)) since ϕ_{ijkp} is only a function of the transition time θ_{ijkp} as identified by the application of SBM. Therefore, if a transition does not occur, i.e. $Z_{ijkp} = 0$, then $Z_{ijkp}\phi_{ijkp}(\theta_{ijkp}) = 0$ even if $\phi_{ijkp}(\theta_{ijkp}) \neq 0$, so the cost associated with this transition does not affect the profit. If the transition occurs, i.e. $Z_{ijkp} = 1$, then the cost, which is equal to $\phi_{ijkp}(\theta_{ijkp})$, affects the profit.

4.2. Solution algorithm

The above problem can not be solved directly since the value functions are not known explicitly. We will follow a cutting plane method to solve the problem. Specifically, we will approximate the value functions with hyperplanes. From Geoffrion (1971), it is known that if the value function ϕ_{ijkp} is convex and we solve the problem in Eq. (14) for $\bar{\theta}_{ijkp} = \theta_{ijkp}$, we can outer approximate ϕ_{ijkp} as follows:

$$\phi_{ijkp}(\theta_{ijkp}) \geq \phi_{ijkp}(\bar{\theta}_{ijkp}) + \partial\phi_{ijkp}(\bar{\theta}_{ijkp})(\theta_{ijkp} - \bar{\theta}_{ijkp}) \quad \forall \theta_{ijkp} \geq \theta^{min}_{ij} \tag{16}$$

where $\partial\phi(\bar{\theta}_{ijkp})$ is the subgradient of the value function for $\theta_{ijkp} = \bar{\theta}_{ijkp}$ and is equal to the negative of the optimal Lagrange multiplier λ_{ijkp} for the equality constraint $\theta_{ijkp} = \bar{\theta}_{ijkp}$.

Given this approximation, if we solve the dynamic optimization problems for different values of θ_{ijkp} we can approximate the function ϕ_{ijkp} and the problem:

$$\underset{\theta_{ijkp}}{\text{minimize}} \quad \phi_{ijkp}(\theta_{ijkp}) \tag{17}$$

is equivalent to Geoffrion (1970a,b):

$$\begin{aligned} &\underset{\theta_{ijkp}}{\text{minimize}} \quad \eta_{ijkp} \\ &\text{subject to} \quad \eta_{ijkp} \geq \phi^{\nu}_{ijkp}(\bar{\theta}^{\nu}_{ijkp}) - \lambda^{\nu}(\theta_{ijkp} - \bar{\theta}^{\nu}_{ijkp}) \forall \nu = 1, \dots, \mathcal{V} \end{aligned} \tag{18}$$

where $\mathcal{V} = \{\nu_1, \nu_2, \dots, \nu_n\}$ is the number of points used to approximate the value function and the overbar denotes a fixed value. The integrated optimization problem can be written as:

$$\begin{aligned} &\text{maximize} \quad \Phi_1 - \textstyle\sum_{ijkp} Z_{ijkp}\eta_{ijkp} - \sum_{ijp} Zp_{ijp}\eta_{ijN_sp} \\ &\text{subject to} \quad \text{Eqs. (1), (2), (3), (4), (5), (9)} \\ &\qquad \eta_{ijkp} \geq \phi^{\nu}_{ijkp} - \lambda^{\nu}_{ijkp}(\theta_{ijkp} - \bar{\theta}^{\nu}_{ijkp}) \quad \forall i, j, k, p, \nu \in \mathcal{V} \end{aligned} \tag{19}$$

We note that the tangent approximation corresponds to the Benders cuts (Geoffrion, 1972). We will follow a Generalized Benders Decomposition approach to solve this problem. The master problem is the relaxed planning/scheduling problem and the subproblems are independent dynamic optimization problems for each transition, slot, and period. The dynamic optimization problems are solved only for the transitions that occur, i.e. $(i, j, k, p) \in \{(i, j, k, p) | Z_{ijkp} = 1\}$, $(i, j, p) \in \{(i, j, p) | Zp_{ijp} = 1\}$. Once the subproblems are solved, the following Benders cuts are added in the master problem:

$$\eta_{ijkp} \geq \phi_{ijkp} - \lambda_{ijkp}(\theta_{ijkp} - \bar{\theta}_{ijkp})$$

if $Z_{ijkp} = 1$ and

$$\eta_{ijN_sp} \geq \phi_{ijN_sp} - \lambda_{ijN_sp}(\theta_{ijN_s} - \bar{\theta}_{ijN_sp})$$

if $Zp_{ijp} = 1$, where the overbar denotes a fixed value. The steps that are followed to solve the problem are presented in Algorithm 1. In this approach at every iteration one cut is added for every transition that occurs, therefore multiple cuts are added per iteration. This approach is known in the literature as multicut Benders decomposition (Birge and Louveaux, 2011).

Algorithm 1 Multicut Generalized Benders Decomposition based on the learnt structure.

Require: Optimization problem

1: Set $UB = \infty, LB = -\infty$
2: Set tolerance and optimality gap (tol)
3: Initialize the algorithm by fixing the production sequence and obtain the transitions that occur, transition times, Lagrangean multipliers λ_{ijkp}, ϕ_{ijkp} and add tangent approximation (Line 10)
4: **while** $(UB - LB)/LB \geq$ tol/100 **do**
5: Solve the master problem (Eq. 19), obtain UB and transitions
6: Solve the dynamic optimization problems (Eq. 14) that correspond to $Z_{ijkp} = 1, Zp_{ijp} = 1$
7: Obtain Lagrangean multipliers λ_{ijkp}, ϕ_{ijkp}, Φ_1, Φ_2
8: Update lower bound $LB = \max\{LB, \Phi_1 - \Phi_2\}$
9: Add following tangent approximation in the relaxed problem:
10:
$$\begin{aligned} &\text{if} \quad Z_{ijkp} = 1 \quad \text{add} \quad \eta_{ijkp} \geq \phi_{ijkp} - \lambda_{ijkp}(\theta_{ijkp} - \bar{\theta}_{ijkp}) \\ &\text{if} \quad Zp_{ijp} = 1 \quad \text{add} \quad \eta_{ijN_sp} \geq \phi_{ijN_sp} - \lambda_{ijN_sp}(\theta_{ijN_sp} - \bar{\theta}_{ijN_sp}) \end{aligned}$$
11: **end while**
12: **return** Upper, lower bound and variable values

We can exploit further the structure of the problem to accelerate its solution. Specifically, since η is defined for all $(ijkp)$, the approximation of the transition from i to j in slot 1 is also valid in all the other slots and periods. Therefore, we propose an accelerated hybrid multicut algorithm where in each iteration we add the constraints:

$$\eta_{ijk'p'} \geq \phi_{ijkp} - \lambda_{ijkp}(\theta_{ijk'p'} - \bar{\theta}_{ijkp}) \ \forall i, j, k' \in N_s, p' \in N_{per}$$

if $Z_{ijkp} = 1$ and

$$\eta_{ijk'p'} \geq \phi_{ijN_sp} - \lambda_{ijN_sp}(\theta_{ijk'p'} - \bar{\theta}_{ijN_sp}) \ \forall i, j, k' \in N_s, p' \in N_{per}$$

if $Zp_{ijp} = 1$, where the overbar denotes a fixed value. In this approach, at each iteration, for each transition that occurs multiple cuts are added. We note that the addition of multiple cuts per iteration is a common strategy in decomposition based solution methods for MINLP problems (Su et al., 2015; Kronqvist et al., 2016). In these cases the solution of the master problem provides a pool of solutions which can be used to solve multiple subproblems which lead to the addition of multiple cuts per iteration. In the proposed *hybrid* multicut GBD approach, the subproblems are solved based on the global solution of the master problem but the cut for a transition between product i and j in slot k and period p is used to approximate the value functions for the specific transition for all slots and periods. The steps that are followed to solve the problem are presented in Algorithm 2. For both algorithms (multicut and

Algorithm 2 Hybrid Multicut Generalized Benders Decomposition.

Require: Optimization problem

1: Set $UB = \infty, LB = -\infty$
2: Set tolerance and optimality gap (tol)
3: Initialize the algorithm by fixing the production sequence and obtain the transitions that occur, transition times, Lagrangean multipliers λ_{ijkp}, ϕ_{ijkp} and add tangent approximation (Line 10)
4: **while** $(UB - LB)/LB \geq$ tol/100 **do**
5: Solve the master problem (Eq. 19), obtain UB and transitions
6: Solve the dynamic optimization problems (Eq. 14) that correspond to $Z_{ijkp} = 1, Zp_{ijp} = 1$
7: Obtain Lagrangean multipliers λ_{ijkp}, ϕ_{ijkp}, Φ_1, Φ_2
8: Update lower bound $LB = \max\{LB, \Phi_1 - \Phi_2\}$
9: Add following tangent approximation in the relaxed problem:
10: if $Z_{ijkp} = 1$ add $\eta_{ijk'p'} \geq \phi_{ijkp} - \lambda_{ijkp}(\theta_{ijk'p'} - \bar{\theta}_{ijkp})$ $\forall i, j, k' \in N_s, p' \in N_{per}$
if $Zp_{ijp} = 1$ add $\eta_{ijk'p'} \geq \phi_{ijN_sp} - \lambda_{ijN_sp}(\theta_{ijk'p'} - \bar{\theta}_{ijN_sp})$ $\forall i, j, k' \in N_s, p' \in N_{per}$
11: **end while**
12: **return** Upper, lower bound and variable values

Table 1
Operating conditions and product price for the first case study.

Product	$c^{ss}\,(mol/L)$	$Q^{ss}\,(L/h)$	Production rate
A	0.24	200	150
B	0.2	100	80
C	0.30	400	278
D	0.39	1000	607

hybrid multicut), the relaxed problem is a Mixed Integer Nonlinear Program (MINLP) with bilinear terms in the objective function ($Z_{ijkp}\eta_{ijkp}$, $Zp_{ijp}\eta_{ijN_sp}$) and in Eq. (9) ($Z_{ijkp}\theta_{ijkp}$, $Zp_{ijp}\theta_{ijN_sp}$) solved with Gurobi (Gurobi Optimization, LLC, 2021). We note that this problem can be transformed into a Mixed Integer Linear Program (MILP) by linearizing the bilinear terms. Specifically we can replace every bilinear term, e.g. $Z_{ijkp}\eta_{ijkp}$ with $\eta \in [\underline{\eta}_{ij}, \bar{\eta}_{ij}]$ as follows

$$\begin{aligned} \min\{0, \underline{\eta}_{ij}\} &\leq \delta_{ijkp} \leq \bar{\eta}_{ij} \\ \underline{\eta}_{ij} Z_{ijkp} &\leq \delta_{ijkp} \leq \bar{\eta}_{ij} Z_{ijkp} \\ \eta_{ijkp} - (1 - Z_{ijkp})\bar{\eta}_{ij} &\leq \delta_{ijkp} \leq \eta_{ijkp} - (1 - Z_{ijkp})\underline{\eta}_{ij} \\ \delta_{ijkp} &\leq \eta_{ijkp} + (1 - Z_{ijkp})\underline{\eta}_{ij}. \end{aligned} \tag{20}$$

The computation of $\underline{\eta}_{ij}, \bar{\eta}_{ij}$ is presented in the Supplementary material. Similarly we can linearize the $Z_{ijkp}\theta_{ijkp}$ bilinear terms. Although this leads to a MILP, we found that for small planning horizons solving the master problem with the bilinear terms (using Gurobi) is faster than solving the MILP model. Hence, in the first case study (Section 5) the master problem is a MINLP whereas in the second case study (Section 6) we use the MILP model. The subproblems are nonlinear optimization problems solved with IPOPT (Wächter and Biegler, 2006) and the values of the dual variables that are used are the ones returned by IPOPT. The algorithm is implemented in Python using Pyomo (Hart et al., 2017).

Remark 1. In the proposed algorithms the hyperplanes that approximate a value function are valid under the assumption that the value function is concex. For the isothermal CSTR considered in Section 3, when four products can be produced, the value function for each transition from product 1 to the other products is shown in Fig. 2 and the Benders cut for the transition from product 1 to product 2 is shown in Fig. 3 (the steady state values of the concentration and inlet flowrate are presented in Table 1). From these figures we observe that the value functions are convex and the Benders cuts are valid understimators.

Remark 2. Given the convexity of the value functions, the proposed multicut and hybrid multicut algorithms can be used to

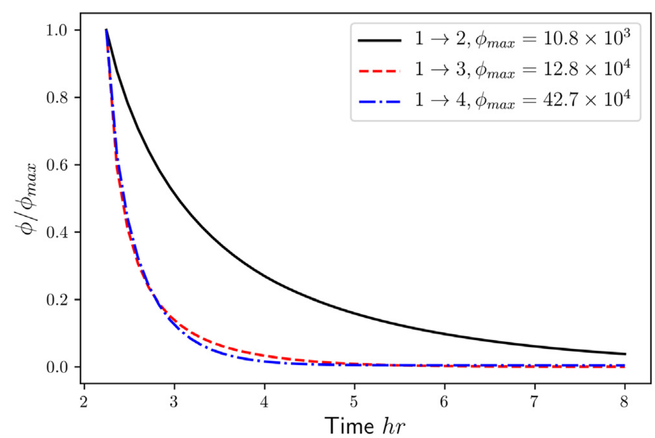

Fig. 2. Transition cost for a transition from product 1 to products 2,3,4. The x axis is the transition time and the y axis the scaled cost. The steady state values of the state and manipulated variable are given in Table 1.

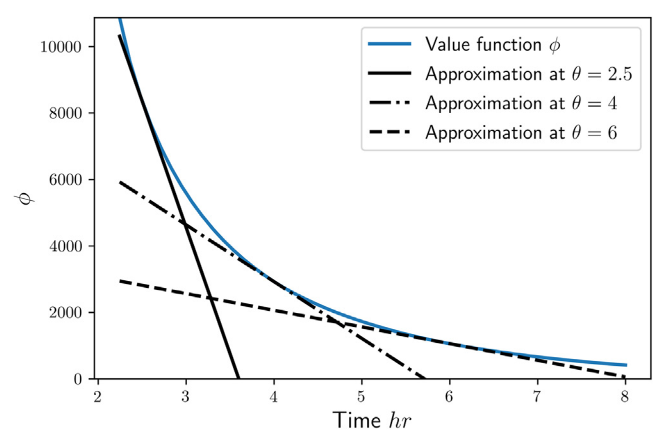

Fig. 3. Approximation of the value function for three different values of θ.

solve the problem to global optimality since the Benders cuts are valid understimators of the value functions. However, the solution of the integrated problem to global optimality requires that the subproblems are also solved to global optimality. Although this can be achieved using global optimization solvers like BARON (Kılınç and Sahinidis, 2018), this can increase the CPU time in cases where the subproblems have a large number of variables/constraints and

Table 2
Operating and transition cost for the first case study, $C^{inv} = 0.026$, $a_u = 1$.

Product	C^{oper}		C^{trans}			
	$p = 1$	$p = 2$	A	B	C	D
A	13	13	0	100	60	120
B	22	12	150	0	50	80
C	35	45	200	150	0	100
D	29	19	90	100	120	0

Table 3
Product demand for the first case study.

Prod.	Demand (mol/week)		Price (\$/*mol*)	
	$p = 1$	$p = 2$	$p = 1$	$p = 2$
A	8000	9000	200	220
B	4000	3600	160	140
C	7000	8000	130	150
D	6000	11,000	110	110

nonconvex terms. In the case studies presented in this paper we solve the subproblems with IPOPT and therefore global optimality cannot be guaranteed. We also note that in the general case, where the value functions are not convex the proposed algorithms can still be applied but global optimality cannot be guaranteed even if the subproblems are solved to global optimality.

Remark 3. The idea of replacing the transition cost with its value function has been previously pursued in literature. In Shi et al. (2015), the dynamic optimization problem was solved for different values of the transition time and a flexible recipe approach was followed to solve the integrated planning, scheduling, and dynamic optimization problem. Similarly in Charitopoulos et al. (2017) a surrogate model was used to approximate the transition cost. A similar approach was followed in Chu and You (2014a), where a cooperative game theoretical approach was followed and the problem was formulated as a two level game. The first level agent solves the scheduling problem and the second level agent solves the dynamic optimization problem by considering only its objective value. The value function of the dynamic optimization problem was approximated using piece-wise linear functions. In the above approaches the transition cost and value of the objective function obtained are approximate. In our approach, the proposed algorithm provides the exact solution of the problem.

5. Case study 1: Isothermal CSTR

In the first case study we consider the isothermal CSTR whose dynamic behavior is described by Eq. (11). We assume that four products must be produced in two planning periods, each composed of four slots. The economic data of the problem, adapted from Gutiérrez-Limón et al. (2014), can be found in Tables 1, 2, 3. We solve the problem with the proposed formulation and multicut and hybrid multicut decomposition based solution algorithms and compare them with the application of Generalized Benders Decomposition based on the structure found in Mitrai and Daoutidis (2021) using the formulation of the integrated problem proposed in Gutiérrez-Limón et al. (2014). The formulation of the integrated problem and formulation of GBD (Mitrai and Daoutidis, 2021) can be found in the Supplementary material. In this case study, we constrain the rate of change of the manipulated variable for the dynamic optimization problems through the following constraints:

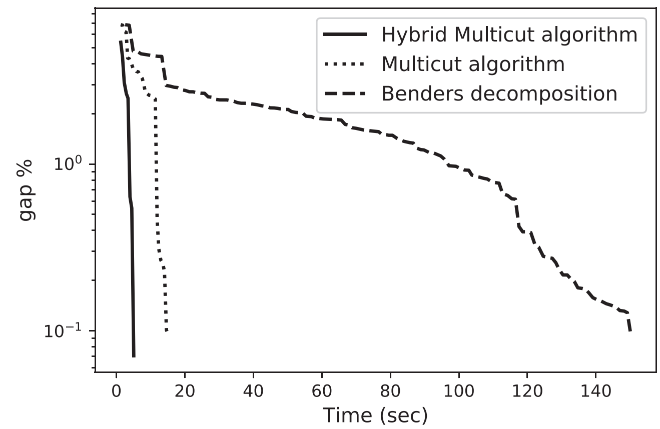

Fig. 4. Evolution of the gap for the proposed algorithms and GBD (Benders decomposition) based on Gutiérrez-Limón et al. (2014), Mitrai and Daoutidis (2021) for the first case study.

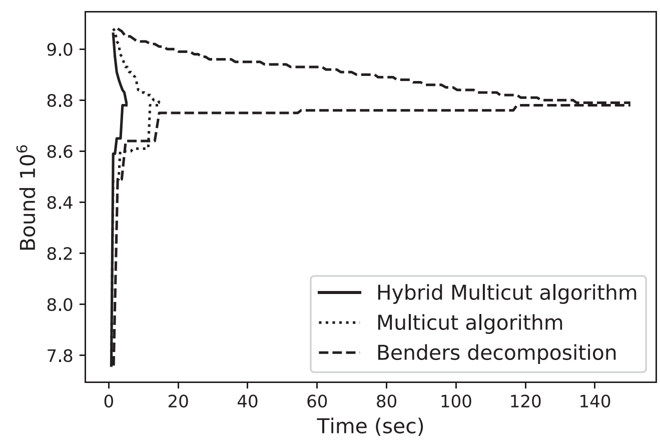

Fig. 5. Evolution of the upper and lower bounds for the proposed algorithms and GBD (Benders decomposition) based on Gutiérrez-Limón et al. (2014), Mitrai and Daoutidis (2021) for the first case study.

$$\begin{aligned}
&u^m_{ijfckp} - u^m_{ijf-1,ckp} \leq U^{max}_m(t^d_{ijfckp} - t^d_{ijf-1,ckp}) \\
&\qquad \forall m, i, j, f \geq 1, c, k, p \\
&u^m_{ijfckp} - u^m_{ijfc-1,kp} \leq U^{max}_m(t^d_{ijfckp} - t^d_{ijfc-1,kp}) \\
&\qquad \forall m, i, j, f, c \geq 1, k, p \\
&u^m_{ijfckp} - u^m_{ijf-1,ckp} \geq U^{min}_m(t^d_{ijfckp} - t^d_{ijf-1,ckp}) \\
&\qquad \forall m, i, j, f \geq 1, c, k, p \\
&u^m_{ijfckp} - u^m_{ijfc-1,kp} \geq U^{min}_m(t^d_{ijfckp} - t^d_{ijfc-1,kp}) \\
&\qquad \forall m, i, j, f, c \geq 1, k, p,
\end{aligned} \tag{21}$$

where $U^{\max}_m, U^{\min}_m$ is the maximum and minimum change for manipulated variable m. The dynamic model is discretized using 20 finite elements with 3 collocation points. For all algorithms the optimality gap was set equal to 0.1%, and the initial production sequence was $A \to B \to C \to D$ for both periods. The master problem in the first iteration has 592 variables and 445 constraints and the dynamic optimization problem for each transition, slot and period has 265 variables and 326 constraints.

The evolution of the optimality gap and the upper and lower bound with the CPU time for the different algorithms is presented in Fig. 4, 5. Based on the results, GBD based on the formulation and decomposition from Gutiérrez-Limón et al. (2014), Mitrai and Daoutidis (2021) converges after 150 CPU seconds (131 iterations) and the value of the objective function is 8.781×10^6. The multicut algorithm converges after 15 CPU seconds (28 iterations) lead-

Table 4
Production results for the for the first case study.

Slot	Product	Production amount (mol)	Production time (hr)	Transition time (hr)
Period 1				
1	B	4000	50.0	0.98
2	A	8000	53.3	1.21
3	C	14,176	51	1.58
4	D	6000	9.8	0
Period 2				
Slot	Product	Production amount (mol)	Production time (hr)	Transition time (hr)
1	D	29,968	49.3	1.87
2	C	823	2.9	1.55
3	A	9000	60	2.24
4	B	4000	50	0

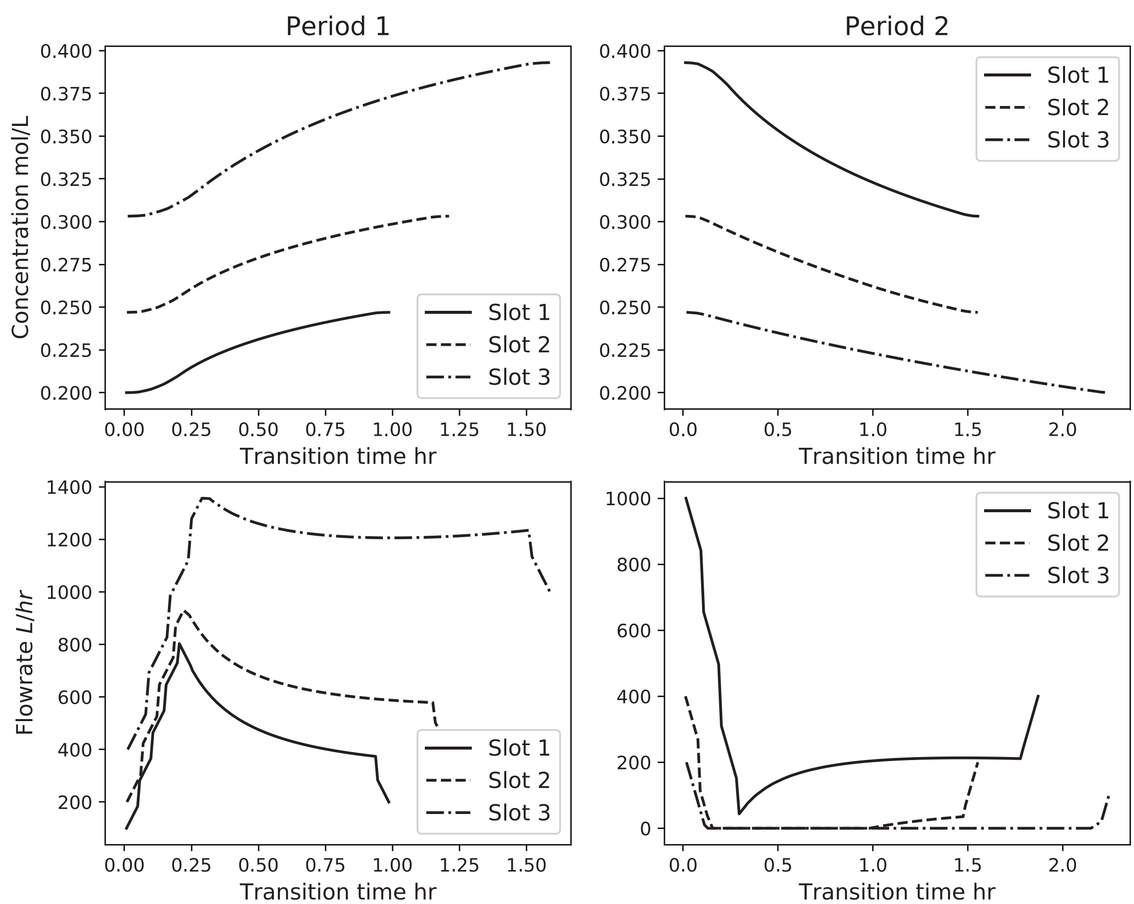

Fig. 6. Concentration and inlet flowrate profiles for each slot and period for the first case study.

ing to a 90% reduction in CPU time and the objective function is 8.782×10^6. From Fig. 5 we observe that the multicut algorithm reduces the bounds faster even though initially the lower bound obtained from GBD is better. The hybrid multicut algorithm converges after 5 s (8 iterations) leading to a 96% reduction in CPU time compared to GBD and 66% compared to the multicut algotirhm. The solution that is obtained is the same as the one obtained from the multicut algorithm. The difference in the solution time is due to the fact that in the hybrid multicut algorithm, in each iteration more information is added in the master problem through the multiple cuts for each transition. In GBD and the multicut algorithm, in each iteration the Benders cut provides information only about the specific production sequence and transition time. The production results obtained from the proposed algorithm are presented in Table 4, and the concentration and inlet flowrate profiles are presented in Fig. 6. From the production results, we see that the demand is satisfied and product D is overproduced in the second period. Additionally, product C is overproduced in the first period in order to satisfy the demand in the second period where the operating cost is higher, compared to the first period. Finally, no transition occurs between the two periods leading to a reduction in the cost and increase in the profit.

6. Case study 2: MMA polymerization reactor

In the second case study we will consider a methyl methacrylate (MMA) polymerization process. The states of the system are the concentration of the monomer c_m, the concentration of the initiator c_i, concentration of dead chains D_0 and mass concentration of dead chains D_1. The input is the flowrate of the initiator F_i and

Table 5
Parameters of the dynamic model for the MMA rector.

Parameter	Value
F	10 m^3/h
V	10 m^3
f^*	0.58
k_p	2.5 10^6 $m^3/(kmol\ h)$
k_{td}	1.09 10^{11} $m^3/(kmol\ h)$
k_{fm}	2.45 10^3 $m^3/(kmol\ h)$
k_i	1.02 10^{-1} h^{-1}
c_i^{in}	8 $kmol/m^3$
c_m^{in}	6 $kmol/m^3$
M_m	100.12 kg/kmol

Table 6
Steady state and production rate values for the MMA rector.

	Products			
Steady state value	1	2	3	4
c_m	3.07	3.22	3.33	3.43
c_i	0.14	0.12	0.1	0.09
D_0	0.019	0.016	0.014	0.012
D_1	292	277	267	257
Y	15,000	17,000	18,500	20,000
F_i	0.2	0.16	0.14	0.12
Prod. rate (kg/hr)	123	76.4	50.8	35.2

the output is the molecular weight of each product Y. Based on the value of the initiator inlet flowrate, products with different molecular weight can be produced. The dynamic behavior of the system is described by the following differential equations (Chu and You, 2013b):

$$\begin{aligned}
\frac{dc_m(t)}{dt} &= -(k_p + k_{fm})Pc_m(t)\sqrt{c_i(t)} + \frac{F(c_m^{in} - c_m(t))}{V} \\
\frac{dc_i(t)}{dt} &= -k_i c_i(t) + \frac{F_i(t)c_i^{in} - Fc_i(t)}{V} \\
\frac{dD_0(t)}{dt} &= (0.5k_{tc} + k_{td})P^2 c_i(t) + k_{fm}Pc_m(t)\sqrt{c_i(t)} - \frac{FD_0(t)}{V} \\
\frac{dD_1(t)}{dt} &= M_m(k_p + k_{fm})Pc_m(t)\sqrt{c_i(t)} - \frac{FD_1(t)}{V} \\
Y(t) &= D_1(t)/D_0(t) \\
P &= \sqrt{\frac{2f^* k_f}{k_{td} + k_{tc}}}
\end{aligned} \tag{22}$$

The parameters of the dynamic model can be found in Table 5 (Chu and You, 2013b). We will assume that four products must be produced in three planning periods. The steady state values of the states, inlet flowrate and molecular weight are presented in Table 6. In this case, the dynamic model is discretized using 20 finite elements and 3 collocation points. The dynamic optimization problems for each slot has 741 variables and 689 constraints and in the first iteration the master problem has 1368 variables and 2966 constraints. We solve the problem using the proposed multicut and hybrid multicut algorithms and GBD based on Gutiérrez-Limón et al. (2014), Mitrai and Daoutidis (2021). The algorithms are initialized by fixing the product sequence to $1 \to 2 \to 3 \to 4$ for all periods and the optimality gap tolerance is set to 0.1%. The economic data of the problem are presented in Tables 6, 7, 8.

The evolution of the optimality gap and the upper and lower bound with the CPU time for the different algorithms is presented in Fig. 7, 8. The multicut algorithm converges after 90 CPU seconds (17 iterations), the hybrid multicut algorithm converges after 35 s (7 iterations) and the value of the objective function is 5.06×10^6. GBD based on Gutiérrez-Limón et al. (2014), Mitrai and Daoutidis (2021) converges after 425 CPU seconds (71 iterations) and the value of the objective function is 4.84×10^6. The production sequence that is obtained from this algorithm is the same as the initial guess, leading to lower value of the objective function compared to the solution obtained by the multicut and hybrid multicut algorithm. In this case, the hybrid multicut algorithm reduces the CPU time by 91 %, the multicut algorithm by 78% and the value of the objective is improved by 4.5%. Similar to the previous case study the multicut and hybrid multicut algorithms improve the upper and lower bounds faster compared to GBD. Also, the addition of multiple cuts per transition in the hybrid multicut

Table 7
Operating and transition cost for the second case study, $C^{inv} = 0.026$, $a_u = 10^6$.

	C^{oper}			C^{trans}			
Product	$p=1$	$p=2$	$p=3$	A	B	C	D
1	23	10	15	0	150	120	180
2	30	25	20	160	0	180	160
3	45	55	40	150	100	0	90
4	50	29	20	110	100	120	0

Table 8
Product demand and price for the second case study.

	Demand (kg/week)			Price ($/kg)		
Prod.	$p=1$	$p=2$	$p=3$	$p=1$	$p=2$	$p=3$
1	2500	2200	2150	300	280	250
2	2200	1400	1800	180	150	160
3	3000	3500	2500	160	190	180
4	1000	2000	1500	120	120	130

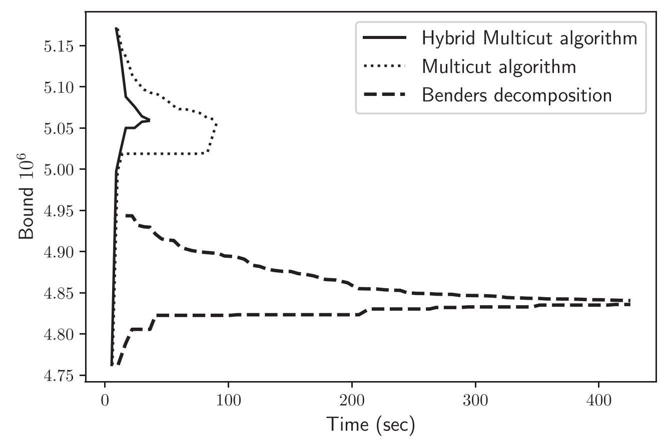

Fig. 7. Evolution of the upper and lower bound for the different algorithms for the second case study.

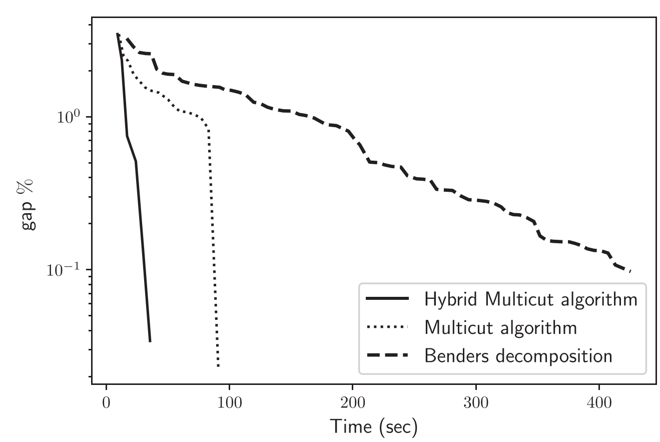

Fig. 8. Evolution of the optimality gap for the different algorithms for the second case study.

Table 9
Production results for the second case study.

Slot	Product	Production amount (*kg*)	Production time (*hr*)	Transition time (*hr*)
Period 1				
1	4	1000	28.36	1.10
2	3	4013	78.86	1.14
3	2	2200	28.76	1.41
4	1	3481	28.28	0
Period 2				
1	1	3481	28.28	1.95
2	2	2200	28.76	1.69
3	3	2486	48.85	1.66
4	4	2000	56.72	0
Period 3				
1	4	2000	56.72	1.10
2	3	3500	68.77	1.25
3	2	1000	13.07	1.41
4	1	3156	25.64	0

Table 10
Convergence results for the MMA reactor for different planning periods.

	4 weeks	5 weeks	6 weeks	7 weeks	8 weeks	9 weeks	10 weeks
Hybrid Multicut algorithm							
Master problem[a]							
Variables	1824 (400)[b]	2280 (500)[b]	2736 (600)[b]	3192 (700)[b]	3648 (800)[b]	4104 (900)[b]	4560 (1000)[b]
Constraints	3959	4952	5945	6938	7931	8924	9917
Objective ($\times 10^6$)	7.57	9.66	10.70	12.24	14.7	17.64	21.58
CPU time (sec)	56	72	123	100	161	128	247
Master prob.	14.2	20	54	28.8	62.5	41.3	106
Subproblem	41.8	52	68	71.2	98.5	86.7	141
Iterations	7	6	7	6	7	5	6
Multicut algorithm							
Master problem[a]							
Variables	1824 (400)[b]	2280 (500)[b]	2736 (600)[b]	3192 (700)[b]	3648 (800)[b]	4104 (900)[b]	4560 (1000)[b]
Constraints	3959	4952	5945	6938	7931	8924	9917
Objective ($\times 10^6$)	7.57	9.66	10.70	12.24	14.7	17.64	21.5
CPU time (sec)	156	199	464	289	681	613	1193
Master prob.	42.58	72.94	212.32	111	306	256	612
Subproblem	113.15	126.06	251.68	178	375	357	571
Iterations	23	21	28	17	27	19	30
Generalized Benders Decomposition from (Gutiérrez-Limón et al., 2014; Mitrai and Daoutidis, 2021)							
Master problem[a]							
Variables	865 (400)[b]	1081 (500)[b]	1297 (600)[b]	1513 (700)[b]	1729 (800)[b]	1945 (900)[b]	2161 (1000)[b]
Constraints	865	1086	1307	1507	1725	1943	2616
Objective ($\times 10^6$)	7.27	9.27	10.2	11.5	14	16.7	20.6
CPU time (sec)	908	1812	2087	5095	6800	9748	11,246
Master prob.	22	42	47	106	256	247	314
Subproblem	886	1170	2040	4989	6544	9488	10,932
Iterations	96	165	179	252	418	424	451

[a] First iteration.
[b] Binary variables.

algorithm leads to improved performance compared to the multicut algorithm (see Fig. 7). The production results obtained with the proposed approach are presented in Table 9 and the profiles of the output and manipulated variables are presented in Fig. 10. From the production results, we observe that no transitions occur between the time periods leading to a reduction in the transition cost. Product *C* is overproduced in the first period where the operating cost is lower compared to the second time period and product *D* is overproduced in the last period.

Finally, we solve the problem for different numbers of planning periods and the convergence results are presented in Table 10. In all the cases the algorithms are initialized by fixing the production sequence to $1 \rightarrow 2 \rightarrow 3 \rightarrow 4$ for all periods and the optimality gap tolerance is set to 0.1%. The economic data can be found in the Supplementary Material.

From the results we observe that for all cases the proposed algorithms solve the problem faster than GBD and the solution that is obtained is better, i.e. the value of the objective function is higher. Specifically, the multicut algorithm reduces the CPU time up to 94% (for 7 planning periods) and the hybrid multicut algorithm up to 98% (for 9 planning periods). Both algorithms provide better results since the value of the objective function is increased up to 6.4% for 7 planning periods. For all algorithms an increase in the number of planning periods leads to an increase in

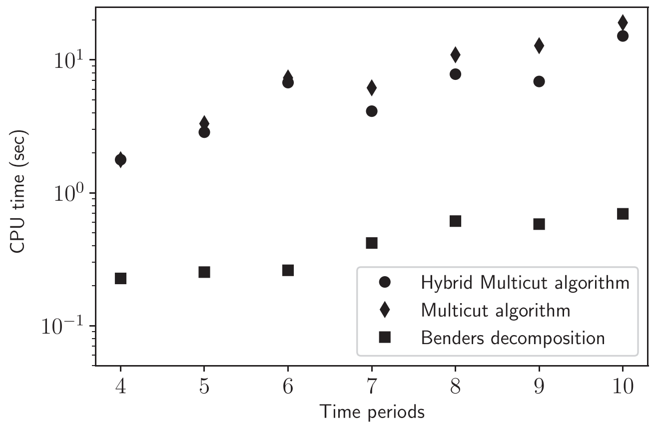

Fig. 9. Average computational time per iteration for the solution of the master problem for different planning periods.

the CPU time. For the proposed algorithms this increase is caused by the increase in the number of variables/constraints in the master problem. For example, the solution of the master problem requires 43% of the CPU time for the hybrid multicut algorithm for 6 planning periods and 53% of the CPU time for the multicut algorithm for 10 planning periods, whereas for the GBD algorithm the solution of the master problem requires (on average) 2.5% of the CPU time. However, the overall CPU time for the proposed algorithms is lower since fewer iterations are required, i.e. the master problem and subproblems are solved fewer times. Comparing the performance of the hybrid multicut and multicut algorithm, from Fig. 9 we observe that the solution time of the master problem per iteration is similar, however since the hybrid multicut algorithm requires fewer iterations the total CPU time for the solution of the problem and the solution of the master problem is lower.

We note that the dynamic optimization problems that are solved in each iteration for all algorithms are independent and can be solved in parallel. Although this will lead to a reduction in the total CPU time, it will not affect the computational performance of the hybrid multicut algorithm compared to GBD, since this parallelization will reduce the computational time for the solution of the subproblems. The solution time of the master problem will not be affected. From Table 10 we can see that for the cases considered the total solution time of the master problem in the hybrid multicut algorithm is lower than the total solution time of the master problem in the GBD algorithm. Therefore, the solution time of the hybrid multicut algorithm will still be lower than the solution time of GBD. Finally, based on these results we note that for a large number of products/planning periods the limiting step in the proposed algorithm will be the solution of the master problem. In such cases one must employ different acceleration techniques for the solution of the master problem, such as using decomposition based solution algorithms like Benders (Benders, 1962) or bilevel (Erdirik-Dogan and Grossmann, 2008; Shi et al., 2015) decomposition.

7. Conclusions

The optimal operation of process systems depends on the solution of problems that involve different time scales, the integration of which leads to large scale optimization problems. In this work, we proposed a new formulation of the integrated planning, scheduling, and dynamic optimization problem for continuous systems. In this approach, all the possible transitions are con-

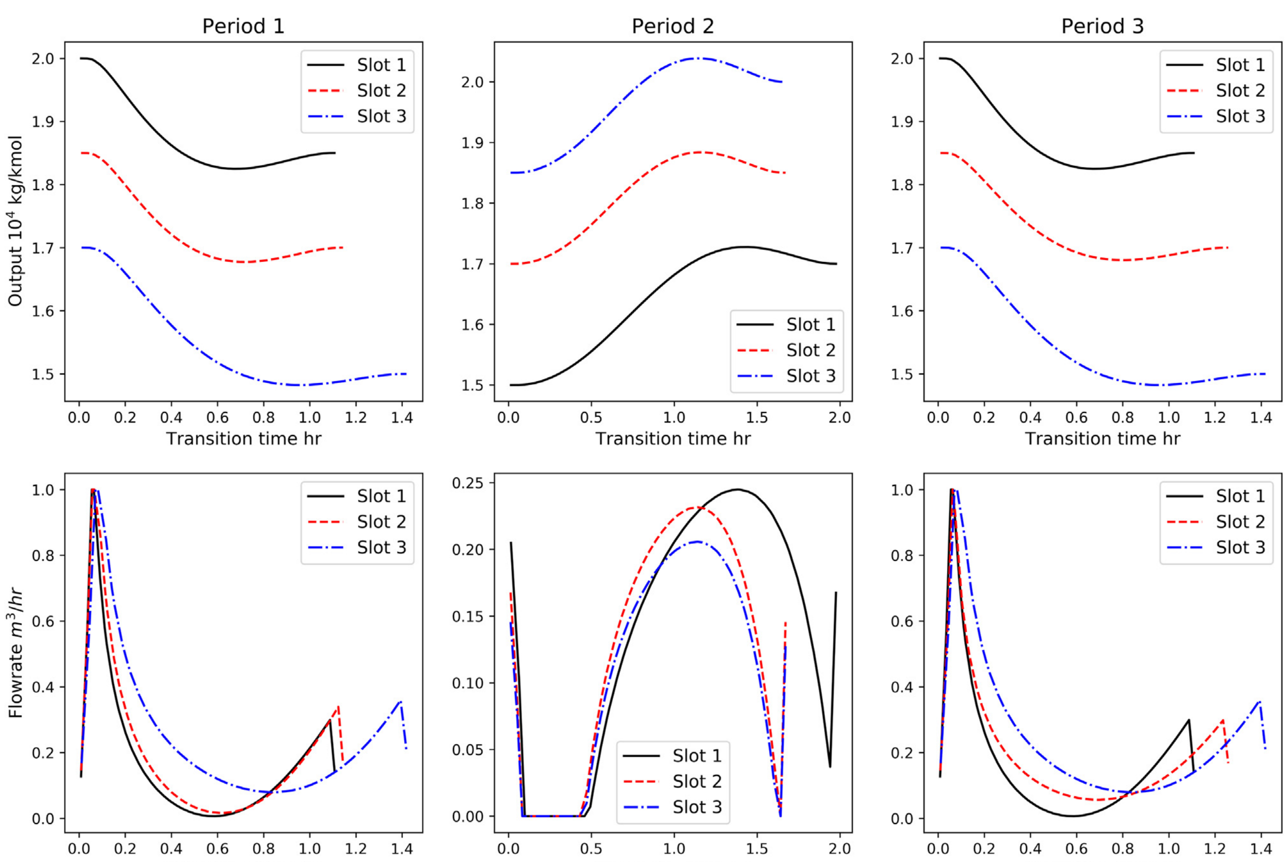

Fig. 10. Inlet flowrate and output profile for the second case study.

sidered simultaneously. Using SBM we analyzed the structure of the problem and proposed a multicut and a hybrid multicut Generalized Benders Decomposition algorithm. Through case studies we showed that the proposed problem formulation and multicut and hybrid multicut GBD algorithms can reduce the necessary CPU time and find a better solution compared to the application of GBD using other formulations. Finally, we point out some extensions of the proposed problem formulation and decomposition based solution approach in the remarks below.

Remark 4. In this work we considered the case of planning, scheduling, and dynamic optimization. The same problem formulation and solution approach can be followed in the case of the integration of scheduling and dynamic optimization for continuous systems for different problems such as cyclic/ non-cyclic schedules and single and parallel lines.

Remark 5. In the case studies considered, the production planning and scheduling problem was modelled using a slot based formulation. We can also follow a Traveling Salesman Problem formulation (Charitopoulos et al., 2017; Liu et al., 2008). In that case the time horizon is discretized into periods and in each period each transition can occur at most once. We can define ϕ_{ijp} as the value function for the dynamic optimization cost for the transition from product i to j in slot p. The value of ϕ_{ijp} will depend on the value of the transition time. Therefore, we can follow the same hybrid multicut GBD algorithm to solve the problem.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Ilias Mitrai: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Data curation, Writing – original draft, Visualization. **Prodromos Daoutidis:** Conceptualization, Methodology, Validation, Formal analysis, Investigation, Writing – review & editing, Supervision, Project administration, Funding acquisition.

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Supplementary material

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