

A BI-LEVEL FORMULATION AND SOLUTION METHOD FOR THE INTEGRATION OF PROCESS DESIGN AND SCHEDULING

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Abstract

Design and operation decisions of manufacturing plants can often be expressed within a hierarchical structure, where optimal decisions at lower operating level provide constraints for the decision making at a higher decision level. In this work, we are addressing the case of a hierarchical design and scheduling optimization problem. The integration of design and scheduling decisions can play a big role in designing economically profitable plants and improving their operational performance. This problem can be expressed as a bi-level problem, where design related decisions occur at the upper level and operational scheduling decisions at the lower level. Since discrete decisions are involved in both optimization levels, the resulting formulation typically corresponds to bi-level mixed-integer programming problems (B-MIP). The solution of B-MIP problems is very challenging, and typically requires the use of global optimization techniques, with many algorithms not able to guarantee of feasibility. To overcome the challenges in solving this class of problems we propose the use of a multi-parametric based algorithm for the solution of bi-level mixed-integer linear and quadratic programming problems, capable of providing the exact and global solution. The main idea of this approach is to treat the lower scheduling problem as a multi-parametric programming problem in which the design decisions are considered as parameters. The resulting parametric solutions can then be substituted into the upper level design problem, which can be solved as a set of single-level deterministic programming problems. Through the developed formulation and algorithm we are able to supply the decision makers with the exact solution of the integrated design and scheduling problem.

Keywords

Design and Scheduling, Multi-parametric programming, Bi-level programming.

Introduction

The integration of design and scheduling decisions can play a big role in designing economically profitable plants and improving their operational performance (Pistikopoulos and Diangelakis, 2016).

Design decisions involve the decisions that must be taken before the plant is operational and are the less likely to change while a possible change usually requires not only a considerable investment but also the permanent cease of

operation. Such decisions include the location and capacity of the production plant, the choice of raw materials and products, and the number and capacity of different units in the plant. At the operating level, scheduling decisions optimize the plant performance and involve the detailed timing of operations and sequencing for a fixed process design (Edririk-Dogan et al., 2007).

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In this work we are focusing on the integration of process design decisions and operation decisions of processing plants. The design and scheduling problem can be expressed as a hierarchical decision problem, where design related decisions occur at the upper level and operational scheduling decisions at the lower level (Lukszo and Heijnen, 2007), (Yue and You, 2015). We formulate this mixed-integer bilevel optimization problem and solve it through a multi-parametric bi-level solution algorithm to arrive to the exact global optimum of the integrated problem.

The remainder of this paper is organized as follows. Bi-level programming is introduced and the challenges in solving such problems are explained, and the solution algorithm used in this work is summarized. A generic bi-level formulation of a design and scheduling problem is then presented. Finally, a small case study is formulated and solved to illustrate the capabilities of the suggested formulation and solution algorithm.

Bi-level programming

Optimization problems that involve two decision makers at two decision levels, such as the design and scheduling problem, can be formulated as bi-level programming problem. Both the design optimization level and the scheduling level involve both continuous and integer variables. In the design level integer decisions include the decision on the choice of products and raw materials, or the number and type of processing units, while continuous decisions involve the capacity of the processing plant. In the scheduling level, integer decision can include the sequence of operations, while continuous decisions can include the detailed timing of this operations.

The general form of a mixed-integer bi-level programming problem is as follows:

$$\begin{aligned}
& \min_{x_1, y_1} F_1(x, y) \\
& \text{s. t. } G_1(x, y) \leq 0 \\
& \quad H_1(x, y) = 0 \\
& \quad x_2, y_2 \in \arg \min_{x_2, y_2} \{F_2(x, y): G_2(x, y) \leq 0, \\
& \quad \quad \quad H_2(x, y) = 0\} \\
& x \in [x_1^T \ x_2^T]^T, \ y = [y_1^T \ y_2^T]^T \\
& x \in \mathbb{R}^n, \ y \in \mathbb{Z}^m
\end{aligned} \tag{1}$$

,where x_1 is a vector of the upper level problem continuous optimization variables, y_1 is a vector of the upper level integer variables, x_2 is a vector of the lower level problem continuous optimization variables, y_2 is a vector of the lower level integer variables, x is a vector of all continuous variables and y is a vector of all integer variables.

Bi-level programming problems are very challenging to solve, even in the linear case (shown to be NP-hard by Hansen et al. (1992) and Deng (1998)). For classes of problems where the lower level problem also involves

discrete variables, such as the case of design and scheduling integration where the scheduling problem involves integer variables, the complications are further increased, typically requiring global optimization methods for their solution and often result to approximate solutions that does not guarantee feasibility.

To overcome the difficulties Avraamidou et al. (2017a) presented an algorithm for the global and exact solution of linear and quadratic bilevel mixed-integer problems. This is described in the following section.

Bi-level mixed-integer optimization through multi-parametric programming

The integration of process design and operation formulated in the previous section corresponds to a bi-level mixed-integer programming (B-MIP) problem, Eq. (1). The multi-parametric based algorithm for the solution of B-MILP and B-MIQP problems suggested by Avraamidou et al. (2017) will be used in this work for the solution of B-MIP problems. The main idea behind this approach is to treat the lower level problem (operation level) as a multi-parametric mixed-integer linear programming (mp-MILP) problem, where the upper level variables (design decisions) are considered as parameters.

This approach has been applied for the solution of an array of hierarchical process systems engineering applications, such as the integration of Planning and Scheduling (Avraamidou and Pistikopoulos 2018a), supply chain optimization (Avraamidou and Pistikopoulos, 2017b), and hierarchical model predictive control (Faisca et al. 2007) (Avraamidou and Pistikopoulos, 2017c). It has been also implemented in a MATLAB® based toolbox, the Bi-level Parametric Optimization (B-POP) toolbox (Avraamidou and Pistikopoulos, 2018b). The main steps of the algorithm for the solution of B-MIP problems with linear lower level problem are summarized in Table 1.

Table 1. Multi-Parametric based algorithm for the solution of B-MIP problems

Step 1	Establish integer and continuous variable bounds.
Step 2	Transform the B-MIP into a binary B-MIP.
Step 3	Recast the lower level problem as a mp-MILP, in which the optimization variables of the upper level problem are considered as parameters.
Step 4	Solve the resulting mp-MILP problem to obtain the optimal solution of the lower level as explicit functions of the upper level variables
Step 5	Substitute each multi-parametric solution into the upper level problem to formulate k single level MIP problems.
Step 6	Solve all k single level problems and compare their solutions to select the exact and global optimum.

Table 2. Notation

Sets and indices	
i	Time slot (1, ..., N)
k	Product (1, ..., N)
j	Stage (1, ..., M)
Upper level Variables	
n_j	Integer variable for the number of units in stage j
P_k	Production target of product k
Ca	Plant capacity
Lower level Variables	
$c_{i,j}$	Completion time of i th product in stage j
$y_{i,k}$	Binary variable to denote if product k is made at i th time slot (sequence)
$w_{i,k}$	Auxiliary variable
Constants	
$A_{j,k}$	Processing time factor of product k in stage j
d_k	Demand of product k
C_j^{InvC}	Capacity investment cost
C_j^{InvU}	Unit investment cost for stage j
C_k^{Rev}	Selling price of product k
C_k^{Oper}	Operating cost of product k
P_k^L	Lower bound on the production target of product k
P_k^U	Upper bound on the production target of product k

Bi-level formulation for the integration of Process Design and Scheduling

Bi-level formulations have been used extensively in operations research for several years. In this section, we will present a bi-level formulation for the integration of process design and scheduling, where design-related decisions occur at the upper level, and scheduling-related decisions at the lower level optimization problem. The notation used throughout the formulation can be found in Table 2.

Upper level problem – Design

A design problem generally aims at designing a profitable plant by making long term decisions. Those decisions include the location or capacity of the plant, the type of products it is producing, the pathways to produce these products, and the type and number of units needed.

Equation (2) presents a simplified objective function example of a plant design optimization problem.

$$\min_{n_j, P_k, Ca} - \sum_{k=1}^N C_k^{Rev} P_k + \sum_{k=1}^N C_k^{Oper} P_k + \sum_{j=1}^M C_j^{InvU} n_j Ca \quad (2)$$

,where the first term corresponds to the revenue gained from selling the products, the second term to corresponds to the operating costs and the final term to the investment costs required to purchase process units. Note that the objective function here is not linear as the last term (investment costs) is bilinear.

The design decisions for this example include the choice of the number of units in each processing stage, and the production target of each product.

Lower level problem – Scheduling

The scheduling problem optimizes the plant performance by determining the detailed timing of operations and sequencing so as to meet a performance criterion, for example minimizing the makespan.

The scheduling model generally involves two types of constraints, sequencing constraints that typically denote which products are produced in the different time instances, and assignment constraints that determine the completion times of the products at different stages. The formulation of the scheduling problem (3) presented here is a modification of the formulation developed in Ryu et al. (2007).

$$\begin{aligned} \min_{c_{i,j}, y_{i,j}} \quad & c_{N,M} \\ \text{s. t.} \quad & \sum_{i=1}^N y_{i,k} = 1 \quad \forall k \\ & \sum_{k=1}^N y_{i,k} = 1 \quad \forall i \\ & c_{i,1} \geq \sum_{k=1}^N y_{i,k} A_{1,k} P_k \quad \forall i \\ & c_{i,j} \geq c_{i,j-1} + \sum_{k=1}^N y_{i,k} A_{j,k} P_k \quad j > 1, \forall i \\ & c_{i,j} \geq c_{i-n_j,j} + \sum_{k=1}^N y_{i,k} A_{j,k} P_k \quad i > n_j, \forall j \end{aligned} \quad (3)$$

In this formulation, we are assuming that the processing time of each product at each stage is a linear function of the production target, P_k .

The objective function of problem 3 is to minimize $c_{N,M}$, that is the completion time of the last product in the last stage and corresponds to the makespan. The first equality constraint ensures that each product is assigned at one position in the production sequence. The second equality constraint ensures that each position in the sequence is assigned to one product. The third constraint is an inequality constraint and indicates that the completion time of the first stage for all products is greater than the processing time needed. The fourth and fifth constraints indicate that a product in a stage can only be processed if the product and the corresponding unit are available at the same time.

The last three bilinear constraints are linearized by introducing an auxiliary variable, $w_{i,k} = y_{i,k}P_k$, and are updated with the following constraint set (4).

$$\begin{aligned}
c_{i,1} &\geq \sum_{k=1}^N A_{1,k} w_{i,k} \quad \forall i \\
c_{i,j} &\geq c_{i,j-1} + \sum_{k=1}^N A_{j,k} w_{i,k} \quad j > 1, \forall i \\
c_{i,j} &\geq c_{i-n_j,j} + \sum_{k=1}^N A_{j,k} w_{i,k} \quad i > n_j, \forall j \\
P_k - P_k^U(1 - y_{i,k}) &\leq w_{i,k} \leq P_k - P_k^L(1 - y_{i,k}) \\
y_{i,k}P_k^L &\leq w_{i,k} \leq y_{i,k}P_k^U \\
P_k^L &\leq P_k \leq P_k^U
\end{aligned} \tag{4}$$

The third constraint in the set is only active for $i > n_j$. Since n_j is considered an optimization variable, a reformulation is needed. Big-M constraints are formulated to activate and deactivate this constraint for different values of i and n_j . The integer variable n_j is transformed into a set of binary variables, m_j^α , using the procedure described in Floudas (1995) (Section 6.2.1 - Remark 1) to allow for the formation of Big-M constraints.

One can observe that the design optimization variables, n_j and P_k , appear in the constraints of the scheduling problem. This indicates that solving the two problems separately can result in a sub-optimal or even infeasible solution. Therefore, a bi-level formulation and a global solution algorithm for bi-level problems will be able to supply the decision makers with the optimal solution of the design and scheduling problem. The final problem formulation corresponds to a bi-level mixed-integer linear programming problem.

Illustrative Case Study

Based on the proposed formulation and algorithm, a small case study is solved for illustration purposes. The case study considers the design and scheduling integration of processes that consists of two stages (a reaction stage and a separation stage, Figure 1) for the production of three products (A, B, and C). At the design phase the number of units for each stage is decided along with the capacity or production target of the processing plant. At the operating stage scheduling decisions are made, that include the sequence of the production of the three products and the start and finish times of each production stage for each product. The constants used for this case study are presented in Table 3, Table 4 and Table 5.

The maximum number of units for both of the production stages is set to three (Figure 1) as the number of products being produced is three. Furthermore, bounds are set for the maximum and minimum production capacity of

the three products and this are set to 20 and 10 tons respectively.

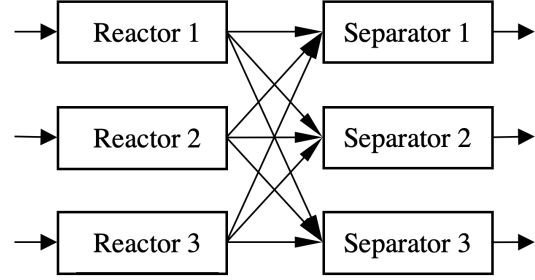


Figure 1. A schematic representation of the process configuration of the illustrative example

Table 3. Processing time data

Product, k	Processing time factor, $A_{j,k}$ (h/Ton)	
	Stage 1 ($j=1$)	Stage 2 ($j=2$)
A	0.1	0.3
B	0.07	0.2
C	0.1	0.25

Table 4. Operating cost and Demand data

Product, k	Operating Cost, C_k^{oper} (\$/Ton)	Demand, d_k (Ton)	Selling Price (\$/Ton)
A	30	20	600
B	33	19	720
C	27	17	880

Table 5. Unit investment cost data

Stage, j	Cost, C_j^{InvU} (\$/Ton)
Reactor, $j=1$	300
Separator, $j=2$	600

Solution method

Following the algorithm presented Table 1, the first and second steps are skipped as the problem is already a binary B-MILP.

For the third step, the lower level scheduling problem, Eq. (3) and Eq. (4) is solved as a multi-parametric problem where the design decisions, number of units (n_j),

production target of each product (P_k) and production capacity (Ca), are considered as parameters.

The solution of the multi-parametric problem resulted into the complete profile of optimal solutions of the lower scheduling level problem as explicit functions of the variables of the higher design level problem, with corresponding boundary conditions for different regions in the parametric space (critical regions, CR). The solution consists of 25 critical regions and a fraction of them is given in Table 6 and illustrated through a 3-D plot (P_A vs P_B vs P_C) of the parametric space in Figure 2, by fixing the number of units (n_j) to $n_1 = 1$ and $n_2 = 3$ (one reactor and 3 separators).

Table 5. Partial solution of the lower level scheduling problem

CR	Definition of the CR	Lower level variables
C1		$c_{1,1} = 0.07P_A$
		$c_{1,2} = 0.27P_B$
	$0.359P_A + 0.252P_B - 0.899P_C \leq 0$	$c_{2,1} = 0.1P_A + 0.07P_B$
	$-0.926P_A + 0.216P_B - 0.309P_C \leq 0$	$c_{2,2} = 0.4P_A + 0.07P_B$
	$-0.408P_A + 0.816P_B - 0.408P_C \leq 0$	$c_{3,1}$
	$10 \leq P_A \leq 20$	$= 0.1P_A + 0.07P_B + 0.1P_C$
	$P_B \geq 10$	$c_{3,2}$
	$10 \leq P_C \leq 20$	$= 0.1P_A + 0.07P_B + 0.35P_C$
	$n_1 = 1, n_2 = 3$	$y_{1,A} = 0, y_{1,B} = 1$
		$y_{1,C} = 0, y_{2,A} = 1$
C2		$y_{2,B} = 0, y_{2,C} = 0$
		$y_{3,A} = 0, y_{3,B} = 0$
		$y_{3,C} = 1$
		$c_{1,1} = 0.07P_A$
		$c_{1,2} = 0.27P_B$
	$0.359P_A + 0.252P_B - 0.899P_C \leq 0$	$c_{2,1} = 0.1P_A + 0.07P_B$
	$-0.926P_A + 0.216P_B - 0.309P_C \leq 0$	$c_{2,2} = 0.4P_A + 0.07P_B$
	$0.408P_A - 0.816P_B + 0.408P_C \leq 0$	$c_{3,1}$
	$10 \leq P_A \leq 20$	$= 0.1P_A + 0.07P_B + 0.1P_C$
	$P_B \leq 20$	$c_{3,2} = 0.27P_B + 0.25P_C$
	$10 \leq P_C \leq 20$	$y_{1,A} = 0, y_{1,B} = 1$
	$n_1 = 1, n_2 = 3$	$y_{1,C} = 0, y_{2,A} = 1$
		$y_{2,B} = 0, y_{2,C} = 0$
		$y_{3,A} = 0, y_{3,B} = 0$
		$y_{3,C} = 1$

In step 5, the computed solutions (Table 5) are then substituted into the upper design level problem to formulate new single-level deterministic mixed-integer bilinear programming problems. More specifically, the expressions for the optimization variables of the lower scheduling level, $c_{i,j}$ and $y_{i,j}$, are substituted in the upper design level in terms of the design optimization variables, n_j and P_k , and

the definition of critical regions is added in the upper level as a new set of constraints.

For Step 6, the resulting single level MIP problems are solved using CPLEX algorithm. The solution of a fraction of the single level problems created is presented Table 6.

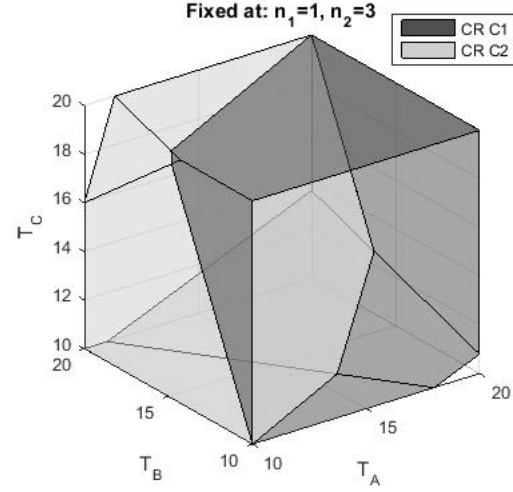


Figure 2. 3-D plot of the parametric space for fixed number of units

As a final step, the solutions of all the single level problems are compared. The solution with the minimum objective function value corresponds to the global minimum of the original bi-level programming problem. For this case the optimum lies in CR A1 and CR A2, that result to the same upper and lower objective functions but have different sequence for the production of the three products. The upper level objective is -\$21284 and the lower level objective is 15.08 hr. The optimal design variables are $P_A = 19$, $P_B = 19$, $P_C = 17$, $Ca = 19$, $n_1 = 1$, $n_2 = 1$. The optimal sequence of production is either B-A-C or B-C-A.

It is worth noting here that optimistic, pessimistic and degenerate solutions can be found using the proposed methodology, supplying the decision maker with all optimal solutions.

Conclusions

In this work we were able to formulate and solve a Design and Scheduling integration problem as a bi-level mixed integer programming problem. Through the proposed algorithm we were able to get the global solution of the bi-level problem that considered both design and operational decisions.

Table 6. Single level solutions of a fraction of the CRs created in Step 4.

CR	Upper level Objective Function	Lower level Objective Function	Production Sequence	Fraction of the Variables
A1	-21248	15.080	B-A-C	$n_1 = 1,$ $n_2 = 1,$ $P_A = 19,$ $P_B = 19,$ $P_C = 17$
A2	-21284	15.080	B-C-A	$n_1 = 1,$ $n_2 = 1,$ $P_A = 19,$ $P_B = 19,$ $P_C = 17$
B1	-10370	8.840	B-A-C	$n_1 = 1,$ $n_2 = 2,$ $P_A = 17,$ $P_B = 17,$ $P_C = 17$
B2	-10370	9.350	C-A-B	$n_1 = 1,$ $n_2 = 2,$ $P_A = 17,$ $P_B = 17,$ $P_C = 17$
...				
C1	-170	9.350	C-A-B	$n_1 = 1,$ $n_2 = 3,$ $P_A = 17,$ $P_B = 17,$ $P_C = 17$
C2	-170	8.840	B-A-C	$n_1 = 1,$ $n_2 = 3,$ $P_A = 17,$ $P_B = 17,$ $P_C = 17$
...				

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