Bilevel optimization of mixed-integer nonlinear integrated planning and scheduling problems using the DOMINO framework

Hasan Nikkhah,a,b Vassilis M. Charitopoulos,c Styliani Avraamidou,d Burcu Beykala,b

aDepartment of Chemical & Biomolecular Engineering, University of Connecticut, Storrs, CT, 06260, USA

bCenter for Clean Energy Engineering, University of Connecticut, Storrs, CT, 06269, USA

cDepartment of Chemical Engineering, Sargent Centre for Process Systems Engineering, University College London, Torrington Place, London WC1E 7JE, UK

dDepartment of Chemical & Biological Engineering, University of Wisconsin-Madison, Madison WI, 53706, USA

beykal@uconn.edu

Abstract

We study the solution of integrated planning and scheduling problems that are formulated as bilevel programming problems with mixed-integer nonlinear lower levels using data-driven optimization algorithms. Due to their inherent interdependence, multi-scale nature, and volatile market conditions, decision-making in such multi-level supply chain networks poses challenging task. Traditionally, these problems are addressed sequentially but, this approach often results in production schedules that are not feasible. Motivated by this, we formulate enterprise-wide decision-making problems with linear production planning and mixed-integer nonlinear scheduling level as a bilevel optimization problem. We solve the resulting integrated problem using the DOMINO framework which is a data-driven optimization strategy to handle general constrained bilevel optimization problems. We demonstrate our approach on case studies with varying complexities from crude oil scheduling using a continuous-time formulation to scheduling of continuous manufacturing processes using a traveling salesman problem formulation. The results show that DOMINO can address bilevel programming problems with high-dimensional mixed-integer nonlinear lower levels and can be applied to complex integrated enterprise-wide optimization problems, regardless of the lower-level formulation type.

**Keywords**: Data-driven optimization, mixed-integer nonlinear programming, bilevel programming, enterprise-wide optimization, production planning, scheduling.

* 1. Introduction

Production planning and scheduling are distinct decision-making levels within enterprise-wide optimization that operate over different timescales; nevertheless, they are intricately interconnected (Harjunkoski et al., 2014). This is because the targets set by the planning problem directly influence the scheduling decisions on the production level. While the planning functionality evaluates the market demand and establishes production goals accordingly, production scheduling determines the sequencing and allocation of tasks to specific production units based on the planning targets. In process industries, a prevalent approach to solving such integrated planning and scheduling problems involves a sequential tactic. This strategy entails solving the higher-level and longer-term planning problems first to establish the production targets for meeting the demands, followed by solving the shorter timescale scheduling problem to fulfill these targets. However, a significant drawback of this approach is that the decisions are taken without the accounting for the interdependence of the two problems, leading to over-optimistic decisions that may be realized in practice (Grossmann, 2005). This means that the planning decisions may result in schedules that cannot be feasibly executed within the capacity of the production units (Li and Ierapetritou, 2010). This challenge can be addressed by considering planning and scheduling problems simultaneously (Maravelias and Sung, 2009; Charitopoulos et al., 2018).

This intrinsic connection between planning and scheduling levels can be mathematically expressed using bilevel programming (Eq.1). Nevertheless, NP-hardness, nonconvexity, and discontinuity in bilevel programs lead to significant algorithmic challenges that are yet to be addressed (Beykal et al., 2021). One prevalent approach involves transforming bilevel formulations into a single-level formulation and subsequently treating it as a conventional optimization problem. As the optimality of the lower-level problem is a constraint on the upper problem, Karush-Kuhn-Tucker (KKT) optimality conditions can be used for the reformulation of general bilevel programs. Nonetheless, scheduling formulations at the lower-level problem that include mixed-integer variables prevent the use of KKT-based reformulation.

|  |  |
| --- | --- |
|  | (1) |

We have previously shown that such challenges can be resolved using data-driven optimization with the DOMINO framework and achieve near-optimal solutions for general constrained bilevel optimization problems with continuous linear, continuous nonlinear, mixed-integer linear, and integer nonlinear lower levels (Beykal et al., 2020; Beykal et al., 2021; Beykal et al., 2022). Expanding on our previous results, in this work, we study integrated planning and scheduling problems with mixed-integer nonlinear (MINLP) lower levels and investigate the effects of two different scheduling formulations, continuous-time and traveling salesman problem (TSP) on the overall bilevel optimization performance.

* 1. Methods
     1. Planning and Scheduling Formulations
        1. Scheduling of Crude Oil Refinery Operations (Continuous-time Formulation)

We use the crude oil unloading system formulation presented in Jia et al. (2003) which comprises several components, including marine vessels utilized for transporting crude oil, storage tanks, charging tanks to blend the crude oil, and crude oil distillation units (CDUs) where hydrocarbons are separated into downstream feedstocks (Fig. 1). When the marine vessels arrive at the refinery docks, the crude oil is unloaded from the vessels and transferred to the storage tanks. The crude oil in the storage tanks is then transferred to the charging tanks to produce the oil blend that is required by the crude oil distillation units. The objective of this scheduling problem is to minimize the total operating cost subject to capacity, flowrate, allocation, sequence, duration, and time horizon constraints, as well as the nonlinear component balance, and demand for oil blends from charging tanks which define the bilevel feasibility. This makes the lower-level scheduling an MINLP with 56 binary variables, 367 continuous variables, and 1112 constraints considering 4 event points. Detailed model equations and parameters can be provided upon request.

Figure 1. Superstructure of the oil flow network in the crude oil case study.

2.2.2. Scheduling of a Multiproduct CSTR Process (TSP-based Formulation)

In this example, we study the continuous methyl methacrylate polymerization process from Charitopoulos et al. (2017), where six different grades of polymers are produced via free-radical polymerization in an isothermal CSTR. The reactor is fed with the monomer, toluene (solvent), and azo-bis-isobutyronitrile (initiator) to carry out the polymerization reaction as shown in Fig. 2. The goal of the scheduling problem is to determine the optimal sequence of grade transitions among these six polymers that minimize the production cost (i.e., total operational, raw material consumption cost during transition periods, and raw material cost) subject to allocation, sequencing, symmetry breaking, timing, and production constraints to satisfy the demand from the planning level (i.e., bilevel feasibility). Different than Eq. (1), in the bilevel integrated planning and scheduling formulation of this problem, the planning (leader) objective is taken as the maximization of the planning profit. The lower-level problem is an MINLP with 174 binary variables, 313 continuous variables, and 390 constraints. Detailed model equations and parameters can be found in Charitopoulos et al. (2017; 2018) .

Figure 2. Multiproduct CSTR for scheduling different polymer grade production.

2.2.3. The Planning Problem

The planning level of the crude oil operations case study minimizes the total inventory and scheduling operating cost over the entire time horizon *T* as shown by eq. (2).

|  |  |
| --- | --- |
|  | (2) |

We assume that there is no backlog cost, but if negative inventories are encountered at any *t* period, the respective product inventory across the entire planning period is penalized by adding the minimum missing inventory to make it positive. The planning level is also subject to production target constraints retrieved from the scheduling level to ensure the products are being produced, and demand constraints where the production target *P* and the starting day inventory *I*t-1 should meet the product (*s*) demand *D* (Eq. 3).

|  |  |
| --- | --- |
|  | (3) |

Finally, the relative optimality gap of the scheduling level is imposed as a constraint on the planning level, where we used a tight relative optimality gap of 1E-6. For the multiproduct CSTR case study, we use the same inventory penalization approach, demand constraint, and lower-level optimality constraints. However, the objective function considers total planning profit instead of the planning cost.

* + 1. Solution Strategy – The DOMINO Framework

We use the DOMINO framework (Beykal et al., 2020) to solve the resulting bilevel LP-MINLP integrated planning and scheduling model. This algorithm uses a data-driven optimization subroutine to sample the upper-level decision variables and solve the lower-level problems to global optimality at these sampling points using a deterministic global optimization solver. In this work, we use the DOMINO framework with the NOMAD algorithm that uses a progressive barrier constraint handling approach. To start the algorithm, a random initial point for the production targets for products is provided within the bounds of the decision variables. Then, scheduling problems are solved to global optimality for this point to retrieve the objective function value of the planning and the violations for the inventory, demand, production target, and optimality gap constraints. This information is then used by NOMAD to proceed with its algorithmic iterations of search and poll until it converges to a solution. We execute this algorithm 10 times for each case study, starting with a different random initial point. In the crude oil case study, we have three products that we assume the randomly generated demand for 7 days is known with an initial starting inventory of 10 units. We also assume the planning level is cyclical in nature, with the production target for the last day needing to fulfill the demand for that day and generate the inventory for the first day of the subsequent planning cycle. The planning problem has 18 decision variables, which DOMINO-NOMAD will determine and are subject to 43 grey-box constraints (i.e., scheduling constraints that involve planning variables, demand, and optimality gap constraints). For the multiproduct CSTR case study, we have 6 products with known demand for two weeks with an initial inventory of 10 units for each product. Therefore, this problem's data-driven complexity is 12 decision variables and 37 grey-box constraints. Both scheduling case studies are modeled in GAMS and solved with BARON (Sahinidis, 1996) at the lower level.

* 1. Results

The results with the best objective function value over the 10 random runs are presented in Figures 3 and 4 for the crude oil and the multiproduct CSTR studies, respectively. Figure 3 shows that, across the 7-day planning period, the demand for oil blends is met with the optimized production targets, and the production is satisfied with globally optimal schedules. We observe that the solution has a much higher production target on the first day for the oil blend 1, which is reserved as inventory to meet the higher demand on Day 2 of crude oil operations. For oil blend 2, we see that the demand is met by daily production, and the inventory levels are minimal throughout the planning horizon. This is because the storage and charging tank capacity in the crude oil blending system is high enough to process the required blends for the CDUs. Only for the last planning period do we see that the system produces more oil blends than demand. This is to ensure the planning is carried out in a cyclic fashion where the first-day inventory of the following planning week is produced on the last day of the previous planning period. Although not shown here, the oil blend 3 profiles show similar trends where demand is met, and scheduling levels are guaranteed globally optimal. These results indicate that DOMINO can solve highly complex enterprise-wide optimization problems with a bilevel feasibility guarantee subject to more than 1000 scheduling constraints.

A graph of a diagram

Description automatically generated with medium confidence

Figure 3. Demand, production, and inventory profiles for: (a) Oil blend 1 (b) Oil blend 2. Computational time to reach solution is 144 h (maximum wall time).



Figure 4. Demand, production, and inventory profiles for: (a) Polymer grade 1; (b) Polymer grade 2; Polymer grade 3; and Polymer grade 4. Computational time to reach solution is 44.13 h.

Likewise in Figure 4, we observe that the demands for different polymer grades are satisfied for the 2-week planning horizon with guaranteed optimal production schedules. Different than the crude oil operations results, we observe that some inventory is carried over within the planning period, yet still at minimal amounts. This is expected as the optimization algorithm minimizes the cost of overproducing and carrying over excess inventory. For the other two polymer grades not shown in Figure 4, we also observe the same trends where the demand is met over the 2-week planning horizon with globally optimal production schedules. When we look at the variability in the objective function value across the 10 random runs, we observe that the standard error is 0.0002. This shows that we consistently converge to the same solution even when the data-driven optimizer

is initialized from different starting points. Overall, these two case studies demonstrate that our data-driven optimization approach is highly flexible and independent of any specific formulation, and it can address high dimensional integrated planning scheduling problems with a feasibility guarantee subject to MINLP complexity at the lower level.

* 1. Conclusions

In this study, we use the DOMINO framework and the NOMAD algorithm for solving bilevel integrated planning and scheduling problems with mixed-integer nonlinear lower levels. Two different scheduling formulations are tested at the lower-level problem with varying complexity. First, the continuous-time formulation of a crude oil blending system is analyzed. Second, a traveling salesman problem-based formulation of multiproduct CSTR is studied. The results show that DOMINO-NOMAD identifies guaranteed feasible solutions for both case studies, regardless of the scheduling formulation type. We have also shown that the algorithm can address highly complex and highly dimensional enterprise-wide optimization with scheduling problems subject to thousands of constraints. By explicitly incorporating the optimality gap at the planning level, we ensure that the bilevel feasibility is ensured by the data-driven optimizer, ultimately providing globally optimal schedules for the production level. In the future, we will investigate the performance of other data-driven optimizers and improve the efficiency of the algorithm for a computational speed-up.

**Acknowledgments**

Financial support from U.S. National Institutes of Health (NIH) grant P42 ES027704 and EPSRC grants EP/V051008/1 & EP/W003317/1 is gratefully acknowledged.

References

B. Beykal, S. Avraamidou, E.N. Pistikopoulos, 2021, Bi-level mixed-integer data-driven optimization of integrated planning and scheduling problems, Comput. Aid. Chem. Eng., 50, 1707-1713.

B. Beykal, S. Avraamidou, E.N. Pistikopoulos, 2022, Data-driven optimization of mixed-integer bi-level multi-follower integrated planning and scheduling problems under demand uncertainty. Comput. Chem. Eng., 156, 107551.

B. Beykal, S. Avraamidou, I.P.E. Pistikopoulos, M. Onel, E.N. Pistikopoulos, 2020, DOMINO: Data-driven optimization of bi-level mixed-integer nonlinear problems, J. Global Optim., 78, 1-36.

V.M. Charitopoulos, V. Dua, L.G. Papageorgiou, 2017, Traveling salesman problem-based integration of planning, scheduling, and optimal control for continuous processes, Ind. Eng. Chem. Res, 56(39), 11186-11205.

Charitopoulos, V. M., Papageorgiou, L. G., & Dua, V. (2019). Closed-loop integration of planning, scheduling and multi-parametric nonlinear control. Comput. Chem. Eng., 122, 172-192.

I.E. Grossmann, 2005, Enterprise‐wide optimization: A new frontier in process systems engineering, AIChE J., 51(7), 1846-1857.

I. Harjunkoski, C.T. Maravelias, P. Bongers, P.M. Castro, S. Engell, I.E. Grossmann, J. Hooker, C. Méndez, G. Sand, J. Wassick, 2014, Scope for industrial applications of production scheduling models and solution methods, Comput. Chem. Eng., 62, 161-193.

N. V Sahinidis, 1996, BARON: A general purpose global optimization software package, J. Global Optim, 8, 201-205.

Z. Jia, M.G. Ierapetritou, J.D. Kelly, 2003, Refinery short-term scheduling using continuous time formulation: Crude-oil operations. Ind. Eng. Chem. Res. , 42(13), 3085-3097.

Z. Li, M.G. Ierapetritou, 2010, Production planning and scheduling integration through augmented Lagrangian optimization, Comput. Chem. Eng., 34(6), 996-1006.

C.T. Maravelias, C. Sung, 2009, Integration of production planning and scheduling: Overview, challenges and opportunities, Comput. Chem. Eng., 33(12), 1919-1930.