

# On the Combinatorial Structure of Network-based Discrete-time Mixed-integer Programming Chemical Production Scheduling Models

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## Abstract

The present work includes a critical analysis of an extensive computational study of mixed-integer programming (MIP) scheduling models and a presentation of results on the combinatorial structure of discrete-time MIP models.

First, we summarize the results from an extensive computational study including more than 1,000 problem instances (Sundaramoorthy and Maravelias, 2011). We focus on medium- to large-scale problems and problems with large scheduling horizons. Using these results, we provide insights into the time partitioning in both discrete- and continuous-time formulations, as well as the relationship between formulation size and solution quality. We also comment on formulation flexibility and solution efficiency. Interestingly, our results refute some of the widely accepted beliefs in the area; e.g., discrete-time models seem to perform better than their continuous-time counterparts even in problems with variable processing times. Most importantly, we show that formulation tightness, as opposed to formulation size, is the most important characteristic. We conclude that discrete-time models have a number of advantages, suggesting that further research on the solution of these models, theoretical and algorithmic, is needed.

Second, motivated by our computational findings, we study the structure of discrete-time MIP models. We discuss how chemical manufacturing facilities can be represented as dynamic networks and then converted into time-expanded networks with side constraints (Maravelias, 2012). Based on this representation, we show that material balance constraints of the MIP models correspond to generalized flow balances in time-expanded networks. We discuss the implications of conversion coefficients in tasks with multiple inputs and outputs. We also show that assignment constraints lead to side constraints that are equivalent to clique constraints in the time-expanded task-graph of the facility. Finally, we discuss how variable batch sizes lead to fixed charge network structures. Our analysis can be useful in two ways. First, it suggests that the integration of methods for known combinatorial optimization problems or the extension of these methods is likely to lead to better solution approaches for the general chemical batch scheduling problem. Second, it provides insights into the structure of discrete-time MIP models which can be used to tune accordingly commercial MIP solvers. Based on the aforementioned insights, we outline some general solution approaches for discrete-time models.

Sundaramoorthy, A.; Maravelias, C. T. Computational Study of Scheduling Approaches for Batch Process Networks. *Industrial and Engineering Chemistry Research*, 50(9), 5023-5040, **2011**.  
Maravelias, C. T. On the Combinatorial Structure of Discrete-time MIP Formulations for Chemical Production Scheduling. *Computers and Chemical Engineering*, in press, **2012**.