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An efficient MILP framework for integrating nonlinear process dynamics and control in optimal production scheduling calculations

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ABSTRACT

The emphasis currently placed on enterprise-wide decision making and optimization has led to an increased need for methods of integrating nonlinear process dynamics and control information in scheduling calculations. The inevitable high dimensionality and nonlinearity of first-principles dynamic process models makes incorporating them in scheduling calculations challenging. In this work, we describe a general framework for deriving data-driven surrogate models of the closed-loop process dynamics. Focusing on Hammerstein–Wiener and finite step response (FSR) model forms, we show that these models can be (exactly) linearized and embedded in production scheduling calculations. The resulting scheduling problems are mixed-integer linear programs with a special structure, which we exploit in a novel and efficient solution strategy. A polymerization reactor case study is utilized to demonstrate the merits of this method. Our framework compares favorably to existing approaches that embed dynamics in scheduling calculations, showing considerable reductions in computational effort.

1. Introduction

Competitive pressure from global market forces has placed a heightened emphasis on information exchange, coordination, and integration of all decision-making layers of the chemical supply chain. Significant developments in this area, supported by advances in computer hardware, data exchange, storage, and optimization algorithms, have already led to substantial economic benefits for chemical operations (Grossmann, 2005). This coordination often extends to inclusion of power grid and power supply networks such as distributed energy systems (Diangelakis and Pistikopoulos, 2017) into the operation and control of chemical systems.

Two essential layers in the decision-making hierarchy of a chemical enterprise are production scheduling and process control. The interface between scheduling and control represents, in effect, an interaction between business-driven decisions (scheduling) with situation- and safety-driven decisions (control) (Baldea and Harjunkoski, 2014). Integrating these activities is therefore key in maximizing operational profits by meeting demand and ensuring that production targets (i.e., the setpoints transmitted to the control system) are met safely in the presence of disturbances and operational uncertainties. Integrating scheduling and control decisions has been shown to improve operations for several industrial entities, including, polymer and metal production, wastewater treatment, air separation, and energy storage systems (Engell and Harjunkoski, 2012; Touretzky and Baldea, 2014; Touretzky et al., 2016).

Integrating scheduling and control becomes particularly important when a chemical plant operates in fast-changing markets (e.g., markets with real-time electricity pricing). In order to operate more profitably under such circumstances, the plant must be able to quickly change production rates or product grades, taking advantage of excess production capacity and product storage facilities when available. This is reflected in fast and frequent changes in scheduled production targets, often over time intervals shorter than the (closed-loop) time constant of the process. As a result, the process may permanently operate in a transient mode (as opposed to being predominantly at or close to a steady state). Under these circumstances, it is crucial that the scheduling calculations account explicitly for the dynamics of the process and the performance of its control system, such that the aforementioned scheduled transitions are feasible and economically optimal (Baldea and Harjunkoski, 2014).

Any approach for integrating scheduling and control must combine the long scheduling time horizon with the frequent execution

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Sets

Sets

i	scheduling time slot
j	dynamics time slot
j'	dynamics time slot
g	product grade
k	piecewise linear breakpoints
m	Lagrangian relaxation iteration

Continuous variables

t	time
t_C	cycle time
t_i	length of scheduling time slot i
t_g^P	production time of each product
t_{gi}^P	production time of each product in slot i
p_g	amount of product g produced
t_i^{ss}	steady state production time
t_i^{trans}	transition time in each slot
t_i^e	ending time for slot i
t_i^s	starting time for slot i
e_{ij}	error
u_i	scale-bridging model input
h_i	Hammerstein block output
$\vec{x}_{ij}$	state variable
$\vec{y}_{ij}$	state-space output
w_{ij}	scale-bridging model output
$\vec{w}_{ij}$	vector of scheduling-relevant variables
$\vec{w}_{ij}^{inv}$	vector of storage-relevant variables
λ_{ijk}	special ordered sets of type 2 variable
s_{gij}	storage holdup
t_{gi}^{st}	time spent in storage by product g in slot i
$f_{st_{gij}}^{in/out}$	flow into/out of storage of product g
RIE_{ij}	reverse-integrated error
$\gamma_{i,m}$	complicating constraint violation

Integer variables

z_{gi}	binary variable defining production schedule
$b_{ij'}$	binary variable defining *RIE*
κ_{ijk}	special ordered sets of type 1 variable

Parameters and coefficients

N_I	number of scheduling time slots
T_I	maximum allotted time per scheduling slot
N_J	number of dynamics time slots
T_J	length of each dynamics time slot
τ_{dom}	dominant system time constant
t_{set}	settling time
α	timescale conversion factor
D_g	demand of product g for each i and j
P_g	production rate of product g
$Price_i$	associated operating costs for product g over time
M	large number used in big-M linearization
pw_{ijk}	value of the piecewise linear function at breakpoint k
bp_{ijk}	breakpoint k of piecewise linear function
Λ	*RIE* tolerance
Θ	Lagrangian relaxation (LR) termination tolerance
$LD_{i,m}$	Lagrange multiplier
$\Gamma_{i,m}$	positive parameter for Lagrangian multiplier calculation
S_j	finite step response (FSR) model parameter

of the control system, thus accounting for both (longer term) economic performance and (short term, real-time) safety and stability requirements. The multiple time-scale nature of this problem results in stiff models that are computationally intensive (Baldea and Harjunkoski, 2014). Furthermore, first-principles dynamic process models are almost invariably nonlinear and high-dimensional (Wang and Shan, 2007). Together, these features represent a considerable challenge to the effective integration of scheduling and control, including solving the resulting problems in a practical amount of time.

Motivated by the above, in this work, we propose a novel computationally-efficient scheduling formulation which integrates scheduling and process dynamics/control information.

The key contributions of this paper are:

- a general framework for developing *(exact) linearizations* of low-order, data-driven representations of the closed-loop process dynamics (introduced in our previous work by Pattison et al., 2016), based on commonly-employed model classes, such as Hammerstein–Wiener (HW) and finite step response/finite impulse response (FSR/FIR) models.
- a production scheduling formulation for continuous processes, incorporating these models. Importantly, this scheduling problem is formulated as a mixed-integer linear program (MILP), and can be solved using powerful solvers currently available.
- a Lagrangian relaxation (LR) scheme for increased computational efficiency in solving the aforementioned scheduling problem.

A polymerization case study is included to demonstrate the proposed approach.

The article is organized as follows: we begin with a review of the relevant literature concerning the integration of production scheduling and process control. The next section contains an overview of scheduling techniques and a presentation of the model classes (HW and FSR) considered. This review is followed by methods for linearization of the selected models. From here, the model dimensions are reduced using their unique structural properties, and the MILP scheduling problem is given with a computationally-efficient LR strategy. Following the theoretical content, a case study is presented on optimal scheduling in a polymerization reactor.

2. Literature review

When presented with the need to account for process dynamics, conventional scheduling problem formulations typically circumvent computational efficiency issues by capturing dynamic information in terms of estimated transition times between products in a set product wheel, and/or constraints concerning the maximum rate of change for, e.g., production rate transitions (Zhang and Grossmann, 2016; Maravelias, 2012). However, these techniques inherently assume the process reaches steady-state prior to set-point changes, and that it operates (mostly) at steady state. These premises are no longer valid when set-point changes occur at frequencies comparable to or higher than the dominant time constant in the process, and may therefore result in dynamically infeasible transition sequences (Pattison et al., 2016; Chu and You, 2012). Further, transition time estimates and transition rate constraints are often chosen to be very conservative (to account for safety and equipment limitations), typically resulting in a suboptimal solution. An evolution of these basic concepts consists of separating a production time slot into two sub-intervals, transition from the previous slot and steady-state operation, estimating transition dynamics or calculating them offline by enumerating all possible pairwise switches (transitions) (Nyström et al., 2005; Tong et al., 2015). While this is relatively manageable for systems with