Computers and Chemical Engineering 113 (2018) 139–151

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

A simulation-based optimization framework for integrating scheduling and model predictive control, and its application to air separation units

Lisia S. Dias[a], Richard C. Pattison[b], Calvin Tsay[b], Michael Baldea[b,c,*], Marianthi G. Ierapetritou[a,*]

[a] Department of Chemical and Biochemical Engineering, Rutgers University, 98 Brett Road, Piscataway, NJ 08854, United States
[b] McKetta Department of Chemical Engineering, The University of Texas at Austin, 200 E. Dean Keeton St., Austin, TX 78712, United States
[c] Institute for Computational Engineering and Sciences, The University of Texas at Austin, 201 E. 24th St., Austin, TX 78712, United States

ARTICLE INFO

Article history:
Received 31 May 2017
Revised 7 March 2018
Accepted 13 March 2018
Available online 14 March 2018

Keywords:
Scheduling of production
Process control
Integrated scheduling and control
Model predictive control
Air separation units

ABSTRACT

The integration of dynamic process models in scheduling calculations has recently received significant attention as a mean to improve operational performance in increasingly dynamic markets. In this work, we propose a novel framework for the integration of scheduling and model predictive control (MPC), which is applicable to industrial size problems involving fast changing market conditions. The framework consists on identifying scheduling-relevant process variables, building low-order dynamic models to capture their evolution, and integrating scheduling and MPC by, (i) solving a simulation-optimization problem to define the optimal schedule and, (ii) tracking the schedule in closed-loop using the MPC controller. The efficacy of the framework is demonstrated via a case study that considers an air separation unit operating under real-time electricity pricing. The study shows that significant cost reductions can be achieved with reasonable computational times.

1. Introduction

Globalization and extensive information exchange supported by new technologies have given rise to an environment with fast changing market conditions, which must be taken into account in order to achieve optimal process operation. In the process systems engineering community, the search for the optimal operation has been translated to optimizing the decision-making processes across the entire enterprise. The decision-making processes can be analyzed in a hierarchical structure as presented in Fig. 1 (considering a process with product inventory). Traditionally, decisions made in upper levels of this hierarchy are communicated to lower levels, and each decision-making problem is (optimally) solved separately and independently. However, (overall) sub-optimal and infeasible solutions can be avoided by proper integration of different levels of the hierarchy (Baldea and Harjunkoski, 2014). In this work, we focus on strategies for the integration of scheduling and control problems.

The benefits that such integration can bring are intuitive, given that the dynamics of a process governed by a particular control strategy can significantly affect the behavior of scheduling relevant-variables, influencing, e.g., the time required for transitions between production setpoints and the associated operational costs. Initial efforts in the area followed the intuitive route of including the dynamic model of the process as an additional set of constraints in the scheduling problem. The result is a mixed-integer dynamic optimization problem (MIDO), and its solution provides the optimal production sequence and optimal control moves required to implement the schedule. The MIDO problem is typically discretized, resulting in a Mixed Integer Nonlinear Program (MINLP) using, for example, collocation or implicit Runge Kutta methods. This approach was proposed by Flores-Tlacuahuac and Grossmann (2006), and it was extended by Terrazas-Moreno et al. (2007) and Zhuge and Ierapetritou (2012). Alternatively, Nyström et al. (2005) proposed a decoupled modeling approach which consisted in formulating the scheduling problem (master problem) as a Mixed Integer Linear Programming (MILP) and the control problem (primal problem) as Dynamic Optimization. The problem is solved through iterations between the master and primal problems. This approach was later extended to a multiple parallel lines application by Nyström et al. (2006). These

* Corresponding authors.
E-mail addresses: mbaldea@che.utexas.edu (M. Baldea), marianth@soemail.rutgers.edu, marianth@soe.rutgers (M.G. Ierapetritou).

https://doi.org/10.1016/j.compchemeng.2018.03.009

Nomenclature

Indices

i	Time intervals for the simulation problem
n	Time slot of the scheduling problem
k	Sample number of the MPC problem

Sets

I	Set of time intervals
N_n	Set of scheduling slots
W	Set of scheduling relevant variables

Variables

α	Split fraction
F_p^i	Product flow rate at sample period i
$F_p^{sp,n}$	Product flow rate setpoint at sample period n
F_{feed}^i	Feed air flow rate at sample period i
$F_{inv,in}^i$	Inlet flow rate to the inventory at sample period i
k_{PHX}	Split fraction in the PHX
I_p	Product purity (modeled in term of impurity concentration)
L_{drain}	Liquid drain rate in the reboiler
M_{inv}^i	Inventory holdup at sample period i
M_{reb}	Liquid level in the reboiler
R_{col}	Fraction of vapor product sent to the condenser
$\Delta T_{reboiler}$	Temperature driving force in the reboiler
u_p	Manipulated variables
u_p^{sp}	Setpoint for manipulated variables
x_p	Differential states
y_p	Outputs
y_p^{sp}	Setpoint for output variables

Parameters

$F_p^{sp,initial}$	Initial product flow rate setpoint
$F_{p,min}^{sp}$	Lower bound for the product flow rate setpoint
$F_{p,max}^{sp}$	Upper bound for the product flow rate setpoint
$\bar{F}^i$	Demand rate at sample period i
M_{inv}^0	Initial inventory holdup
M_{inv}^{min}	Minimum inventory holdup
M_{inv}^{max}	Maximum inventory holdup
N	Prediction horizon for MPC
p^i	Electricity price at sample period i
P_f	Terminal penalty matrix
Q	Output penalty matrix
R	Input penalty matrix
s	Limiting factor for changes in setpoint
τ	Scheduling time slot duration
t_{end}^n	End time for scheduling time slot n
t_{start}^n	Start time for scheduling time slot n
T_s	Sample time for the MPC problem
T_m	Scheduling horizon
u_{min}	Lower bound for manipulated variables
u_{max}	Upper bound for manipulated variables
y_{min}	Lower bound for output variables
y_{max}	Upper bound for output variables

approaches, however, face considerable computational challenges associated with the use of high-fidelity representations of the process dynamics and the complexity, nonlinearities and discontinuities that this brings to the scheduling problem. In view of these difficulties, You and coworkers proposed a series of strategies to improve the computational efficiency when solving the integrated scheduling and control problem (Chu and You, 2013a, 2013b).

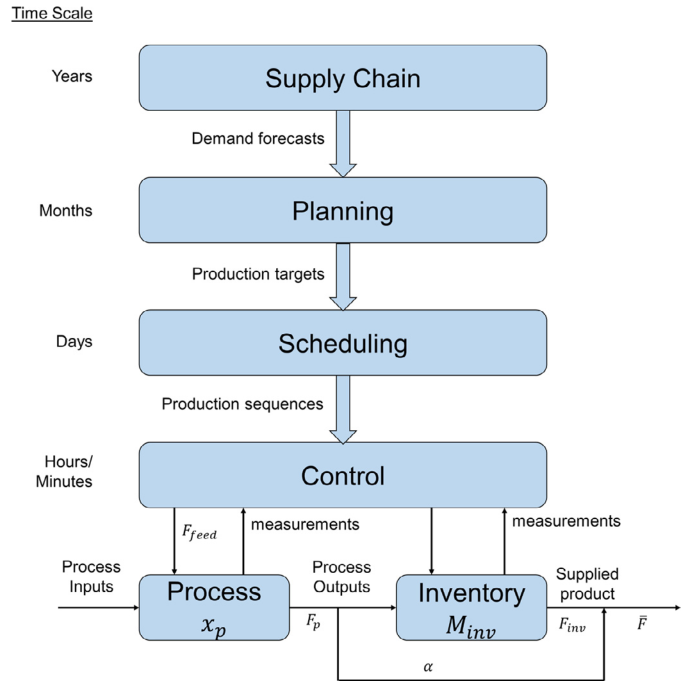

Fig. 1. The decision-making hierarchy in an enterprise with product inventory.

It is important to notice that, in general, issues related to the stability and safety of the dynamic process (a problem extensively studied in the control literature) have not been accounted for in integrated frameworks. This can be verified by analyzing the integrated models proposed in the literature; the majority of the respective works only consider the dynamics of the process for the transition periods. In general, a constraint establishing that the state and control variables should achieve their steady state values at the end of the transition period is imposed, and an implicit assumption that the system remains at the steady state values from that point forward is made. Such manipulation reduces the complexity of the integrated model and allows the schedule to be optimized without previous knowledge of the transition times, which should otherwise be obtained in an iterative procedure. However, it is clear from a control perspective that achieving such steady state values does not guarantee that the system remains stable, especially when considering open-loop unstable steady states. Finally, most of the existing integrated frameworks assume there is no model mismatch between the dynamic model and the process, and the control actions are usually computed offline. Such assumption is typically violated in practice, and can cause instability and safety constraint violations when implementing the integrated scheduling and control solutions.

Motivated by these issues, Zhuge and Ierapetritou (2014) proposed to integrate scheduling and model predictive control (MPC) by including explicit control laws in the scheduling problem, where control laws were derived using multi-parametric programming techniques. MPC would then address the control objective of guaranteeing stability, robustness, safety and fast tracking, while the integrated scheduling model accounted for economic objectives. Furthermore, Zhuge and Ierapetritou (2015) proposed an integrated framework that consisted of the use of two control loops for the online integration of scheduling and control. An integrated problem at the outer loop generated the production schedule and the state references for the inner loop. The inner loop tracked state references using fast model predictive control, and the exact control solution was computed online. Recently, Du et al. (2015) noticed that the use of the detailed dynamic models of the process