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A dynamic optimization framework for integration of design, control and scheduling of multi-product chemical processes under disturbance and uncertainty

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ABSTRACT

A novel dynamic optimization framework is presented for integration of design, control, and scheduling for multi-product processes in the presence of disturbances and parameter uncertainty. This framework proposes an iterative algorithm that decomposes the overall problem into flexibility and feasibility analyses. The flexibility problem is solved under a critical (worst-case) set of disturbance and uncertainty realizations, whereas the feasibility problem evaluates the dynamic feasibility of each realization, and updates the critical set accordingly. The algorithm terminates when a robust solution is found, which is feasible under all identified scenarios. To account for the importance of grade transitions in multi-product processes, the proposed framework integrates scheduling into the dynamic model by the use of flexible finite elements. This framework is applied to a multi-product continuous stirred-tank reactor (CSTR) system subject to disturbance and parameter uncertainty. The proposed method is shown to return robust solutions that are of higher quality than the traditional sequential method. The results indicate that scheduling decisions are affected by design and control decisions, thus motivating the need for integration of these three aspects.

1. Introduction

Multiproduct processes are widely used in different sectors due to their versatility and convenience, e.g. oil & gas (Harjunkoski et al., 2009), pharmaceutical (Nie and Biegler, 2012), and polymer production (Harjunkoski et al., 2009; Terrazas-Moreno et al., 2008). To remain competitive, companies are required to operate their systems at nearby optimal conditions that can efficiently produce their products under environmental, safety and product specification constraints. Most major chemical companies have invested in large computing networks that are dedicated to solving large-scale process optimization problems (Seferlis and Georgiadis, 2004). Obtaining a solution for design, control, and scheduling can be quite challenging, as the problems are typically very large, and there are many aspects to a process which can impact the process economics. There are multiple approaches for obtaining solutions, each of which vary in solution quality and computational time.

The simplest approach to address optimal process design, scheduling and control for large process networks is the sequential approach, where the design, control, and scheduling of the system are all considered separately (Patil et al., 2015; Zhuge and Ierapetritou, 2012). This approach is popular in many industries (Mohideen et al., 1996) because solutions can be obtained very quickly, due to independence of the sub-problems. Although the sequential method is fast, there are many limitations. Since each sub-problem is solved independently, the interactions between design, control, and scheduling are typically neglected, even though it has been recognized that these interactions can be significant (Flores-Tlacuahuac and Grossmann, 2011; Pistikopoulos and Diangelakis, 2015; Zhuge and Ierapetritou, 2012). Furthermore, assumptions need to be made in each sub-problem, e.g. steady-state operation or adding overdesign factors, and these assumptions may be invalid or return expensive plant designs. Hence, the solution generated by the sequential approach is likely to be suboptimal, and may become dynamically infeasible in some cases leading to the specification of invalid designs and scheduling sequences (Chu and You, 2014a). These limitations have motivated the development of a more reliable and robust method of determining design, control, and scheduling.

The simultaneous approach is a more advanced method of integrated optimization. In this approach, the design, control, and scheduling are optimized simultaneously, for the purpose of

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Nomenclature

Indices

g	Index of product grades $(1, 2, \ldots, G)$
i	Index of production/transition regions in time $(1, 2, \ldots, I)$
j	Index of finite elements in time $(1, 2, \ldots, J)$
k	Index of collocation points in time $(1, 2, \ldots, K)$
ω	Index of realizations for process disturbances $(1, 2, \ldots, N)$
θ	Index of realizations for parameter uncertainty $(1, 2, \ldots, M)$
a	Index of inequality constraints
n	Iteration number of decomposition algorithm

Parameters

I	Number of regions in time
J	Number of finite elements in each region in time
K	Number of collocation points in each finite element
N	Number of realizations for process disturbances
M	Number of realizations for parameter uncertainty
$\mathcal{A}$	Matrix of orthogonal collocation weights
$\boldsymbol{f}$	Vector function of closed loop non-linear process model equations
$\boldsymbol{g}$	Vector function of inequality constraints
$\boldsymbol{h}$	Vector function of equality constraints
$\boldsymbol{\alpha}$	Infeasibility of inequality constraints $\boldsymbol{g}$ at each point in time
Φ_n	Maximum infeasibility in iteration n
$\boldsymbol{\psi}$	Function to map the production sequence to a set-point profile
$\zeta^{\theta,\omega}$	Weight or probability of occurrence for realization (θ, ω)
t	Time

Variables

Δt_i	Length of time region i
δt_i	Length of every finite element in time region i
$\boldsymbol{x}(t)$	Vector of process states at time t
$\boldsymbol{u}(t)$	Vector of process inputs at time t
$\boldsymbol{y}(t)$	Vector of process outputs at time t
$y^{\boldsymbol{sp}}(t)$	Vector of process output set-points at time t
$\boldsymbol{x}_{ijk}$	Vector of process states in region i, finite element j, and collocation point k
$\boldsymbol{x}_{ijk}^{\theta,\omega}$	Vector of process states in region i, finite element j, and collocation point k, corresponding to realization (θ, ω) of process disturbance and parameter uncertainty
$\boldsymbol{u}_{ijk}^{\theta,\omega}$	Vector of process inputs in region i, finite element j, and collocation point k, corresponding to realization (θ, ω) of process disturbance and parameter uncertainty
$\boldsymbol{y}_{ijk}^{\theta,\omega}$	Vector of process outputs in region i, finite element j, and collocation point k, corresponding to realization (θ, ω) of process disturbance and parameter uncertainty
$(\boldsymbol{y}^{sp})_{ijk}$	Vector of process output set-points in region i, finite element j, and collocation point k
z	Objective variable
$\boldsymbol{\kappa}$	Vector of design decisions
$\boldsymbol{\Lambda}$	Vector of control decisions
$\mathscr{B}$	Binary matrix for sequence scheduling
$\boldsymbol{\eta}$	Vector of process disturbances
$\boldsymbol{P}$	Vector of uncertain parameters
$\mathcal{D}$	Vector of all design, control, and scheduling decisions $\{\boldsymbol{\kappa}, \boldsymbol{\Lambda}, \mathrm{B}, \Delta\mathbf{t}\}$
$\boldsymbol{c}$	Set of critical realizations of process disturbance and parameter uncertainty
$\boldsymbol{\beta}$	List of process set-points, in order of production
$\mathbf{Y}^{\mathrm{sp}}$	List of process output set-points, unordered

considering interactions. This approach has the potential to provide attractive solutions, which are more optimal and reliable (Chu and You, 2014b; Mendez et al., 2006; Nie et al., 2015; Patil et al., 2015). While several studies have considered integration of design and control (Ricardez-Sandoval et al., 2009; Sakizlis et al., 2004; Yuan et al., 2012), integration of scheduling has not been deeply explored. In the case of multi-product plants, it can be advantageous to account for scheduling decisions at the design stage since it dictates the dynamic transitions between the different products to be produced, which in turn, depend on design and control (Bhatia and Biegler, 1996; Flores-Tlacuahuac and Grossmann, 2011; Pistikopoulos and Diangelakis, 2015). For large-scale problems, the simultaneous approach has a high computational cost due to the large number of variables involved, including the integer variables considered in the scheduling formulation. The problem can be complicated further by considering dynamic evolution of the system subject to process disturbances and uncertainty in the model parameters. Solving the simultaneous problem explicitly is challenging due to the reasons described above; therefore, decomposition algorithms that account for different aspects of the integration of design, control and/or scheduling have been proposed to arrive at economically attractive solutions (Chu and You, 2013; Heo et al., 2003; Mohideen et al., 1996; Sanchez-Sanchez and Ricardez-Sandoval, 2013; Seferlis and Georgiadis, 2004; Zhuge and Ierapetritou, 2016). Currently, there is no commercial software which is specifically designed to solve these types of problems (Pistikopoulos and Diangelakis, 2015).

Typically, the decomposition algorithm consists of two sub-problems: a flexibility analysis and a feasibility analysis (Sakizlis et al., 2004; Sanchez-Sanchez and Ricardez-Sandoval, 2013; Seferlis and Georgiadis, 2004). In the flexibility sub-problem, a solution is chosen such that total cost is minimized and all constraints are satisfied, subject to a critical set of process disturbances and parameter uncertainty. In the feasibility sub-problem, the solution from the flexibility sub-problem is tested for feasibility at all realizations of disturbance and uncertainty. If the solution is determined to be invalid (i.e. infeasible for one or more realizations), the critical set is updated, and the algorithm returns to the flexibility problem. The algorithm terminates when all realizations are feasible at the given solution.

As shown in Table 1, previous publications typically focus on either design and control, design and scheduling, or control and scheduling. Due to problem complexity, few publications address the integration of design, control, and scheduling. In one of the first studies, the design, control, and scheduling of a methyl-methacrylate process are optimized simultaneously (Terrazas-Moreno et al., 2008). The scheduling decisions include production order and transition times, which account for process dynamics. The formulation includes uncertainty, as values that are selected from a discrete set. Process disturbances were not considered. In lieu of a closed-loop control scheme, the profile of the manipulated variable was directly obtained from dynamic optimization. In another study (Patil et al., 2015), the integration was applied to multiproduct processes under disturbance and uncertainty. Decisions were made on equipment sizing, steady-state operating conditions, control tuning, production sequence, and