Integration of Design and Control for a large scale flowsheet

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Abstract

In order to design a process that operates close to tighter boundaries safely, much attention has been devoted to the integration of design and control, in which the design decisions, dynamics, and controlled performance are considered simultaneously in optimal fashion. However, rigorous methods for solving design and control simultaneously meet challenging mathematical formulations which become computationally intractable. In an earlier paper of our group, a new mathematical formulation to reduce the combinatorial complexity of integrating design and control was introduced. We showed that substantial reduction in the problem size can be achieved by embedded control for specific process designs. In this paper, we extend the embedded control to the plantwide process. This case will demonstrate the current capabilities of the methodology with integrated design and control under uncertainty.

Keywords: Integrated design and control, embedded optimization, uncertainty, dynamic feasibility

1. Introduction

Rigorous incorporation of the process dynamics is important for operational safety and efficiency. By considering dynamic controllability and operability for uncertain condition in early design stage, we can achieve better overall performance of the system than classical approaches which only consider steady state, thus dynamic constraint violations cannot be detected. Integration of process design and control pursues minimizing cost, while guaranteeing smooth process operation in spite of dynamic disturbances and process uncertainty. Integration of design and control has received attention in the scientific community for the last 30 years. And several remarkable methodologies have been developed. Excellent reviews of integrated design and control methodologies can be found elsewhere (Sakizlis et al., 2004; Seferlis & Georgiadis, 2004).

One main difficulty of integration of design and control for large-scale processes stems from the large computational time requirement which makes it impossible to apply current optimization algorithms. Recently, we proposed a new method entitled embedded control optimization (Malcolm et al., 2007).

In this paper, the embedded control optimization methodology is enhanced to incorporate moving horizon estimator for achieving better dynamic process performance compared to our earlier fixed horizon state estimation. Also a plantwide scale of process-isomerization flowsheet is solved to provide a realistic example for the capability of this methodology.

This paper is organized as follows. Section 2 briefly reviews methodology of embedded control optimization. Section 3 demonstrates the application of embedded control
optimization for integrated design and control of an isomerization process flowsheet. This paper closes with conclusions.

2. Methodology

Mathematical problem decomposition for design under uncertainty

The conceptual problem of the integration of process design and control under uncertainty is a stochastic infinite dimensional mixed integer dynamic optimization problem. To solve these integrated design and control problems requires expensive computational time, integer decisions, and non-convex equations introduced by feedback pose an extreme challenge to existing mathematical programming techniques. To overcome the intractability of the original problem, Pistikopoulos and co-workers proposed a problem decomposition algorithm as shown in Figure 1 (Mohideen et al., 1996). In this decomposition technique, the optimal design choices are solved stochastically in a discrete sampling space. Because the discrete sampling space may not contain all critical scenarios, a separate search for critical constraint violations needs to be performed. Accordingly the rigorous feasibility test explores whether the current design is feasible in the entire uncertain space. If a new critical scenario is identified, this critical situation is added to the discrete sample spaces. Thus, this decomposition technique is composed of three steps- sampling step (A), main optimization step (B) and dynamic feasibility test step (C). For this feasibility analysis, several methods can be used. (Dimitriadis & Pistikopoulos, 1995; Grossmann & Floudas, 1987; Moon et al., 2008; Swaney & Grossmann, 1985).

![Figure 1. Decomposition algorithm for integrated design and control under uncertainty. Main optimization problem (B) is separated from flexibility test. (Mohideen et al., 1996)](image)

Embedded control optimization

Even though the problem decomposition substantially reduces the problem size, it still remains a challenge due to combinatorial complexity of the NP-hard search space. Specifically, the control decisions such as the insertion of feedback loops, or pairing of manipulated and control variables cause a combinatorial explosion in the possible process design and control realizations. We therefore propose to separate the design
decisions from the control decisions. The master level fixes design decisions such as reactor dimensions, residence time, reactor length and diameter that govern dynamic process performance. No control decisions are made at this level. For a given design, we assess its dynamic process performance by solving the process dynamics problems rigorously. Moreover, the optimal control action is calculated with relatively ease way because it operates on linear state space models which are updated dynamically in each time step. In our algorithm, a Linear Quadratic Regulator (LQR) computes the best control action to minimize a cost function. We map the nonlinear dynamic process model to linear state space model using linear identification methods. This identification is executed in every step of the discretized time horizon. The required input-output data sets are obtained by sampling the dynamic system model with suitably chosen sampling intervals. The adaptive identification involves the solution of a least square fitting problem. For solving this problem, the sequential least squares method was used in previous paper (Malcolm et al., 2007). In this paper, we used a Moving Horizon Estimation (Haseltine & Rawlings, 2005). It estimates the state and parameters using a moving data window of fixed size. When new observation becomes available, new data are added to the data window and the same amount of oldest data is removed from the window. It provides a generic approach to the state and parameter estimation which can be applied both linear and nonlinear processes. Next section, we will show effectiveness of embedded control optimization by designing isomerization process flowsheet.

3. Case study-Integrated Design and Control of isomerization process flowsheet

This section will demonstrate the effectiveness of embedded control optimization for an entire flowsheet. We show the large scale case study- for integrated design and control of an isomerization process under uncertainty (Luyben et al., 1998).

Isomerization Process description

Isomerization process converts normal butane to isobutene, as shown in Eqn. (1).

$$nC_4 \rightarrow iC_4$$  

(1)

The isomerization flowsheet consists of a reactor, a heat exchanger, and two distillative separation columns as shown in Figure 2. An input feed is the mixture of $nC_4$ and $iC_4$. It also has small amount of propane ($nC_3$) and isopentane ($iC_5$). Since the input feed already has some amount of $iC_4$, it does not enter reactor directly. It enters Deisobutanizer column (DIB) and some of $iC_4$ is separated from input feed. The propane, the lightest component also comes out in the distillate stream. Because of similar volatilities of iso/normal butane, it is hard to separate. Thus, relatively higher number of tray and reflux ratio is required. The bottom stream of DIB goes into the purge column in which, most of $iC_4$ is purged to bottom stream. The upper stream of the purge column is vaporized and goes into reactor by passing the heat exchanger. In the reactor, some of normal butane is converted to isobutene in the vapor phase shown in (2).

$$R = kC_{nC_4}, \quad k = k_0 \exp\left(\frac{\lambda}{RT}\right)$$  

(2)

where $R$ is reaction rate, $k$ is temperature-dependent reaction rate constant, $k_0$ is pre-exponential factor, $\lambda$ is activation energy, $T$ is the reactor temperature in Rankin.
In the heat exchanger, heat transfer between input stream of reactor and output stream of reactor is occurred. The input feed of the reactor is heated with heat of output stream. However since this heat exchange does not heat input feed sufficiently, a furnace is used to heat input stream to the desired temperature. The effluent of reactor is fluidized in the condenser and goes into DIB. It is fed at a higher tray than the fresh feed because the concentration of \( iC_4 \) in the reactor effluent is higher than in the fresh feed.

Operational constraints and control action strategy

We set two quality constraints and one safety constraint for operating this process. These constraints are adopted from Luyben et al. (1998). For the product quality, the mole fraction of \( nC_4 (x_1) \) of final product should be less than 2%. For complete elimination of heaviest inert \( iC_5 \), the mole fraction of \( iC_5 (x_2) \) at top stream of purge column should not exceed 0.1%. For safety, the reactor pressure \( (x_3) \) should never exceed 700 psia to prevent explosion. To satisfy quality and safety constraints, we use reflux ratio \( (u_1) \) and vapor ratio of DIB column \( (u_2) \), reflux ratio of purge \( (u_3) \), and input temperature of reactor \( (u_4) \) as manipulated variables.

\[
\begin{align*}
    x_1 & \leq 0.02 \\
    x_2 & \leq 0.001 \\
    x_3 & \leq 700
\end{align*}
\]

Among these constraints, violation of (5) is unacceptable at any times under any circumstances. On the other hand, it is impossible to keep the product specifications exactly at the set point target in a real operation. Therefore, the quality constraints for bottom and product streams are soft. However, the optimal process should deviate as little as possible for this target.

Design variables

To optimize this problem we consider four main design variables - Reactor volume size \( (D_1) \), Total tray number of DIB \( (D_2) \), Total tray of purge column \( (D_3) \), Heat exchanger size \( (D_4) \). While larger values of these design variables ease the separation task, it increases the capital cost. Therefore we should consider the trade off between controllability and the capital cost.
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Uncertainty scenarios
To account for uncertainty in the process operations, several expected uncertainty scenarios are considered. We assume two dynamic scenarios: varying compositions of nC_4 and iC_4 in input feed, and the increase of the feed rate at certain time (t=1,500) by 15 percent. For time-invariant uncertainty, we wish to investigate the impact of two main uncertain parameters associated with chemical reactions. The first parameter is the pre-exponential factor, k_0, and the second is the heat energy of reaction, λ. We assume that 10% of variation exists from nominal points.

Optimal design process
To maximize the performance, while at the same time planning flexible operation, we performed the design optimization under uncertainty as follows. First we collected uncertain samples (step 1) and performed embedded control optimization (step 2). Finally we checked feasibility of design obtained from step 2 (step 3).

First attempt: As a first attempt to perform the stochastic optimization, we chose 10 samples in the uncertain space of reaction conditions and evaluated the probabilities of each parameter set to calculate expected cost. Then we rigorously determined the design and manipulated variables such that the process does not violate the constraints in desired purity limit in every realization of the reaction conditions and design variability in the dynamic performance due to uncertainty. For capital cost, we considered the reactor, the columns, and the heat exchangers. For operating cost, we considered energy consumption in the furnace, condensers, and reboilers. The master level of this problem is to maximize total profit. To solve optimal design problem, a Nelder-Mead simplex method is used in master level of our methodology, and embedded control was used to adjust control decisions. To handle the constraints, penalty function is used. We found the best optimal design after 24 iterations, (D_1=156ft^3, D_2=59, D_3=32, D_4=1,034ft^2).

Next we rigorously tested the steady and dynamic state feasibility of the design specifications obtained previous section. A fully dynamic feasibility test is very challenging, so we used following strategy. At first, we performed a steady state feasibility test. If the current design is feasible in steady state, then rigorous dynamic feasibility test follows steady state feasibility test. We used active constraint strategy for this test (Dimitriadis & Pistikopoulos, 1995; Grossmann & Floudas, 1987). In steady state feasibility test, we found the critical point (k_0=2.66e7, λ=-3,900), which disobey constraints with the design spec. This critical point is located at the vertex of the uncertain region.

Second attempt: We solved the main optimization problem again with ten uncertain parameter set and the critical point. In this time we obtained these optimal values - D_1=432ft^3, D_2=52, D_3=33, D_4=1,011ft^2. We tested feasibility tests again in both steady state and dynamic state. This time no violations were found. Thus we concluded obtained result is the best solution. We presented the simulation result of design obtained in Figure 3. It shows a tight control. x_1 and x_2 go under the set point after t=1,500, x_3 never goes higher than the set point.

4. Conclusions
This paper describes a conceptual framework for design and control integration. This paper enhanced and refined the embedded optimization approach for integrated design and control, originally suggested by our group (Malcolm et al., 2007). Our methodology recasts the problem of design and control integration into a solvable mathematical programming formulation. Moving horizon estimation is used to convert the nonlinear
dynamics into the linear state space model adaptively. With the linear process model; Linear Quadratic Regulator could easily find optimal control analytically. The case study of designing an isomerization process-described control and design integration for large scale flowsheet. We apply our novel methodology to plantwide process successfully.

Figure 3. Simulation result of final optimal design. It shows tight control of all process variables. The pressure never exceed more than 700 psia for all simulation time. The constraints $x_{C5}$ and $x_{C4}$ were stabilized under the set points after $t=1,500$(sec). These constraints are soft constraints, they are not required to be satisfied for all time period but should be satisfied from specific point of time through the end-operation time. So we set them point constraints $r=[t_1, t_2]$ and for this case, $t_1$ is 2,250 and $t_2$ is 2,500 (sec). Here, $t_1$ means the stabilized operation time after control. However, The pressure constraint should be satisfied through all simulation periods ($r=[0, t_2]$).

References