Integrating Systems Design and Control using Dynamic Flexibility Analysis

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Currently, chemical process design and process control are separate disciplines assisting process development at different stages. Design and control decisions are made separately despite the common objective of dissipating the impact of uncertainty to ensure robust plant operation. Experience suggests that designing processes for flexibility against disturbances or parameter variations without considering dynamics under actual control feedback does not guarantee robust performance. Thus, it appears advantageous to address process design and control decisions simultaneously for maximizing performance in face of operational and model uncertainty. Realistic high-performance processes should be optimal in their dynamic operation with realizable control. The lack of integration between design and control objectives at the conceptual level is addressed here. The proposed procedure finds optimal trade-offs between design and control decisions, based on process dynamics and advanced control. A major innovation is a novel embedded control optimization approach. It suggests a two-stage problem decomposition leading to a massive reduction of problem size and complexity. Integration of design and control is expected to have a broad impact on high-performance systems operated close to their limits. Two case studies demonstrate the suitability of the methodology.

Keywords: Design and control integration, uncertainty, dynamic flexibility, optimization

Introduction

In classical process synthesis, design decisions are selected so that the process achieves the desired production goals at nominal conditions.1 Optimal design variable sets are often determined by mathematical programming.2 In industry, these “optimal” values are subsequently relaxed using safety overdesign factors in order to accommodate uncertainty.3 After an optimized and, subsequently, heuristically “overdesigned” process has been obtained, control aims at protecting the process operation against the effect of disturbances. Low-level process variables, such as pressure, temperature or filling levels are typically handled with classical feedback.3–5 Model predictive control (MPC) can also incorporate high-level economic objectives. In both classical and advanced approaches, controller tuning and optimization is...
Can we optimize design and control decisions simultaneously to maximize overall system performance in the presence of operational and model uncertainty? It is interesting to visualize the trade-offs in design and control integration as depicted in Figure 1. In classical process design under uncertainty, it is customary to study steady state performance. However, a rigorous proof for a design to be flexible at steady state is of little value, when dynamic constraint violations may occur. Dynamic constraint violations, however, are not detected by classical flexibility methods.

Second and more importantly, steady flexibility typically does not consider feedback control built into virtually every chemical operation. Tracking the impact of uncertain variables without accounting for the processes’ closed-loop control dynamics does not actually describe process flexibility. Hence, steady-state flexibility analysis without control feedback merely tracks uncertainty from inputs to outputs, but does not really quantify the actual process robustness as shown in Figure 2. The importance of static controls on flexibility was pointed out in pioneering work by Grossman. However, a rigorous proof for a design to be flexible at steady state is of little value, when dynamic constraint violations may occur. Dynamic constraint violations, however, are not detected by classical flexibility methods.

Tractability of Design and Control Integration. Integration of design and control has been achieved for specific cases, such as a simple binary distillation column. The simultaneous search for structural decisions and continuous design variables, optimization control structure, and controller tuning alongside process design exceeds the capability of most existing optimization algorithms. Therefore, new problem formulations are needed to reduce the combinatorial complexity of design and control integration. A novel problem approach will demonstrate a substantial reduction of combinatorial complexity of design and control integration by performing a stochastic design optimization with embedded control.

Previous work

Despite an extensive body of literature in design and control, much work needs to be done to harmonize process design and process control activities. The robust "steady-state" design of manufacturing processes under uncertainty has received ample attention. Several different design flexibility metrics were proposed: deterministic flexibility, resilience index, fuzzy possibility metrics, decision flexibility in production planning, stochastic flexibility. Robust design by minimizing signal-to-noise ratios is discussed elsewhere. Recently, robust design concepts for flexible dynamic performance were generalized. Their binary distillation column considers control structure and tuning decisions alongside continuous design variables like number of equilibrium trays and reflux ratio. Recently, Hoo proposed low-order model identification for control of distributed parameter systems. Seider also advocated the need for design and control integration. Several authors proposed quantitative approaches to ensure stability of nonlinear system with uncertain parameters. The challenges of design and control integration were clearly identified and discussed by several groups.

Classical controller design methods make use of frequency domain transfer function models, and capture model uncertainty in terms of deviations of the frequency response from nominal model response. Amplitude and phase margins and sensitivity functions are used to quantify robust stability and quality of the design. More modern techniques base robust stability analysis and performance design on structured singular values and $H_\infty$ theory. The infinite horizon control approach ($H_\infty$) has a rigorous mathematical basis for predicting stability and robustness properties, but cannot handle parametric uncertainty. These limitations can be overcome by employing modified methods, such as $\mu$-synthesis and $H_\infty$ adaptive control. Primary contribution to robust control theory in chemical processes is found elsewhere. Other work suggests extensions of MPC for plant-wide control, nonlinear systems and robustness. Still, in all approaches, control system design is carried out after the process design has been completed.

The subsequent section will introduce a decision hierarchy for design and control integration. A new problem formulation will be presented in Methodology section. Implementation of the embedded control optimization section will discuss the mathematical implementation of the novel embedded control algorithm. Application section will introduce two case studies to demon-
integrate design and control optimization. Increases the difficulty in obtaining numerical solutions to the equation-oriented mathematical model of the fundamental conservation laws. The variables in the system equations are then partitioned into four categories: (1) design decisions $d$, (2) control decisions $c$, (3) uncertainty sources, $\theta$ and $\xi$, as well as (4) state variables $x$. Table 2 summarizes variables categories of the proposed methodology.

**Level-1: Dynamic modeling, flexibility concepts and structural decisions.**

- Identify state variables, $x$, and formulate conservation laws and constitutive equations. Select design variables, $d$, controls, $c$, and characterize uncertainty sources.
- Perform integrated design and control optimization steps with increasing level of complexity:
  - Mathematical modeling of the uncertain space
  - Dynamic stochastic optimization of the expected performance
  - Steady state flexibility
  - Dynamic flexibility

**Level-2: Design optimization.**

- Perform integrated design and control optimization steps with increasing level of complexity:
  - Mathematical modeling of the uncertain space
  - Dynamic stochastic optimization of the expected performance
  - Steady state flexibility
  - Dynamic flexibility

**Methodology**

This section presents a hierarchical problem formulation to integrate design and control. Then, we introduce a novel mathematical programming framework for its computational solution.

**Hierarchical process and mathematical programs for integrated design and control.**

The proposed hierarchical design procedure has two levels of activities summarized in Table 1. Before any detailed analysis can begin, it is important to create an inventory of relevant state variables and possible manipulated process quantities. In level-1, equation-oriented process models relate state variables to uncertain parameters. The mathematical programming framework of level-2 optimizes design and control decisions to maximize robust expected performance.

**Level-1: Modeling and structural decisions.**

The dynamics of physical processes is best characterized by equation-oriented mathematical model of the fundamental conservation laws and first principles. The variables in the system equations are then partitioned into four categories: (1) design decisions $d$, (2) control decisions $c$, (3) uncertainty sources, $\theta$ and $\xi$, as well as (4) state variables $x$. Table 2 summarizes variables categories of the proposed methodology.

**Level-2: Design optimization.**

- Perform integrated design and control optimization steps with increasing level of complexity:
  - Mathematical modeling of the uncertain space
  - Dynamic stochastic optimization of the expected performance
  - Steady state flexibility
  - Dynamic flexibility

**Sources of Uncertainty $\theta$ and $\xi$.** Uncertain variables are categorized into two sets. Static uncertain parameters $\theta$ vary arbitrarily within an expected value range without adhering to a specific pattern. All uncertain influences changing periodically are represented as known trigonometric functions of time $\xi(t)$. Table 2 proposes suitable mathematical models for different types of uncertainty.

**Table 1. Proposed Decision Hierarchy for Integrated Design and Control.**

<table>
<thead>
<tr>
<th>Level-1: Dynamic modeling, flexibility concepts and structural decisions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Identify state variables, $x$, and formulate conservation laws and constitutive equations. Select design variables, $d$, controls, $c$, and characterize uncertainty sources.</td>
</tr>
<tr>
<td>Level-2: Design optimization</td>
</tr>
<tr>
<td>Perform integrated design and control optimization steps with increasing level of complexity:</td>
</tr>
<tr>
<td>Mathematical modeling of the uncertain space</td>
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<td>Steady state flexibility</td>
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<tr>
<td>Dynamic flexibility</td>
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</tbody>
</table>

**Table 2. Variable Categories in Integrated Design and Control.**

<table>
<thead>
<tr>
<th>Variable Type</th>
<th>Symbol</th>
<th>Type</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>Design</td>
<td>Discrete</td>
<td>Structural decisions:</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$d$</td>
<td>Connectivity</td>
<td></td>
</tr>
<tr>
<td>Control</td>
<td>Continuous</td>
<td>Reactor volume, Column length</td>
<td></td>
</tr>
<tr>
<td>State</td>
<td>Continuous</td>
<td>Temperature, Composition, Pressure</td>
<td></td>
</tr>
<tr>
<td>Uncertainty</td>
<td>$\theta$</td>
<td>Time independent</td>
<td>Parametric uncertainty</td>
</tr>
<tr>
<td></td>
<td>$\xi(t)$</td>
<td>Time dependent</td>
<td>Variations due to seasonal changes</td>
</tr>
</tbody>
</table>

**Figure 3. Variables for integrated design and control (Level-1): Implementable control ($g$: process and equipment constraints $-$ $h_\text{C}$: Conservation law $-$ $h_\text{CTR}$: Control law).**

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