Using Dynamic Flexibility Analysis to Integrate Design and Control under Uncertainty

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Abstract:

Daily process operations are impacted by several short and long-term uncertainties like daily fluctuations and seasonal variations in production levels, such as feed compositions or change in services quality. In order for the process to handle deviations from nominal condition the effect of uncertainties should be adequately incorporated in the conceptual design phase. In addition to parametric uncertainties, uncertainty associated with physical properties and process models add a difficulty to the design problem. Therefore, classic deterministic design based on information at nominal conditions alone may not lead to best process performance in the actual industrial plant. In industrial practice overdesign based in engineering judgment aims at increasing the robustness of a design.

Recent progresses in both theoretical approaches as well as computer power have renewed the interest of many researchers in academia and industry to explore process design under uncertainty with more mathematical rigor. A problem that has not yet been well studied is the distinction between process design versus a controlled process design. The usual practice is design for the worst-case scenario and in a later stage design a control system to handle the uncertainty. This practice usually leads to a robust design but the trade-off between design and control is not exploited leading to non-optimal results. Clearly, this viewpoint brings together a very important aspect, namely the integration of design and control. Unfortunately little systematic control and design of processes under uncertainty is available. Grossmann and co-workers [e.g. Halemane and Grossmann, 1983; Pistikopoulos and Grossmann, 1988b] introduced the concept of integrating design and control to obtain best trade-offs between cost and process flexibility considering a steady state assumption. Pistikopoulos and coworkers [e.g. Pistikopoulos and Dimitriadis, 1995 and Bansal, Perkins and Pistikopoulos, 2002] have shown that considering a steady-state point of view renders an unrealistic control scheme and a dynamic analysis is needed.

In this presentation, we will propose a novel methodology that aim at obtaining best trade-offs between design and control decisions in a dynamic view of process control and design. Our methodology will include the concept of flexible design of controlled systems under uncertainty. We will also demonstrate, with the help of this dynamic approach, that integration of design and control at conceptual level yield better cost performance and higher flexibility as compared to designs, which consider process control separately. In particular we would like to study the impact of periodical uncertainty and the influence of their frequency of occurrence. We will compare the advantages and limitations of our methodology to different deterministic and

probabilistic uncertain design approaches using static-control and illustrate our methodology with the help of benchmark case studies.

Methodology

Our methodology is composed of three specific tasks:

- Task-1: Dynamic Modeling and Flexibility Concepts
- Task-2: Solution of Simultaneous Design and Control Problems

Task-1. Dynamic Modeling and Flexibility Concepts

We integrate design and control of high performance manufacturing processes according to the hierarchical design procedure with three levels of activities summarized in Table 1. In level-1, transient equation-oriented process models relate state variables to uncertain parameters. The mathematical programming framework of level-2 optimizes design and control decisions to maximize the joint objectives. Level-3 further refines attractive candidate design solutions to determine the optimal production quality standard that ideally matches the customer requirements.

Table 1 – Three-level Hierarchical Procedure for integrated design and control

Level-1: Dynamic Modeling, Flexibility Concepts and Structural Decisions: Identify state variables and formulate conservation laws and first principles. Select design variables, controls, and characterize uncertainty sources. Level-2: Design Optimization: Perform Integrated Design and Control Design optimization using the following steps with increasing level of complexity: • Sampling of the uncertain space • Dynamic Stochastic Optimization of the expected cost • Steady state Flexibility • Stability • Dynamic Flexibility

Modeling and Structural Decisions

Basic conservation balances and first principles quantify the dynamics of the physical process. The variables in the system equations are then partitioned into four categories: (i) design decisions, d, (ii) control decisions, c, (iii) uncertainty sources, θ and ξ as well as (iv) state variables, x.

Design decisions, *d.* Design variables, d can be divided into *discrete* structural decisions such as the connectivity of physical units, and *continuous* variables like equipment dimensions or operating conditions. In the condenser example, con-current versus counter-current operation constitutes a discrete decision. The heat exchanger area belongs to the continuous variable set.

Control decisions, *z and c.* For control, two sublevels with increasing detail are proposed. Design with *perfect control* seeks optimal control moves without regard to the controller realization. Perfect control trajectories are denoted as z(t) in Figure 1a and are formally known as second stage decision variables in operations research [e.g. Infanger, 1991 and 1994]. The second layer -*implementable control*- introduces an actual controller framework, see Figure 1b. The *implementable control* stage fixes a particular control strategy alongside its tuning parameters. The control variable set, c, represents alternative controller configurations as well as tuning parameters and set-points. It can be regarded as first stage decisions that do not change with time.

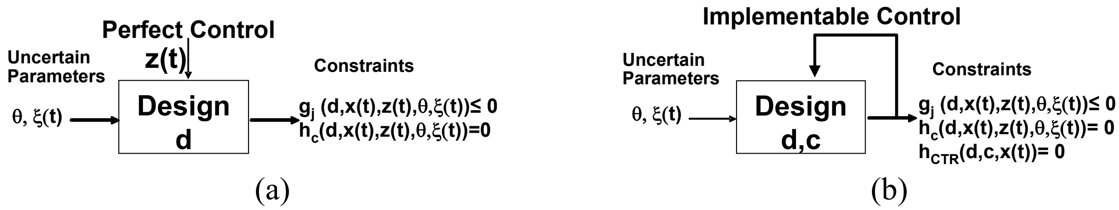

Figure 1 – Variables for Integrated Design and Control (Level-1): (a) Design with Perfect Control – (b) Implementable Control (g_j: Process and Equipment Constraints – h_C: Conservation Laws – h_{CTR}: Control Law)

Sources of Uncertainty, θ and ξ. Uncertain variables are categorized into two sets. Static uncertain parameters θ are time invariant. They may vary within expected bounds without specific pattern in the time domain. All uncertain influences changing periodically in time are collected in the set ξ(t). We propose the models listed in Table 2 to represent different types of uncertainty.

Table 2 – Categorization of uncertainty sources

Uncertainty Type	Mathematical Model	Example
Time-invariant Uncertainty	$\theta^N \pm \Delta\theta$, Probability Distribution Function PDF(θ)	Parametric uncertainty, model uncertainty (e.g. heat transfer coefficient)
Dynamic Periodic Uncertainty	$\xi(t) = A \cdot \sin(\omega t + \phi)$ $A \in [A.low, A.high], \omega \in [\omega.low, \omega.high]$	Temperature variations due to seasonal or daily changes, etc.
Non-Periodical Uncertainty	$\xi(t) = Function(A,t)$ $A \in [A.low, A.high]$	Sudden variations in feed quality (change of feed batch), peak load, etc.

Design Optimization

Design optimization seeks optimal values for design and control variables within a space of uncertain parameters. Numerical optimization algorithms require the discretization of the time domain and the uncertain space. Discretization of control and state variables in the time domain solves the problem only partially, since the number of uncertain parameter realizations is still infinite. However, omitting even a single critical uncertain scenario jeopardizes the rigor of the flexibility test. Moreover, seeking critical constraint violations with mathematical programming algorithms requires strong convexity assumptions which cannot be guaranteed for the highly non-linear integrated design and control problems. Hence, it appears that dynamic flexibility design problems are infinitely large and intractable.

As a remedy, previous research by Imperial College and our group at UIC has lead to a successful mathematical programming approach employing *problem decomposition* and *uncertainty space sampling* techniques [e.g. Bansal et al., 2002; Mohideen et al., 1996; Chakraborty and Linninger, 2003]. The decomposition separates the design variable optimization from the rigorous dynamic flexibility test. Task-2 will propose solutions to integrated design and control with existing numerical optimization algorithms.

Problem decomposition: We decompose the integrated design and control problem into a sequence of an optimal design problem (problem A) followed by a dynamic flexibility test (problem B). Problem A seeks *optimal design decisions* in the time horizon of interest, $t=[0,t_{max}]$

over a specific set of uncertain scenarios, s ∈ Ω. It probabilistic objective typically includes expected operating cost $C_1(.)$ as well as capital cost $C_2(.)$ of the design *d* and the control, *c*. Equality constraints, *h*, include conservational laws and the selected control algorithm, h_{CTR}. Inequalities, *g*, enforce safety, equipment and product constraints at specific instances in time (point constraints) or on average in an integral sense. The sample set includes random realizations of uncertain parameters, θ, and models for periodic uncertainties, ξ(t), mimicking realistic dynamic operating conditions. A probability of occurrence, ω^s, weighs the significance of each event in the stochastic objective function. The solution of problem A determines optimal values of the design and control variable sets.

Critical Scenarios. The optimal design (*d, c*) obtained with problem A is further examined for critical dynamic constraint violations not included in the initial set of samples, s ∈ Ω. The detection of critical scenarios is delegated to the flexibility test problem B, which searches the continuous space of uncertain variables. If the flexibility index, δ^*, is smaller than unity, critical scenarios corresponding to the constraint violations are added to the original sample set, Ω. Depending on the nature of the problem (i.e. convexity of the design space, number of active constraints, etc.) one or more critical points might be identified. Several iterations between design (problem A) and critical scenario search (problem B) may be needed before a design is declared optimal and flexible.

Problem A: Optimal Design Problem (Stochastic Optimization Problem)

$$\min_{\substack{d,\,c,\,z(t)\\ x(t)}} \Gamma = \underbrace{\sum_{t=0}^{t_{\max}} \sum_{s\in\Omega} w^s \cdot C_1\left(d, c, x(t), z(t), \theta^s, \xi^s, t\right)}_{\text{Expected Operating cost}} + \underbrace{C_2(d,c)}_{\text{Capital Cost}} \quad \text{Minimize Total Expected Cost} \tag{1}$$

$s.t.$

$$h_c(d, \dot{x}(t), x(t), z(t), \theta^s, \xi^s, t) = 0, \quad \forall s \in \Omega \quad \text{Conservational Laws} \tag{2}$$

$$h_{CTR}(c, \dot{x}(t), x(t), z(t), t) = 0, \qquad \dot{x}(0) = x^0 \quad \text{Control Algorithm} \tag{3}$$

$$g_j(d, x(t), z(t), \theta^s, \xi^s, t) \le 0 \qquad \forall s \in \Omega \quad \text{Process and Product Constraints} \tag{4}$$

Problem B: Rigorous Dynamic Flexibility Test Problem (Deterministic Optimization Problem)

$$\delta^*_{dyn} = \max \delta \quad \text{Flexibility Index} \tag{5}$$

$$\text{s.t.} \max_{\theta\in T,\ \xi(t)} \min_{z(t)} \max_{t\in[0,\ t_{\max}]} g(d, x(t), z(t), \theta, \xi(t), t) \tag{6}$$

$$T = \left\{\theta / \theta^N - \delta\Delta\theta^- \le \theta \le \theta^N + \delta\Delta\theta^+\right\} \tag{7}$$

Constraints (2)-(4) of problem A

Task 2- Solution of the Simultaneous Design and Control Problems

The integrated design and control problem will be decomposed into smaller sub-problems for its numerical solution. Figure 2 suggests a hierarchy of increasing level of complexity, for ensuring a gradual refinement of the design from simple to harder problems. First, sampling (2.1) discretizes the infinite uncertain space. A stochastic dynamic mathematical program defined over the finite sample set optimizes design and control decisions for minimum expected cost (2.2). The preliminary optimal design is then examined for critical scenarios in the whole uncertain space by a deterministic flexibility procedure (2.3). We propose to establish feasibility for steady state conditions first. Critical scenarios causing failure are added to the sample set and the design is optimized again. Flexible steady systems are tuned to ensure dynamic stability (2.4) by suitable control adjustments or if unsuccessful by re-designed. Stable systems are submitted to a dynamic flexibility test (2.5) to identify transient constraint violations. Critical dynamic scenarios are added to the uncertainty samples. Repeated iterations through the hierarchy progressively narrow the search space with the goal of arriving at an integrated design with minimum expected cost and dynamic flexibility.

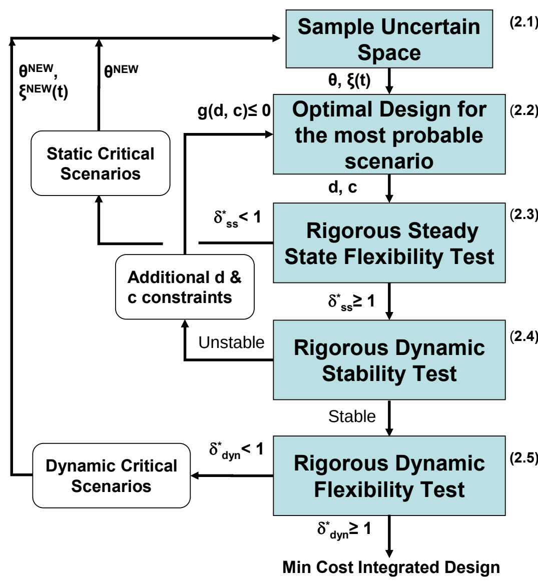

Figure 2 –Proposed Integrated Design and Control Methodology (Level 2)

Uncertain Space Discretization. Parameter uncertainty introduces another infinite dimension to the continuous time dynamic optimization problem. We propose scenario sampling for converting the infinite uncertain space into a discrete mathematical form. The decomposition of the uncertain space provides a simple method to compute expected performance. We have successfully reduced the design space for synthesis of separation flowsheets by using stratified sampling techniques [Chakraborty and Linninger, 2003]. Bootstrapping techniques determined the necessary sample sizes. The size reductions gained by this scheme render acceptable accuracy at reasonable computational effort. Alternatively some researchers report success in modeling the uncertain space with global multi-dimensional integration methods [Pistikopoulos and Grossmann, 1988a].

Time Discretization. We will investigate two alternative numerical solutions strategies as depicted in Figure 3: Global discretization and Control Vector Parameterization. The problem decomposition makes it amenable to dedicated solution algorithms. Discretization of the time domain on finite elements with orthogonal polynomials converts the differential algebraic constraints into a set of algebraic equations defined on discrete collocation nodes [Villadsen and Michelsen, 1978, Biegler, 1984]. This global discretization method substantially reduces the problem size and transforms a dynamic optimization problem into a Non-linear Program (NLP or MINLP) for which state-of-the-art algorithms are available. We intend to explore advanced MINLP solvers such as BARON [2005], DICOPT [Kocis and Grossmann, 1989] or MINOPT [2005]. Further problem size reduction is possible by dynamically adjusting length, number and order of the finite elements [Tanartkit and Biegler, 1995]. Successful applications in design problems under uncertainty are documented in the open literature [Zhang et al., 2004].

Alternatively, the system of dynamic constraints (DAE) can be integrated with specialized variable step-size routines. The master optimization program performs branching and bounding on top of a *gradient-based* search to adjust design variables and the discrete set of control actions. This technique known as control vector parameterization delegates the accurate evaluations of the state variable trajectories to a DAE integrator routine such us DASPK [2005], DAEPACK [2005] or DASOLV [Jarvis and Pantelides, 1993]. We have also successfully integrated numerical DAE solvers into large-scale non-linear programs to solve dynamic kinetic inversion problems [Tang et al., 2005].

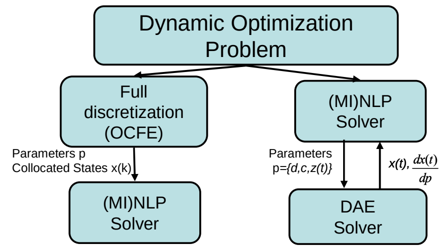

Figure 3 - Different approaches to solve a dynamic optimization problem

Stability. While system performance is optimized on a finite time horizon as described above, the joint design and control system should be stable. However, asymptotic stability criteria for non-linear dynamic systems are mathematically difficult to solve. Several authors have made contributions to test stability of general dynamic processes [e.g. Kokossis and Floudas, 1994ab; Vidyasagar, 2002; Mönnigmann and Marquardt, 2003]. A recent alternative stability determination developed by Ydstie based on the process entropy will also be explored for its suitability in integrated design [Alonso et al., 2002]. We propose two avenues to examine dynamic stability: (i) the first one is based on *matrix metrics* of the Jacobian [Vidyasagar, 2002]; (ii) and alternative route would ensure that the system has reached steady within an *open final time problem*.

Identification of Critical Scenarios. A key requirement for justifying uncertainty analysis with advanced mathematical methods is its rigor in identifying critical scenarios. We have found that existing approaches [e.g. Bansal et. al, 2002] fail to identify whole families of worst case scenarios related to constraint violations caused by critical disturbance frequencies. To illustrate the risk of these disturbance frequencies, a VOC condenser was subjected to periodical inputs of known amplitude but varying frequencies. Using the proposed methodology a critical frequency of coolant temperature oscillations was computed rigorously. This frequency-critical worst-case scenario led to larger overshoots than any series of step changes of equal magnitude as displayed in Figure 4. This phenomenon is known as *critical resonance* and can cause failure. Approaches to find all "transient" critical scenarios for robust dynamic processes design are currently missing and will be addressed in this research. We propose to engage lower order surrogates in order to detect potential disturbance resonances.

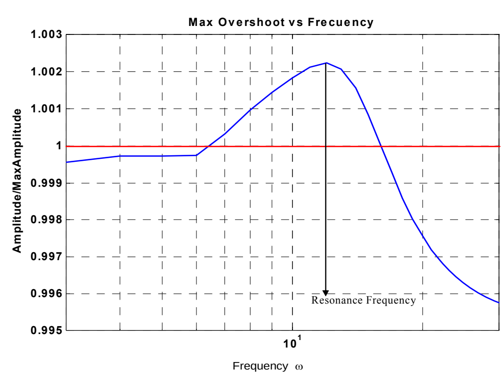

Figure 4 – Frequency plot of the dimensionless output

Significance

Currently, chemical process design and control are separate disciplines assisting process development at different stages. Design and control decisions are made independently despite the common aim of ensuring robust plant operations. The lack of confidence in existing methods is underscored by the industrial practice of process overdesign without ascertaining the actual level of robustness or controllability. A systematic framework for simultaneous process and control system design does not exist yet.

We adopt an *integrated* view of process control and design decisions under realistic dynamic operating conditions. We create a concise decision-making hierarchy allowing designers to arrive at key structural decisions for the process flowsheet and control layout. Rigorous mathematical programming approaches are proposed for optimizing parametric design variables as well as structural alternatives.

Our work foresees an inductive exploration of different types of uncertainty such as model uncertainty, physical parameter uncertainty, varying product demand, operational and external disturbances. We suggest a systematic classification of the functional time-dependency and periodicity of uncertainty sources. The methodology incorporates advanced control options such as non-linear Model Predictive Control or RTDA controller technique developed by the Co-PI [Ogunnaike and Mukati, 2004; Mukati and Ogunnaike, 2004].

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