AIChE Wiley InterScience DISCOVER SOMETHING GREAT

Integrating Systems Design and Control using Dynamic Flexibility Analysis

Andrés Malcolm, Jamie Polan, and Libin Zhang
Laboratory for Product and Process Design, Dept. of Chemical Engineering, University of Illinois at Chicago, Chicago, IL 60607

Babatunde A. Ogunnaike
Dept. of Chemical Engineering, University of Delaware, Newark, DE 19716

Andreas A. Linninger
Laboratory for Product and Process Design, Dept. of Chemical Engineering and Bioengineering, University of Illinois at Chicago, Chicago, IL 60607

DOI 10.1002/aic.11218
Published online July 2, 2007 in Wiley InterScience (www.interscience.wiley.com).

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.
 AIChE J, 53: 2048–2061, 2007
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.

After an *optimized and, subsequently, heuristically "over-designed"* 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.[3–7] Model predictive control (MPC) can also incorporate high-level economic objectives. In both classical and advanced approaches, controller tuning and optimization is

Correspondence concerning this article should be addressed to A. A. Linninger at linninge@uic.edu.

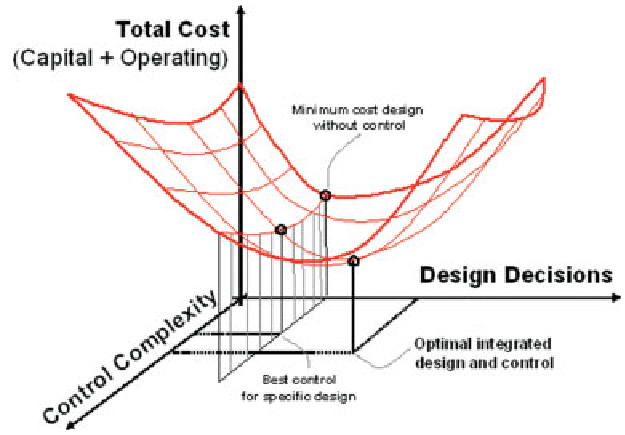

Figure 1. Conceptual representation of the trade off between control and design decisions.

Only integration of design and control can be expected to achieve the overall optimum chemical process. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

limited by process dynamics already fixed in the design phase.

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.[8–11] 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.[8–11] Designing processes without considering feedback control could lead to arbitrary process overdesign or under performance. Consequently, flexible process design should include dynamic design as well as control issues. *Design under uncertainty is inseparable from robust process control*.

Tractability of Design and Control Integration. Integration of design and control has been achieved for specific cases, such as a simple binary distillation column.[12–14] 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.[15–18] Several different design flexibility metrics were proposed: deterministic flexibility index,[8–11,19–23] resilience index,[24] fuzzy possibility metrics,[25,26] decision flexibility in production planning,[27] stochastic flexibility.[28–30] Robust design by minimizing signal-to-noise ratios is discussed elsewhere.[31,32]

Recently, robust design concepts for flexible dynamic performance were generalized.[13,14,33–35] 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.[36] Seider also advocated the need for design and control integration.[37] Several authors proposed quantitative approaches to ensure stability of nonlinear system with uncertain parameters.[38–41] The challenges of design and control integration were clearly identified and discussed by several groups.[42]

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.[43–48] 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_∞ theory.[49–54] The infinite horizon control approach (H_∞) 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 μ-synthesis[51] and H_∞ adaptive control.[55] Primary contribution to robust control theory in chemical processes is found elsewhere.[56–58] Other work suggests extensions of MPC for plant-wide control, nonlinear systems and robustness.[59–65] 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-

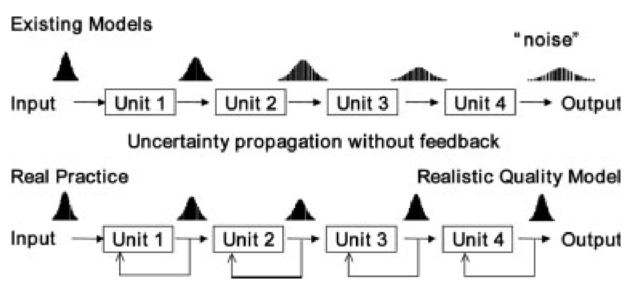

Figure 2. Feedback control helps to dissipate uncertainty.

Control consideration and dynamics should not be ignored in flexible process design methods; but are not accounted for in classical design for flexibility.

Table 1. Proposed Decision Hierarchy for Integrated Design and Control

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.

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
- Stability
- Dynamic flexibility

Table 2. Variable Categories in Integrated Design and Control

Variable Type	Symbol	Type	Example
Design	d	Discrete	*Structural decisions: Connectivity*
		Continuous	*Reactor volume, Column length*
Control	c	Discrete	*Control configuration, Control type*
		Continuous	*Set points, Control tuning parameters*
State	x	Continuous	*Temperature, Composition, Pressure*
Uncertainty	θ	Time independent	*Parametric uncertainty*
	$\xi(t)$	Time dependent	*Variations due to seasonal changes*

strate the applicability of the proposed methodology. The article closes with conclusions and suggestion for future work.

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, θ and ξ, as well as (4) state variables x. Table 2 summarizes variables categories of the proposed methodology.

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 case of a polymerization reactor, the choice of batch or plug-flow reactor would constitute a discrete decision. The reactor size, operating temperature, and pressure are continuous variables.

Control Decisions c. For control, we consider the closed-loop system dynamics operating under actual control strategies as depicted in Figure 3. 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. The mathematical model of the *control law*, h_{CTR}, relates state variables to the control variable set c. Unfortunately, the feedback increases the difficulty in obtaining numerical solutions to the integrated design and control optimization.

Sources of Uncertainty θ and ξ. Uncertain variables are categorized into two sets. Static uncertain parameters θ 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 3 proposes suitable mathematical models for different types of uncertainty.

Level-2: Design optimization

Numerical optimization algorithms require the discretization of the time domain and the uncertain space. Even after time discretization, the spectrum of uncertain parameters is still infinite. However, for flexibility analysis to be rigorous, not a single critical parameter realization must be omitted. The detection of critical constraint violations with mathematical programming algorithms is often divergent due to discontinuities and nonconvexities in the problem space. Hence, it appears that *dynamic flexibility design problems are infinitely large and intractable*.

Problem Decomposition. As a remedy, previous research has lead to a successful mathematical programming approach employing *problem decomposition* and *uncertainty space sampling* techniques.[13,35,66,67] The decomposition separates design optimization from examining process flexibility. In this work, we also decompose the integrated design and control problem into an *optimal design problem* (Problem-A) followed by a *dynamic flexibility test* (Problem-B). Problem-A seeks an *optimal design* like process design and control decisions, that maximize performance within a specific set of uncertain scenarios $s \in \Omega$. Its probabilistic objective typically includes expected operating cost $C_1(.)$, as well as capital cost

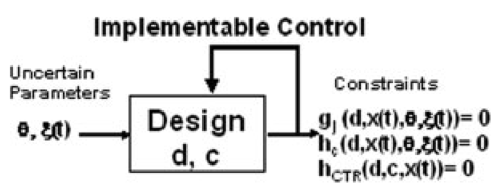

Figure 3. Variables for integrated design and control (Level-1): Implementable control (g_j: process and equipment constraints — h_C: Conservation law — h_{CTR}: Control law).

Table 3. Categorization and Mathematical Models of Uncertainty Sources

Uncertainty Type	Mathematical Model	Example
Time-invariant uncertainty	$\theta^N \pm \Delta\theta$, *Probability distribution function* (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.

$C_2(.)$ in the time horizon of interest $t = [0, t_{\max}]$. Equality constraints include conservation laws h_c, and the selected control algorithm h_{CTR}. Inequalities g, enforce safety, equipment and production constraints at specific instances in time, or in an integral sense as in endpoint constraints. The sample set includes relevant realizations of uncertain parameters, θ, and models for periodic uncertainties $\xi(t)$, mimicking realistic dynamic operating conditions. A probability of occurrence, ω^s, measures the likelihood of each uncertain scenario.

Problem-A: Optimal design problem (stochastic optimization problem)

$$\min_{d,c,x(t)} \Gamma = \underbrace{\int_{t=0}^{t_{\max}} \int_{s\in\Omega} \omega^s \cdot C_1(d,c,x(t),\theta^s,\xi^s,t)\,ds\,dt}_{\text{Expected Operating Cost}} + \underbrace{C_2(d,c)}_{\text{Capital Cost}} \qquad \text{Minimize Total Expected Cost} \qquad (1)$$

s.t.

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

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

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

If no solution to the design problem exists, it means that the quality specifications are not attainable and have to be relaxed. On the other hand, successful feasible solutions to the optimal design problem only means that the process does not fail in any scenario included in the current *discrete* sample space. It does not guarantee *dynamic process feasibility* for critical events that may occur in the *continuous* uncertain space. To ensure robust operation of a candidate solution within the *entire uncertain space*, a separate search is necessary.

Rigorous Search for Critical Scenarios. The flexibility test is a rigorous mathematical program to discover critical events. Problem-B calculates the scalar flexibility index δ_{dyn}. A flexibility index larger than unity, $\delta_{dyn} \ge 1$, signifies that the design is robust for all possible realizations of the uncertain variables. A flexibility index smaller than unity $\delta_{dyn} < 1$, means that at least one parameter variation causes failure. In addition, constraints active in Problem-B identify critical worst scenarios in which the candidate solution fails. Thus, the solution of Problem-B either *guarantees dynamic flexibility*, or *produces additional critical scenarios* that need to be considered in the design optimization. Accordingly, the scenario space for the design problem (Problem-A) is augmented with critical scenarios identified rigorously with the help of solving Problem-B.

Problem-B: Rigorous dynamic flexibility test problem (deterministic optimization problem)

$$\delta^*_{dyn} = \max \delta \qquad \text{Flexibility Index} \qquad (5)$$

s.t.

$$\max_{\theta\in T,\,\xi(t)} \max_{t\in[0,\,t_{\max}]} g(d,\dot{x}(t),x(t),\theta,\xi(t),t) \le 0 \qquad (6)$$

$$T = \{\theta/\theta^N - \delta\Delta\theta^- \le \theta \le \theta^N + \delta\Delta\theta^+\} \\ Constraints\,(2)-(4)\,of\,Problem-A \qquad (7)$$

Depending on the degree of nonlinearity, or the number of adjustable degrees of freedom in the active constraints, *one or multiple critical scenarios* 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*. This problem decomposition separates the design optimization from the flexibility problem, making the simultaneous design and control problem easier to tackle. However, *proper mathematical programming formulations alone do not guarantee numerical solvability*. Challenges involving the numerical solution of integrated design and control problems, and how to circumvent them are discussed next.

Is the integration of design and control solvable?

As pointed out before, feedback raises the difficulty for converging integrated design and control problem with mathematical programming methods. Feedback may make a process unstable; it also adds severe nonconvexity in objective functions and constraints. Simultaneous optimization of design and control structure along with control tuning in an infinite uncertain space poses a tough challenge for current optimization technology. Classical feedback has several additional drawbacks for multivariable control problems. Each possible pairing between controlled and manipulated variables introduces another integer decision, thus, easily causing a combinatorial explosion of design alternatives and introducing discontinuities in the search space. Moreover, classical PID tuning requires *a priori* knowledge of the system dynamics. In simultaneous design and control, *a priori* system dynamics is unavailable. Previous work approached this problem with brute force by solving the control-tuning problem together with the design optimization.[13,14,35] This direct simultaneous approach depicted in Figure 4a often exhibits convergence failures with existing mixed integer nonlinear

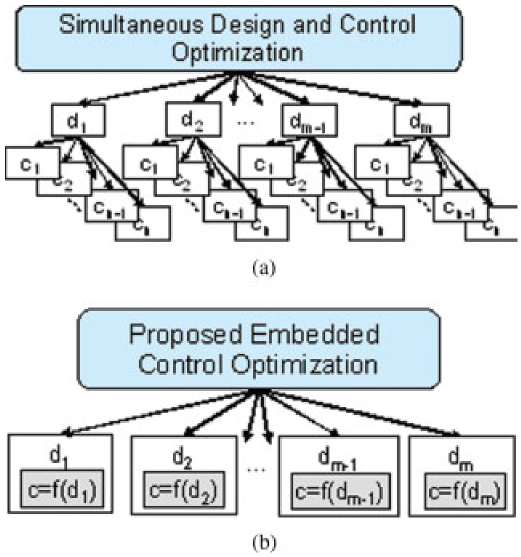

Figure 4. (a) Combinatorial explosion due to alternative control formulations and challenging optimization problems; (b) proposed embedded-adaptive feedback control rendering more tractable optimization problems.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

programming algorithms. Burdening the already challenging dynamic design optimization with additional structural and continuous control variables may not be the best strategy. The next section proposes a novel computational solution strategy to avoid the combinatorial complexity of design and control integration. The solution strategy deploys problem decomposition techniques and a new mathematical programming formulation. This new formulation entitled *embedded control optimization* adaptively optimizes control choices for a given design as depicted in Figure 4b, so that the burden of combinatorics, nonconvexity and stability caused by feedback can be disentangled from the stochastic design optimization.

Mathematical problem decomposition for design under uncertainty

The problem decomposition introduced in the previous section makes the open-ended design space tractable, and converts the design process into concise mathematical programming formulations, amenable to scientific computing methods. The overall methodology depicted in Figure 5 suggests four subproblems, I–IV. It aims at reducing the overall solution effort by following a gradual refinement of design decisions from most important to more detailed, and from simple to difficult.

Uncertain Space Discretization (I). Parameter uncertainty introduces another infinite dimension to the already infinite continuous time dimension in dynamic optimization. We implement scenario sampling for converting the infinite uncertain space into a discrete mathematical form. Replacement of the infinite uncertain space, Ω, with discrete samples for θ and ζ (t) drastically simplifies the evaluation of probability distribution functions of expected performance or cost.

Stochastic-Dynamic Optimal Design (II). The mathematical program of Problem-A defined over the finite sample set optimizes design and control decisions for minimum expected cost. The solution of this probabilistic optimization problem requires discretization of the time domain. We adopt *control vector parameterization* as a numerical solution strategy.[68] The numerical solution of this large-scale probabilistic dynamic optimization deciding design and control simultaneously, is an extremely difficult task. Implementation section will introduce a novel mathematical formulation to tackle this critical point.

Steady-State Flexibility Test (III). We suggest to examine steady state feasibility conditions first. Solution of Problem-B identifies critical scenarios violating design constraints at steady state. Critical scenarios causing failure are added to the sample set. This problem is generally a nonlinear mathematical program for which specialized algorithms have been developed.[21,23,69] Since a system that is infeasible at steady state cannot be dynamically feasible, the steady-state flexibility step reduces the effort for repeated runs of the more expensive dynamic flexibility test (step 4).

Dynamic Flexibility Test (IV). Flexible and stable systems are submitted to a dynamic flexibility test to identify transient constraint violations. Critical dynamic scenarios (θ^{New}, ζ^{New}) are added to the uncertainty samples. $\Omega^{New} = \Omega \bigcup \{\theta^{New}, \zeta^{New}\}$. Thus, the discrete scenario space, initially filled with relevant, but no necessarily critical scenarios, is gradually augmented with critical scenarios identified rigorously by the flexibility tests (Problem-B). Each run through the design optimization (Problem-A) adjusts design and control decisions for best performance in all scenarios including critical scenarios. Repeated iterations through the hierarchy progressively refine the search space with the goal of robustly arriving at an integrated design, and with minimum expected cost and guaranteed dynamic flexibility.

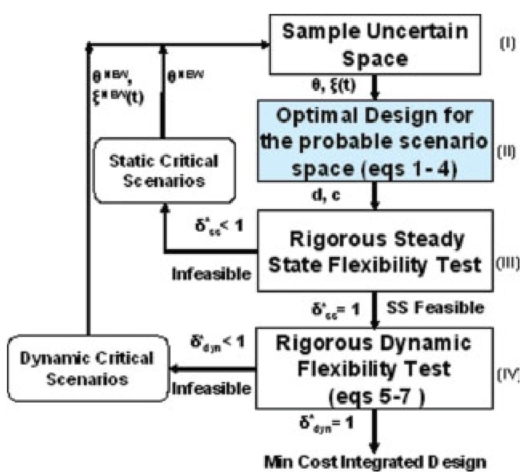

Figure 5. Proposed hierarchy decomposition for flexible design optimization, stages 1–4.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Current optimization techniques often fail when solving process and control optimization simultaneously. We propose to ease the combinatorial complexity of the nonpolynomial hard search space. It delegates control decisions to a suboptimization step which adaptively adjusts suitable control moves for a given design. Thus, control decisions shall be determined implicitly for each candidate design as suggested in Figure 4b. The problem decoupling leads to a massive size reduction without giving up control optimization. Discontinuities caused by control structure, tuning or stability do not directly impact the master optimization. How do we propose to find control actions for a given design? The quality of the control will be ensured by *embedded* control optimization. For each design choice, the embedded control problem will be solved with the help of *dynamically adaptive control optimization* operating under uncertain conditions. We propose to establish a simpler adaptive state space model as a surrogate for the full nonlinear system equations to ease the mathematical complexity of the optimal control problem. Hence, the complete system dynamics will be reduced adaptively to a suitable linear state space model. The linearized state model is used to compute optimal control actions in each time step. The effort for the embedded control optimization is *computationally extremely efficient* for two reasons: First, identification can be implemented sequentially with algorithms based on *sequential least-squares* fitting.[70,71] Second, the computation of optimal control moves of linear state space systems admits an *analytical solution*. Nevertheless, the adaptive nature of the proposed method adequately captures nonlinear process dynamics. The embedded control leads to substantial reduction in problem size and complexity. While adaptive control has been used previously for actual process control, it application as a tool to reduce the numerical challenge of design and control integration has never been before reported in the literature to the best of our knowledge.

Implementation of the embedded control optimization

This section will introduce the mathematical background of the embedded control algorithm composed of two hierarchical optimization loops.

Master Design Optimization Loop. We first describe the dynamic optimal design — step 2 of the methodology — by stochastic design optimization with embedded control. This stage uses the uncertain scenarios and an initial design guess as input as shown in Figure 5. At the master optimization level, design decisions d, are improved to maximize the probabilistic cost function in Eq. 1 of Problem-A. The system dynamics is modeled by sets of differential algebraic equations (DAE); uncertainty sources are described mathematically by the methods illustrated in Table 2. Control decisions are delegated to the embedded control optimization at a second level.

Embedded Control Optimization. The embedded control has three elements as depicted in Figure 6: (1) system identification; (2) state prediction, and (3) optimal control moves follows. This dynamic *identification* step mapping dynamically the equation-based dynamic process model into a linear state space model is executed in every time step of the discretized time horizon. The prediction quality is enhanced by the *observer* step. Finally, optimal control moves are computed by the *regulator*. A description of the embedded control optimization follows.

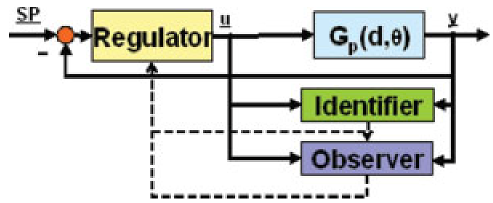

Figure 6. Proposed embedded feedback control with identifier, observer and regulator.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Identifier. Sequential model identification is a robust and fast algorithm that fits dynamic input-output data to a full state space representation Eq. 8. The required input-output data sets are obtained by sampling the highly nonlinear nonconvex equation-based dynamic system model at suitably chosen sampling intervals. The adaptive identification involves the solution of a least-square fitting problem. Fortunately, there exist very inexpensive sequential algorithms.[70–72] Equation 9 correlates the current state $x(k)$ with the past states $x(k-1)$, $x(k-2)$ ... and control movements $u(k-1)$, $u(k-2),\ldots$ through the estimated vector $\hat{a}$. The row vector $\hat{a}$ is composed of scalars α and β, accounting for the influence of the previous states and control moves on the current state as in Eq. 10.

$$x(k) = Ax(k-1) + Bu(k-1) \tag{8}$$

Equation 8 written in compact form, becomes

$$x(k) = z(k)\hat{a}_r^T \tag{9}$$

$$\text{with} \quad z(k) = [-x(k-1)\ldots - x(k-n)u(k-1)\ldots u(k-m)] \quad \text{and} \quad \hat{a} = [\alpha_1\ldots.\alpha_n\,\beta_1\ldots.\beta_m] \tag{10}$$

The solution of least-square fitting problem in Eq. 11 gives the desired state space model.

$$\min_{\hat{a}} \Delta_{\text{LSQ}} = \sum_{k=1}^{r}[x(k) - \hat{x}(k)]^2 = \sum_{k=1}^{r}[x(k) - z(k)\hat{a}^T]^2 \tag{11}$$

Fortunately there exists an analytical solution for the LSQ problem in Eq. 11. Moreover, the state space model $\hat{a}$ can be calculated recursively as a function of the previous model and the new observations. The final update formula is given in Eq. 12, where P_r is the estimation of the covariance of the error matrix. Equation 12 represents the recursive update of the prediction of the vector $\hat{a}$ in terms of previous states and the current observation. The effort for state space identification of $\hat{a}$ requires only matrix multiplications according to Eqs. 9–12. In a process with five measured variables and two states, only five matrix/vector multiplications per identification step are required. Even nonlinear dynamics are captured adequately by adaptive identification in successive time steps.

$$\hat{a}_r = \hat{a}_{r-1} + P_r z_r (x(k) - z_r^T \hat{a}_{r-1}) \text{ with}$$

$$P_r = P_{r-1} + \frac{P_{r-1} z_r z_r^T P_{r-1}}{1 + z_r^T P_{r-1} z_r} \quad (12)$$

Observer. The identification produces a full *state-space model* in each time step, with modest computational effort as shown earlier. The linear state-space model is further refined to predict the system response to previous control moves under the effect of disturbances. In real process control, this step is significant to reduce the effect of measurement noise. In our design application, there is *no* measurement noise as we sample an equation-based model. However, it helps to diminish the *modeling* error between the nonlinear system model and its linear state-space model approximation. Improved predictions are obtained by minimizing the covariance of the estimation error using a Kalman filter. Filtering implies a recursive algorithm to predict future states using current and past information, as well as a disturbance model. The basic equations are the prediction step in Eqs 13 and 14, and the measurement correction step in Eqs. 15–17. The covariance matrix Q, accounts for process noise. The matrix R, is the covariance of the measurement errors, which is it set to zero in our case. K_k is a current weight for the prediction error to be determined by the observer corrections. The matrix C relates the measured variables to the state variables as in Eq. 19. For highly nonlinear dynamics extended Kalman-filter formulation are available, but would augment the computational burden of embedded control optimization.

$$\hat{x}_{k+1}^- = A_k \hat{x}_k + B_k u_k \quad (13)$$

$$P_{k+1}^- = A_k P_k A_k^T + Q_k \quad (14)$$

Measurement update (correction)

$$K_k = P_k^- C_K^T (C_k P_k^- C_K^T + R_K)^{-1} \quad (15)$$

$$\hat{x}_k = \hat{x}_k^- + K_k (y_k - C_k \hat{x}_k^-) \quad (16)$$

$$P_k = P_k^- - K_k C_k P_k^- \quad (17)$$

Regulator. The regulator computes the best control action. This task is relatively easy for linear state-space models proposed in our method. We have used a linear quadratic regulator (*LQR*), that selects control moves to minimize a cost function as given in Eqs. 18 and 19 The objective accounts for *performance loss* according to the matrix S, and punishes the need for *control action* by the matrix τ. The optimality condition of this problem admits an analytical solution; therefore, its computation is inexpensive. Accordingly, the regulator chooses an optimal combination of control moves in terms of gains K^*, for a given design and uncertainty scenario. It also ensures closed-loop stability, and circumvents the combinatorial challenge of control variable pairing. An analytical criterion for the existence of a stable solution is given in appendix A. Extensions to more sophisticated control algorithms like model predictive control are possible. However, more advanced control algorithms come at the price of higher computational time. We suggest the use of simpler control algorithms for screening the search space; the adoption of advanced control laws for later design stages.

$$\min_{K^*} J = \sum_0^\infty (x_k^T \, S \, x_k + u_k^T \mathcal{T} \, u_k) \quad (18)$$

$$\text{s.t } \bar{x}_{k+1} = A\bar{x}_k + Bu_k^* \quad y = Cx_k \quad \bar{u}_k^* = -K^* \bar{x}_k$$
$$\text{with } u_k^* = u_{k-1} + \bar{u}_k^* \quad \text{and} \quad \bar{x}_k = x_k - \textit{Set Point} \quad (19)$$

The problem decomposition drastically reduces the master problem size and complexity. The separation of model equations for design and uncertainties from control strategies is another advantage. Researchers and engineers with experience in equation-oriented modeling may appreciate this feature. Successive iterations of the master design problem gradually improve the structural and parametric design decisions. The overall optimal design is also endowed with optimized control decisions that are enforced in the subordinate embedded control level. The stochastic optimization with the embedded adaptive control dramatically reduces the combinatorial complexity of the integrated design and control problem. Successful implementation of the proposed methodology will be illustrated in the case studies section.

Application of Design and Control Integration

Case Study-A: Design and control optimization of a polymerization reactor

Consider the process for producing poly-methylmethacrylate (PMMA) via free-radical polymerization of methyl methacrylate (MMA), with azo- bis-isobutyronitrile (AIBN) as initiator, and toluene as solvent shown in Figure 7.[73] The mathematical model for conservation of species, energy and polymerization kinetics is given in Eqs. 20 to 25. The state variables listed in Table 4 are: C_m is the dimensionless monomer concentration, C_I is the initiator concentration, D_0 is the bulk zeroth moment, D_1 is the bulk first moment of the polymer chain length, z is the average molecular weight, F_I is the initiator volumetric flow rate, V is the reactor vol-

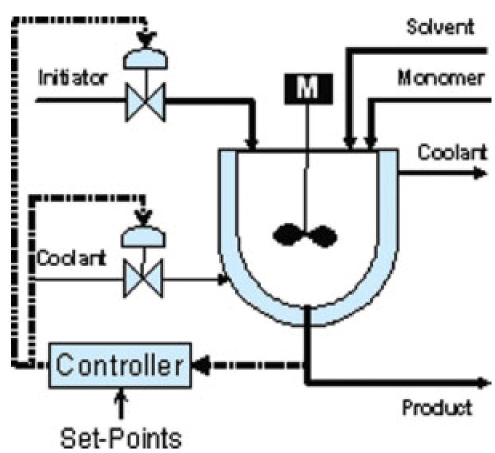

Figure 7. Polymerization reactor shown with multivariable feedback product quality control.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Table 4. Variable Categories in Integrated Design and Control

Variable Type	Symbol	Case Study 1	Case Study 2
Design	***d***	Reactor volume (V) Reactor temperature set point (T_{sp}) Monomer flow (F)	Number of stages (N_s) Feed location (F) Diameter (D)
Control	***c***	Initiator flow (F_I) Coolant flow (F_{cw})	Reflux ratio (R) Reboiler ratio (B)
State	***x***	Monomer concentration (C_m) Initiator concentration (C_I) Polymer zeroth moment (D_0) Polymer first moment (D_1) Reactor temperature (T) Coolant jacket temperature (T_j)	Light liquid composition in tray i (x_{li}) Heavy liquid composition in tray i (x_{li}) Light vapor composition in tray i (y_{li}) Heavy vapor composition in tray i (y_{hi}) Reboiler hold-up (h_{bi}) Condenser hold-up (h_{ci})
Uncertainty	θ	Heat transfer coefficient (U)	Antoine coefficient (B) Feed temperature (T_{feed})
	$\xi(t)$	Monomer concentration (C_m) Coolant inlet temperature (T_{wo})	Feed composition (z_{feed})

ume, F is the monomer/solvent flow rate, T is the reactor temperature, T_j is the cooling jacket temperature, and k_{ij} are temperature-dependent rate constants. More details on the process model and values of constants are given elsewhere (Z_{ij}, f, U, and so on).[74,75] This highly nonlinear system also admits multiple steady states observed in industrial reactors. Multiple steady states and nonlinearity make the system difficult to control with simple control strategies. The integrated optimization will seek to keep the polymer chain normal average molecular weight (NAMW) around 25,000 kg/kmol, by controlling the ratio of the bulk zeroth moment D_0, and the bulk first moment D_1 of the polymer length via simultaneous adjustment of the initiator and coolant flow rates. The nonlinear kinetics of coupled species equations and nonisothermal operation alongside the multivariable control problem presents a complex integrated design and control problem.

$$\frac{dC_m}{dt} = -(k_p + k_{fm})C_m P_0 + \frac{F(C_{m_{in}} - C_m)}{V} \tag{20}$$

$$\frac{dC_I}{dt} = -k_I C_I + \frac{F_I C_{I_{in}} - FC_I}{V} \tag{21}$$

$$\frac{dD_0}{dt} = (0.5k_{Tc} + k_{Td})P_0^2 + k_{fm}C_m P_0 - \frac{FD_0}{V} \tag{22}$$

$$\frac{dD_1}{dt} = M_m(k_p + k_{fm})C_m P_0 - \frac{FD_1}{V} \tag{23}$$

$$\frac{dT}{dt} = -k_p \cdot C_m \cdot \frac{(-\Delta H_P)}{\rho \cdot C_p} \cdot P_0 - \frac{U \cdot A}{\rho \cdot C_p \cdot V}(T - T_j) + \frac{F \cdot (T_{in} - T)}{V} \tag{24}$$

$$\frac{dT_j}{dt} = \frac{F_{cw}}{V_o} \cdot (T_{w_o} - T_j) + \frac{U \cdot A}{\rho_w \cdot c_w \cdot V_o}(T - T_j)$$

$$\text{with } z = \frac{D_1}{D_0}, k_i = Z_i \cdot \exp\left(\frac{-E_i}{R \cdot T}\right), P_0 = \left[\frac{2f^* k_I C_I}{k_{Td} + k_{Tc}}\right]^{0.5} \tag{25}$$

Performance of Embedded Control. The first part of this case study will illustrate in detail the application of the proposed methodology. In order to test the effectiveness of the embedded control optimization algorithm, different designs were obtained by varying the reactor volume, reaction temperature and monomer flow. For these design alternatives, embedded control optimization was carried out for varying input conditions. Figure 8 displays the effective product quality control under the influence of monomer feed concentration disturbances and model uncertainty. The first 1,000 integration steps were devoted to system identification, while the subsequent 4,000 steps performed adaptive model prediction and calculated optimal control action using the embedded control algorithm. As a further illustration, Figure 9 displays satisfactory step responses for two designs with residence time (V/F = 1 and V/F = 0.5) under embedded control for a set point change. When the process design and its dynamics are altered during the master design optimization, the embedded control automatically adapts to the new system dynamics. These results demonstrate the suitability of the adaptive system identification to capture nonlinear system dynamics for different candidate designs.

Integrated Design and Control. Following the proposed methodology, an uncertain space with 30 random samples was considered. The initial guess for the base case was a reactor volume $V = 1\text{m}^3$, an operating temperature of 296 K, and a desired product quality of 25,000 kg/kmol. The initial design and its initial sample set were submitted to the embedded control optimization of Problem-C. The design master loop found in the first round an optimal reactor volume of $V = 0.93$ m^3. The best control set points to achieve the desired polymer quality were found to be 24,978 kg/kmol for the product, and 294 K for the reactor

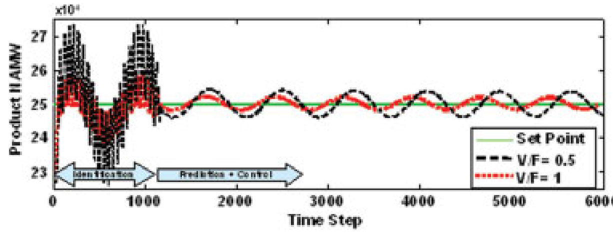

Figure 8. Product NAMW control for different designs and monomer concentration disturbance.

Two designs with different residence time (V/F) were considered (V/F = 1 and V/F = 0.5). [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

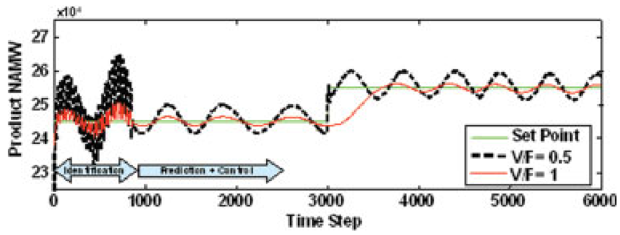

Figure 9. Product quality control for different designs and monomer concentration disturbance.

For illustration the set-point tracking response, two designs with different residence time (V/F) were considered (V/F = 1 and V/F = 0.5). [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

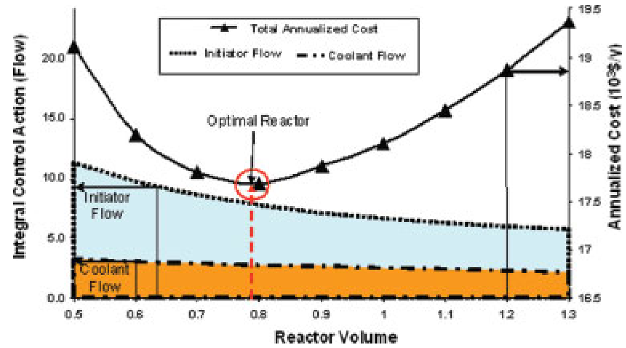

Figure 10. Overall performance of the integrated design and control of polymer quality, larger reactor volumes require less control action.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

temperature control. This tentative design was then tested for flexibility. The flexibility problem detected additional critical scenarios. These critical scenarios were added to the original uncertain scenario set and the master design optimization loop was repeated. Figure 10 shows that the optimal reactor size found in the simultaneous design and control optimization. Other sub-optimal design solutions are also displayed for comparison.

Problem-C: Optimal design problem with embedded control optimization

$$\min_{d} \; Exp[Cost(d, \theta, \xi(t), x(t), u(t))]$$

$$s.t. \; \min_{K^*} J = \sum_{0}^{\infty} (x_k^T \, S \, x_k + u_k^T \mathcal{T} \, u_k)$$

$$s.t. \; x_{k+1} = A_k x_k + B_k u_k^* \; u_k^* = -K^* x_k$$

$$\min_{A_k, B_k} \Delta_{\mathrm{LSQ}} = \sum_{k=1}^{r} [x(k) - \hat{x}(k)]^2 \qquad (26)$$

Our novel procedure converged reliably to the optimal reactor size along with necessary control decisions from arbitrary initial guesses. The optimal solution suggested a smaller reactor than our initial guess. The smaller reactor is more sensitive to disturbances, but permits tighter control. Figure 10 also displays cost, as well as the integral control action of several other reactor sizes. These trends suggest a reduction in necessary control action with increasing reactor volume; thus, confirming that larger reactors are less susceptible to input disturbances. For the illustration, suboptimal designs corresponding to different reactor volumes were explored sequentially; however, the optimal solution was identified independently. Another highly desirable consequence of embedding control technique is the smooth cost and control trajectories. In contrast, the traditional practice of direct and simultaneous design and control optimization often lead to discontinuous jumps in cost and control action, severely hampering the reliability of computational techniques.

Case Study-B: Integrated design and control of a binary distillation column

This second case study demonstrates the effectiveness of the embedded control scheme for the integrated design and control of a binary distillation column accounting for tray equilibria, reboiler and condenser holdups as shown in Figure 11. Open design choices include optimal number of stages, column diameter and feed stage location. The control variables are top and bottoms compositions; manipulated variables are the reflux and reboiler ratios. The desired product and bottoms compositions constitute the process specifications, referred to as design constraints in the Implementation of embedded control optimization section. Product composition outside the quality limits ($x_d \leq 0.995$ or $x_b \geq 0.02$) are considered unacceptable waste and must, therefore, be avoided in any event. The uncertainty sources are varying feed quality and temperature, thermodynamic vapor-liquid equilibrium parameters, and the steam quality in the reboiler. Table 4 lists the different variables and their categories considered for the case studies. The distillation cost models are derived from literature.[76]

Embedded Control Performance. This case study demonstrates the suitability of the proposed embedded control to

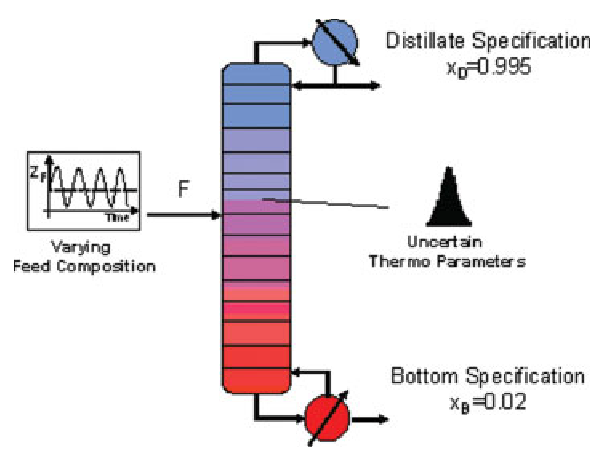

Figure 11. Distillation column of case study 2.

The cutoff quality limits are 0.995 for the distillate and 0.02 for the bottoms. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

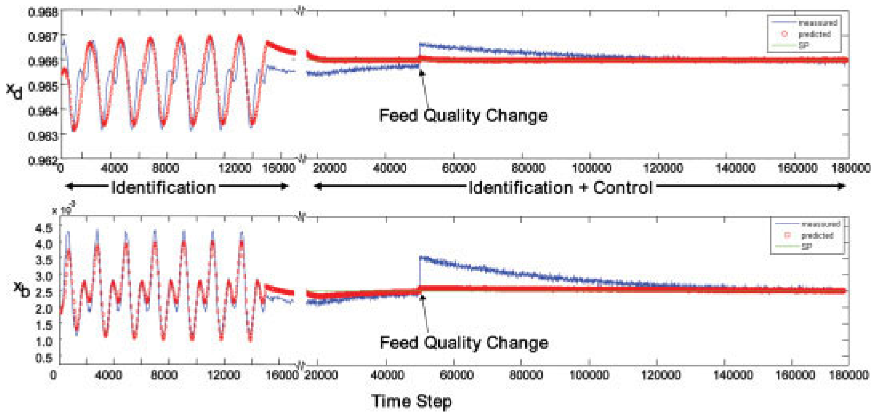

Figure 12. Top and bottom compositions trajectories with the embedded control under a sequence of uncertain scenarios.

One event at $t = 50{,}000$—a sudden change in feed composition—is highlighted for clarity. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

efficiently control a multivariable system. The initial guess for the column had 16 stages and a feed location in stage 7. Figure 12 depicts the measured variables trajectories, in which the first 16,000 time steps were used to identify the system dynamics. Upon stabilization of the identification phase, the embedded control optimization is enabled with an initial set point estimate of 0.996 for the light top composition, and 0.0025 for the bottoms. Figure 13 depicts the performance of the manipulated variables under the influence of the sequence of uncertain events. The step response of the embedded control system to an abrupt change in feed composition occurring at $t = 50{,}000$ is satisfactory, and highlighted for clarity. Note also that control action is necessary throughout the entire time horizon to dissipate the disturbances that were incorporated in the uncertainty scenarios. The plots in Figure 12 and Figure 13 have two timescales in order to better illustrate identification and optimization phases.

Integrated Design and Control. Table 5 summarizes the evolution of the optimal design with embedded control optimization (Problem-C) during the iterations of the integrated design and control algorithm. Starting from the initial design guess, which did not address control quality, the number of stages is gradually reduced in the master optimization procedure. This case study demonstrates the feasibility of considering simultaneously the design together with its control. These results demonstrate the potential improvements attainable by design and control integration, which would lead to more economical processes that safely accommodate all the expected uncertainty without the need for arbitrary overdesign currently practiced in industry.

Computational performance

The total CPU time of the stochastic design optimization with embedded control was typically two to three orders of magnitude faster than the direct and simultaneous optimization approach. The integrated design and control optimization for the polymerization according to Problem-C was implemented with Matlab/Tomlab for rapid prototyping. Tomlab[77] offers Matlab interfaces to access commercial mathematical programming methods (minlpBB, MINOS, CONOPT, SNOPT, CPLEX, Xpress). We expect further dramatic CPU

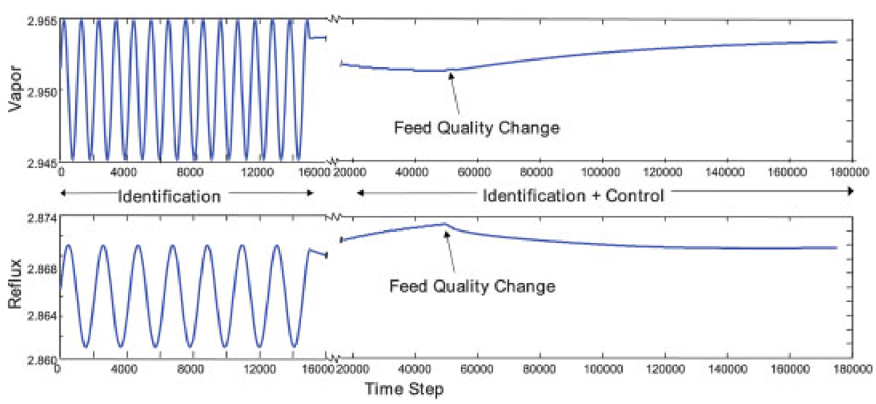

Figure 13. Reflux and stripping flows trajectories (controlled variables) with the embedded control under uncertain scenario realization.

One event at $t = 50{,}000$—a sudden change in feed composition—is highlighted for clarity. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Table 5. Progress of Iterations for the Dynamic Integrated Design and Control Problem

	Iteration			
	Initial	5	10	25
Stages number	16	11	10	9
Feed location	7	5	5	5
Diameter (m)	0.45	0.38	0.35	0.3
Capital cost (k$)	515.07	514.07	514.14	514.44
Operating cost (k$)	300.98	204.91	200.98	192.47
Total cost (k$)	816.07	714.98	719.12	706.91

time reductions when replacing Matlab, which is known to become slow in larger optimization problems. However, the traditional brute force simultaneous design and control optimization did often not converge, even after more than 24 CPU h when using minlpBB. The slow convergence is due to the bigger search space, and the presence of extra integer variables accounting for different control structures. The CPU time for one design of the stochastic design optimization with optimal embedded control took about 60 CPU s for the reactor, and about 160 CPU s for the distillation column as summarized in Table 6. The CPU time was independent of the design variable set and the uncertain scenarios. In contrast, one iteration of the simultaneous design and control optimization consumed more than two CPU h in our computational experiments. The presented computational experiments demonstrate the performance increase and reliability of the proposed embedded control strategy. More importantly the proposed procedure always converged, while the simultaneous effort often failed. The results suggest that the proposed embedded control is a robust technique and necessary milestone toward advancing integrated design and control.

Discussion and limitations of the proposed embedded control methodology

Control Optimality. The stochastic design master optimization with embedded control design is *not* meant to represent the actual control implementation. Rather, it computes an implicit relation of design and control decisions to rapidly screen the infinite design space. It is a "strategy" to recast the integrated design and control problem into a solvable mathematical programming format. In effect, for each design and uncertainty scenarios close-to-optimal control decisions including structural pairing decisions are taken without burdening the master optimization problem. Thus, near optimal control moves are considered in the evaluation of the process performance without solving a control parameter tuning and configuration problem simultaneously, which is prohibitively difficult. Moreover, embedded control ensures closed-loop stability without resolving to troublesome nonlinear stability criteria. Therefore, steps 2, 3 and 4 of Figure 5, significantly benefit from the embedded control optimization.

There is no claim that the embedded control will be globally optimal or that no better control options existed. However, an excellent judgment of *dynamic process performance with control* we believe is possible, based on the proposed integrated design and control strategy. Also the embedded control scheme is not intended to tackle real-time optimization challenges of highly nonlinear process control problems. For developments in real-time optimization, readers should consult different sources.[78–81] Once a superior candidate design has been identified, a detailed control optimization is possible and desirable. A subsequent detailed control optimization is feasible in advanced stages, since many suboptimal structural design decision variables will have been eliminated. Alternatives to the selected control techniques are summarized in Table 7. More sophisticated algorithms, such as subspace identification,[82] Linear MPC, [60–64] parametric MPC[83,84], DMC,[59–65] can further improve control performance for a particular design. Nonlinear state-space estimation could offer potential further advancements of the proposed method. However, these advanced control and identification techniques are not recommended for conceptual design and control integration, since advanced algorithms comes for the price of higher computational cost in each embedded control optimization.

Interaction Between Design and Control Variables. We have noticed that not all first stage variables are independent. In the reactor case study, the operation temperature is intrinsically related to the reactor size; since a change in the residence time requires adjustment of the steady-state relation of these design variables. Therefore, different reactor volumes require corresponding operating temperature set points. Maintaining the same temperature for different sizes could cause the reactor to operate in undesired steady states due to multiplicity. In addition, it may force control action at nominal condition, even if there are no disturbances. A similar problem arises in the second case study where the column diameter, length, operating flows, and desired compositions are not independent variables. Hence, different design choices require corresponding adjustments for all control targets (set points). We propose to initially use engineering insight to establish meaningful design and control variables targets. We have noticed that without attention to reasonable relationships, the numerical convergence of the mathematical programs suffers. As a solution to this problem, the steady state equation-based models were solved to correlate design pa-

Table 6. Computational Performance for the Case Studies in Design and Control Integration

Case Study		Embedded Control Strategy		Simultaneous Solution	
		CPU Time	Convergence	CPU Time	Convergence
Polymerization reactor	Single iteration	60 s	Always	>2hr	Yes, sometimes
	Total	2 hr	Always	>24hr	No
Distillation column	Single iteration	160 s	Always	>2hr	Yes, sometimes
	Total	5.5 hr	Always	>24hr	No

Table 7. List of Methods to Implement Embedded Control Optimization

Problem	Solutions
Identification	Sequential Least Squares
	Subspace Identification
	Neural Networks
Observer	Luenberger Observer
	Kalman Filter
	Extended Kalman Filter
Control	Linear Quadratic Regulator
	DMC
	Linear MPC
	Non-Linear MPC
	Parametric MPC
Optimization	rSQP
	Evolutionary Algorithms

Underlined methods were used for the case studies.

rameters with set points that satisfied the steady state conditions. Base designs with steady-state consistent control set points were used as initial guess for the optimization loop.

Optimal trajectory design. Our novel formulation approach is not limited to static set points. The proposed method can be reformulated to solve for optimal set-point trajectories inside the master optimization problem.

Conclusion and Future Directions

This article advocates the integration of design and control for the consistent attainment of stringent product quality demands. This article presents a decision-making hierarchy that allows designers to arrive at key structural decisions for process flowsheet and control layout, and to optimize them simultaneously for high-performance under realistic uncertain operating conditions. Conceptual approaches to achieve the desired integration of design and control were made possible thanks to a novel problem formulation that implicitly relates closed-loop dynamics with design decisions. As a result, an integrated optimal design with feedback control was obtained. This new integrated design can satisfactorily operate under adverse input conditions, while delivering products within desired quality specifications. Rigorous mathematical programming approaches are presented for optimizing parametric design variables, as well as structural alternatives. The novel design and control integration also provides analytical methods to ensure desired production quality standards in the presence of uncertainty. The case studies suggest that the proposed methodology has the potential to address challenges of realistic industrial complexity. Future work will focus on improving computational methods to globally ascertain the process flexibility using evolutionary and stochastic optimization techniques.

Acknowledgments

Financial support from NSF Grant CBET-0626162 and the Environmental Manufacturing Management (EvMM) fellowship for Andres Malcolm from the UIC Institute for Environmental Science and Policy are gratefully acknowledged. The summer research experience of Jamie Polan was supported by an REU supplement to NSF Grant DMI-0328134.

Notation

A = parameter matrix in state-space model
B = parameter matrix in state-space model
c = control decision
C = measurement matrix
C_m = the monomer concentration, kmol/m^3
$C_{m_{in}}$ = the monomer concentration in the monomer inlet stream, kmol/m^3
C_I = the initiator concentration, kmol/m^3
$C_{I_{in}}$ = the initiator concentration in the initiator inlet stream, kmol/m^3
C_p = heat capacity of the reacting mixture, kJ/kg·K
c_w = heat capacity of water, kJ/kg·K
d = design decisions
D_0 = molar concentration of the bulk zeroth moment of the polymer chain length, kmol/m^3
D_1 = mass concentration of the bulk first moment of the polymer chain length, kg/m^3
E_i = activation energies, kJ/kmol
F = volumetric flow rate of the monomer, m^3/h
F_I = volumetric flow rate of the initiator, m^3/h
F_{cw} = volumetric flow rate of the cooling water, m^3/h
ΔH_p = heat of propagation reaction, kJ/kmol
k_{ij} = temperature-dependent rate constants
K^* = control gain
M_m = molecular weight of the monomer, kg/kmol
Q = covariance matrix
R = covariance matrix
S = weighting matrix
t = time, s
T = the reactor temperature, K
T = weighting matrix
T_j = the cooling jacket temperature, K
U = overall heat-transfer coefficient, kJ/m^3·h·K
V = the reactor volume, m^3
V_0 = overall effective volume of the cooling system, m^3
X = state variable
x_d = distillate composition
x_b = bottom composition
z = the average molecular weight, kg/kmol
Z_i = Frequency factors in Arrhenius equations, kmol/m^3·h

Greek letters

δ = flexibility index
θ = static parametric uncertainty
ρ = density, kg/m^3
ξ = time-dependent uncertainty source or disturbance
Ω = uncertain space

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Appendix A - Existence and Stability of the LQR Solution

Given the *LQR* problem with $T > 0$, and $S = C^T C$, where the pair $(A;C)$ is observable, and the pair $(A;B)$ is controllable, it can be proved that a solution to the steady state *LQR* problem exists.[85] In particular, there exists a unique positive semidefinite solution P^* to the algebraic Riccati Eq. A1. If K^* is defined as in Eq. A2, then the closed loop system is asymptotically stable.[71,72] Self-adaptiveness makes the proposed embedded control applicable even to highly nonlinear processes

$$0 = A^T PA - P - (A^T PB)(B^T PB + T)^{-1}(B^T PA) + S \quad \text{(A1)}$$

$$K^* = (B^T P^* B + T)^{-1}(B^T P^* A) \quad \text{(A2)}$$

Appendix B - Glossary

Flexibility

The ability of a system to operate without violating design constrains even under changing conditions or variations of uncertain parameters. It is the ability to maintain feasible operation over the entire range of uncertain conditions. Synonyms: robustness, feasibility.

Static and dynamic flexibility

Static flexibility signifies that a process can handle all uncertain conditions at steady state. Dynamic flexibility describes processes, whose dynamic performance and transient state trajectories stay within specifications throughout the entire time horizon. Dynamic flexibility implies static flexibility. The converse is not true.

Flexibility index

The flexibility index measures the size of the uncertain parameter variations for which feasible operation can be guaranteed. It is a scalar quantity equal to the normalized deviation from the nominal point at which the nearest critical constraints are violated.

Solvability

Solvability means the existence of a solution satisfying all constraints. The term usually implies the ability to reach this solution by a numerical procedure implemented on a digital computer.

Uncertainty

The possibility of parameters assuming values within a finite range rather than a precise value introduces variable outcomes referred to as uncertainty. The sources of uncertainty in a process may be either internal (such as physical properties, transfer coefficients, and so on), and/or external (such as feed quality, product demands and specifications, prices, and so on). In process control, uncertainty in operating conditions is often referred to as a disturbance.

Manuscript received Oct. 30, 2006, and revision received Apr. 23, 2007.