Optimal Design of Dynamic Systems under Uncertainty

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Fundamental developments of a unified process design framework for obtaining integrated process and control systems design, which are economically optimal and can cope with parametric uncertainty and process disturbances, are described. Based on a dynamic mathematical model describing the process, including path constraints, interior and end-point constraints, a model that describes uncertain parameters and time-varying disturbances (for example, a probability distributions or lower/upper bounds), and a set of process design and control alternatives (together with a set of control objectives and types of controllers), the problem is posed as a mixed-integer stochastic optimal control formulation. An iterative decomposition algorithm proposed alternates between the solution of a multiperiod "design" subproblem, determining the process structure and design together with a suitable control structure (and its design characteristics) to satisfy a set of "critical" parameters/periods (for uncertainty disturbance) over time, and a time-varying feasibility analysis step, which identifies a new set of critical parameters for fixed design and control. Two examples are detailed, a mixing-tank problem to show the analytical steps of the procedure, and a ternary distillation design problem (featuring a rigorous tray-by-tray distillation model) to demonstrate the potential of the novel approach to reach solutions with significant cost savings over sequential techniques.

Introduction

Despite their industrial relevance, flexibility—the ability of a system to readily adjust in order to meet the requirements of changing (usually steady-state) conditions—and controllability— the ability of a system to recover from process disturbances or dynamic plant behavior—have not been considered in most process synthesis tools as distinct design objectives. In contrast to other sectors, such as flexible manufacturing, the common practice in the process industry has traditionally been to base the design on steady-state economics for nominal and fully specified conditions, and then use overdesign factors, design of control systems, and "retrofit" remedies to overcome operability bottlenecks and problems. Nevertheless, it has been realized that such a sequential approach may in fact lead to more expensive or less efficient design options. In this context, flexibility and controllability clearly affect the long-term economic operation of a plant (Grossmann and Morari, 1983).

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During the last 15 years, the problems of including flexibility, controllability, and control-system design at the process synthesis/design stage have started to receive attention. Flexibility in optimal process design under uncertainty has been considered among other aspects in the work of Grossmann and coworkers at Carnegie Mellon (see Grossmann and Straub, 1991, for a recent review); controllability aspects in design are considered, for example, in the recent work of Luyben and Floudas (1994a,b) by a multiobjective optimization framework; control structure selection issues are considered in the work of Narraway and Perkins (1993a,b), and Heath et al. (1994). Recently, Bahri et al. (1996) considered aspects of parametric uncertainty and disturbances in control optimization.

However, synthesis/design approaches that consider both flexibility and controllability aspects are rather limited. Papalexandri and Pistikopoulos (1994a,b) proposed a methodology for the synthesis of optimal and flexible heat-exchanger networks that also satisfy steady-state open-loop controllability criteria in a simultaneous fashion. Walsh and Perkins (1994) introduced an integrated design strategy for including aspects of flexibility in their optimal design and control formulation. Based on a dynamic process description, their approach couples multiperiod design concepts with controllability analysis for fixed system structure (no synthesis considerations). Overviews of recent developments in the area of process design and operations under uncertainty are given in Morari and Perkins (1994), Perkins and Walsh (1994), and Pistikopoulos (1995).

This article will present a conceptual process design framework for addressing the problem of optimal design of dynamic systems under uncertainty, in which flexibility aspects and control design considerations are simultaneously incorporated. The article is structured as follows. First, we introduce the various attributes and the basic nomenclature of the problem by way of a distillation column design problem. We then describe the details of the conceptual process design development. Finally, we propose an iterative decomposition algorithm for the solution of the resulting mixed-integer stochastic optimal-control formulation—the approach is illustrated with two detailed process example problems.

Problem Statement

The process synthesis problem to be addressed in this article can be formally stated as follows:

Given:

(i) A process model, which is described by a set of differential and algebraic equations (DAEs), and appropriate initial conditions.

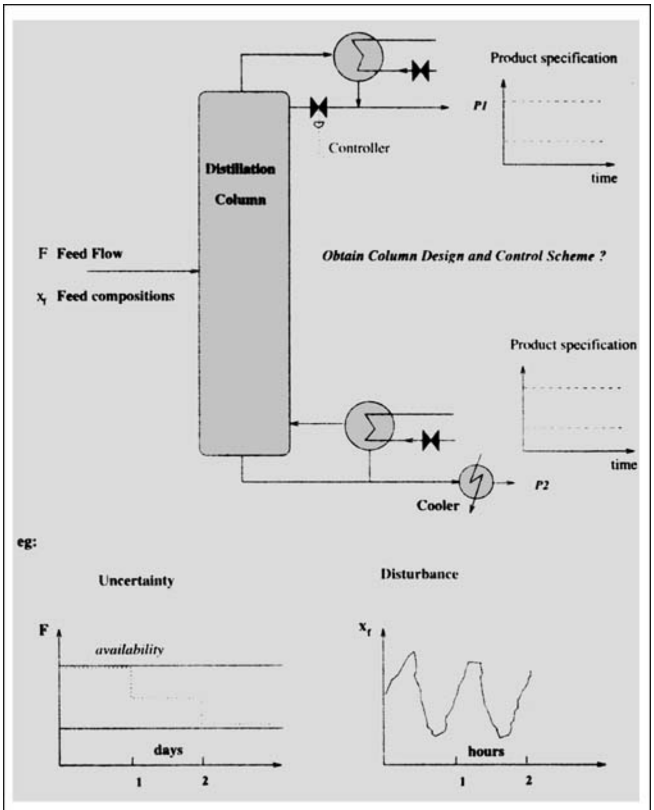

Figure 1. Motivating example.

Table 1. Ternary Separation Feed-Stream Data

Flow (mol/h)	Composition	Temp.
600	$X_{hexane} = 0.08$ $X_{heptane} = 0.12$ $X_{toluene} = 0.80$	60°C

(ii) A set of path and/or interior-point and endpoint constraints, for feasible plant operation (such as product specifications and safety constraints).

(iii) A model for the description of the uncertainty involved in the process, typically described by lower/upper bounds or probability distribution functions.

(iv) A set of process design alternatives (process superstructure).

(v) A set of control alternatives (i.e., a set of potential-manipulated variables and potential measurements–control superstructure) together with a set of control objectives to be achieved and types of controllers to be used in achieving them.

(iv) Cost data associated with equipment, operating, and controller costs.

(vii) A finite time horizon of interest.

The *objective* is then to obtain an optimum set of design variables and a control scheme at minimum total annualized cost, while ensuring feasible operation over the entire time horizon under the specified uncertainty.

In order to gain more insight into the nature of the problem, consider the distillation column of Figure 1, where a ternary mixture of *n*-hexane, heptane, and toluene is to be separated into two product streams. Nominal data for the feed stream flow rate, composition, and temperature are given in Table 1, and specifications of the product flow rates, composition, and temperature are listed in Table 2.

The process model describing the distillation column design and operation is given by a set of DAEs for mass, composition, energy, and equilibrium relationships on a tray-by-tray basis for the three-column compartments, the rectifying/stripping/condenser/reflux-drum, the column base/reboiler and bottom tray sections, respectively. The detailed mathematical model is given in Appendix A.

Feasible operation of the distillation column is ensured by 12 path constraints, the product specifications, flooding and weeping flow-rate requirements, and operating limits for the condenser and reboiler, respectively. These constraints must be met in spite of the presence of variability in the feed stream flow rate (due to process interactions) and feed composition, as given in Table 3. Note that two types of variability are considered, parametric uncertainty (feed-stream flow rate), which can be either time-invariant or varying on long-time-scale, and disturbances (feed compositions), characterized by

Table 2. Product Specifications

Stream	Flow (mol/h)	Composition	Temp.
P1 (distillate)	≥ 76.0	$X_{hexane} \geq 0.60$ $X_{heptane} \geq 0.25$ $X_{toluene} \leq 0.01$	≤ 60°C
P2 (bottoms)	≥ 513.0	$X_{hexane} \leq 0.01$ $X_{heptane} \leq 0.09$ $X_{toluene} \geq 0.90$	≤ 60°C

Table 3. Uncertainty and Disturbance Description

Variable	Range	Time Variation
Feed Rate	600 (±10) mol/h	Uncertainty
Composition		Disturbance
X_{hexane}	0.08 (±10%)	Sinusoidal
$X_{heptane}$	0.12 (±10%)	1-h Period
$X_{toluene}$	$1\text{-}X_{hexane}\text{-}X_{heptane}$	
Cooling water temperature	20°C (±25%)	Sinusoidal 1-h Period

high characteristic frequency (fast uncertainty), as shown in Figure 1.

A degrees-of-freedom analysis reveals that there are three adjustable variables, the reflux-ratio, and the reboiler and condenser heat duties, respectively, which can in principle be adjusted during operation to offset the effects of parametric uncertainty and disturbances. We associate potential proportional-integral (PI) control schemes (see Figure 1) to these three adjustable variables to control the effect of disturbances and feed flow-rate parametric uncertainty.

The objective is then to design the distillation column and the required control scheme at minimum total annualized cost (comprising investment and operating costs including controller costs), able to maintain feasible operation in the presence of the involved variability. This requires the determination of (1) an optimum set of design variables (number of trays, feed-tray location, column diameter, condenser, and reboiler heat-exchanger areas); (2) an optimal control structure (in terms of best selection/pairing of controlled-manipulated variables; for example, condenser duty-heptane distillate composition pairing), and (3) the corresponding optimal values of the controller parameters (such as controller gain, integral time, and actuator offset).

In the next section, the key building blocks for the development of a conceptual mathematical formulation for the problem as stated earlier will be presented in detail.

Conceptual Mathematical Formulation

We consider a process model described by a set of ordinary differential and algebraic equations and inequalities of the following form:

$$\begin{aligned} &\dot{x}(t) = h_l(d,x(t),Z(t),\Theta(t),t) && l \in L \\ &f_q(d,x(t),Z(t),\Theta(t),t) = 0 && q \in Q \\ &x(0) = x_o \\ &g_k(d,x(t),Z(t)\Theta(t),t) \le 0 && k \in K, \end{aligned} \quad (1)$$

where d is the vector of design variables (including 0–1 binary variables) that remain constant at the operation stage; k, l, and q are the index sets of inequality constraints, differential, and algebraic equations, respectively; $x(t)$ is the vector of time-dependent state variables, such that $\dim\{x\} = \dim\{h\}$; Z and Θ are the time-dependent vectors of degrees of freedom and variabilities of the process, respectively; and t denotes time. Two types of inequality constraints are included in the vector g, path constraints, which have to be satisfied throughout the period of operation (such as product specifications), and interior and/or endpoint constraints, which are only imposed at specific times.

Following the discussion in the previous section, we partition the vector of variabilities Θ into two subsets, disturbances, $\nu(t)$, to denote variations with high characteristic frequency, and parametric uncertainty, θ, to denote variations on a longer time scale (for convenience in the presentation, θ and z are considered as time-invariant; yet slow time-varying variables can be treated in an identical way), that is,

$$\Theta(t) \equiv (\nu(t),\theta). \quad (2)$$

We also partition the vector $Z(t)$ of degrees of freedom into two subsets, $u(t)$ corresponding to the ones consumed by controllers in order to reject the disturbances $\nu(t)$, and adjustable variables z denoting the remaining degrees of freedom, which are allowed to compensate for the (slow) uncertain parameters, that is,

$$Z(t) \equiv (u(t),z). \quad (3)$$

By including Eqs. 2 and 3, Eq. 1 can be rewritten as follows:

$$\begin{aligned} &\dot{x}(t) = h_l(d,x(t),z,u(t),\theta,\nu(t),t) && l \in L \\ &f_q(d,x(t),z,u(t),\theta,\nu(t),t) = 0 && q \in Q \\ &x(0) = x_o \\ &g_k(d,x(t),z,u(t),\theta,\nu(t),t) \le 0 && k \in K. \end{aligned} \quad (4)$$

Equation 4 describes the behavior of the time-varying process. However, since Eq. 4 additionally involves uncertainty, θ, and disturbances, $\nu(t)$, a full description of the process behavior requires the consideration of the following two key features:

- feasibility of operation in the presence of any possible realization of θ and $\nu(t)$, and
- control scheme definition.

The feasibility requirement (Dimitriadis and Pistikopoulos, 1995) for a system described by Eq. 4 and by considering a finite time horizon of operation t_f, can be stated as follows: *Ensure that, for any possible profile of θ and $\nu(t)$, there exist profiles of z and $u(t)$ such that the constraints in Eq. 4 are satisfied at any time $t \in [0, t_f]$*; or in a mathematical form:

$$\max_{\substack{\theta \in T \\ \nu(t) \in V(t)}} \min_{\substack{z \in Z \\ u(t) \in U(t)}} \max_{\substack{k \in K \\ t \in [0,t_f]}} g_k[d,x(t),z,u(t),\theta,\nu(t),t] \le 0$$

$$\begin{aligned} &\dot{x}(t) = h_l[d,x(t),z,u(t),\theta,\nu(t),t] && l \in L \\ &f_q[d,x(t),z,u(t),\theta,\nu(t),t] = 0 && q \in Q \\ &x(0) = x_o \\ &t \in [0,t_f] \end{aligned} \quad (5)$$

where

$$T = \{\theta, \theta^l \le \theta \le \theta^u\}, \qquad V(t) = \{\nu(t), \nu(t)^l \le \nu(t) \le \nu(t)^u\}$$

$$Z = \{z, z^l \le z \le z^u\}, \qquad U(t) = \{u(t), u(t)^l \le u(t) \le u(t)^u\}$$

and θ and $\nu(t)$ can be alternatively given via probability distribution functions. Note that the profiles of θ, $\nu(t)$, z, and

$u(t)$ represent an infinite number of decision variables; however, as will be shown in the next section, all time-dependent variables are parameterized to make the number of decision variables finite, yet without assuming any specific knowledge of the uncertainty involved (for example, θ may be considered piecewise constant over a number of finite elements, $\nu(t)$ may be expressed as a function of prespecified form in which one or more parameters are to be determined, such as a sinusoidal function with variable amplitude and/or frequency).

We also introduce a set of constraints for the definition of an appropriate control scheme as follows. The vector of manipulated variables $u(t)$ is related to simple parameterized continuous profiles given by the optimization of PI multiloop controllers (Narraway and Perkins, 1993a,b), where both the control structure and the controller tuning parameters are variables for the optimization. This gives rise to the following set of constraints:

$$u_n = u_{o,n} + \sum_{m \in M} \Delta u_{nm} \tag{6}$$

$$e_{nm} = y_{\text{mes},m} - y_{\text{set},nm}$$

$$\dot{I}_{nm} = \frac{e_{nm}}{\tau_{nm}}$$

$$\Delta u_{nm} = KC_{nm}(e_{nm} + I_{nm})$$

$$KC^l_{nm} X_{nm} \leq KC_{nm} \leq KC^u_{nm} X_{nm}$$

$$\tau^l_{nm} \leq \tau_{nm} \leq \tau^u_{nm}$$

$$\sum_{n \in N} X_{nm} \leq 1$$

$$\sum_{m \in M} X_{nm} \leq 1$$

$$\forall n = 1,2,\ldots,N; \qquad \forall m = 1,2,\ldots,M; \qquad X_{nm} = [0,1]^{n \times m},$$

where X_{nm} is a vector of binary variables denoting whether (or not) a PI controller is used to control output, $y_{\text{mes},m}$, with manipulated variable, u_n. Δu denotes control action and u_o is the actuator offset (at $t = 0$, this corresponds to the steady-state value of u); e denotes the associated error; y_{set} is the controller set point; y_{mes} is the measurement; KC is the controller gain; and τ is the integral time. Note that the introduction of the multiloop PI-control superstructure constraints in Eq. 6 results in the controller set points, y_{set}, being the new set of manipulated variables (replacing $u(t)$), with controller tuning parameters (u_o, KC, τ) and the variables defining the actual control structure (X_{nm}) considered as design variables.

By incorporating Eq. 6, Eq. 5 can be rewritten as follows:

$$\max_{\substack{\theta \in T \\ \nu(t) \in V(t)}} \ \min_{\substack{z \in Z \\ y_{\text{set}}}} \ \max_{\substack{k \in K \\ t \in [0,t_f]}} g_k(d, x(t), z, u(t), \theta, \nu(t), t) \leq 0 \tag{7}$$

$$\dot{x}(t) = h_l[d, x(t), z, u(t), \theta, \nu(t), t] \qquad l \in L$$

$$f_q[d, x(t), z, u(t), \theta, \nu(t), t] = 0 \qquad q \in Q$$

$$x(0) = x_o$$

$$[\text{constraints in (6)}].$$

Note in Eq. 7 that the controller set points y_{set} can in principle be adjusted during operation to absorb the effect of disturbances $\nu(t)$; if this is not a "preferable" option (from an operational viewpoint due to the nonimplementable nature of the resulting control scheme) a constant over time vector y_{set} will be selected for all possible values of $\nu(t)$. Finally, an objective function accounting for the capital costs of the process units and controllers and operating costs, such as hot and cold utilities, is considered of the following form:

$$\min_{\substack{d,X \\ u_o, KC, \tau}} \ \underset{\substack{\theta \in T \\ \nu(t) \in V(t) \\ t \in [0,t_f]}}{E} \left\{ \min_{\substack{z \in Z \\ y_{\text{set}}}} P[d, x(t), z, u(t), \theta, \nu(t), t] + C^T X \right\}, \tag{8}$$

where P is a cost function, and C^T is the vector of control-loop costs. The expectation term in Eq. 8 accounts for the contribution to the cost of all possible realizations of θ and $\nu(t)$ over time; in this context, it represents an average expected cost estimate, which can be determined via a suitable integration scheme (Pistikopoulos, 1995), or alternatively approximated by a weighted summation term over a set of specified periods/critical uncertain parameters (Grossmann and Halemane, 1982; Papalexandri and Pistikopoulos, 1994a,b; Varvarezos et al., 1994). Note also that the inclusion of a term for the control-loop costs in the objective function permits comparison of control structures to be performed based on dynamic economic calculations for optimally tuned controllers. Of course, in practice, an integral error (ISE, IAE, etc.) term for tuning the controller for optimal system response can also be included.

The objective function, Eq. 8, together with the constraint set, Eq. 7, constitute the conceptual mathematical formulation for optimally designing dynamic systems under general uncertainty, denoted as Problem P:

$$\min_{\substack{d,X \\ u_o, KC, \tau}} \ \underset{\substack{\theta \in T \\ \nu(t) \in V(t) \\ t \in [0,t_f]}}{E} \left\{ \min_{\substack{z \in Z \\ y_{\text{set}}}} [d, x(t), z, u(t), \theta, \nu(t), t] + C^T X \right\} \tag{P}$$

s.t.

$$\max_{\substack{\theta \in T \\ \nu(t) \in V(t)}} \ \min_{\substack{z \in Z \\ y_{\text{set}}}} \ \max_{\substack{k \in K \\ t \in [0,t_f]}} g_k[d, x(t), z, u(t), \theta, \nu(t), t] \leq 0$$

$$\dot{x}(t) = h_l[d, x(t), z, u(t), \theta, \nu(t), t] \qquad l \in L$$

$$f_q[d, x(t), z, u(t), \theta, \nu(t), t] = 0 \qquad q \in Q$$

$$x(0) = x_o$$

$$u_n = u_{o,n} + \sum_{m \in M} \Delta u_{nm}$$

$$\Delta u_{nm} = KC_{nm}(e_{nm} + I_{nm})$$

$$e_{nm} = y_{\text{mes},m} - y_{\text{set},nm}$$

$$\dot{I}_{nm} = \frac{e_{nm}}{\tau_{nm}}$$

$$I_{nm}(0)=0 \qquad e_{nm}(0)=0$$

$$KC^l_{nm}X_{nm} \le KC_{nm} \le KC^u_{nm}X_{nm}$$

$$\tau^l_{nm} \le \tau_{nm} \le \tau^u_{nm}$$

$$\sum_{n \in N} X_{nm} \le 1$$

$$\sum_{m \in M} X_{nm} \le 1$$

$$\forall m = 1,2,\dots,M; \qquad \forall n = 1,2,\dots,N; \qquad X_{nm} = [0,1]^{n \times m}$$

$$t \in [0,t_f].$$

Note that Problem P corresponds to a mixed-integer stochastic nonlinear optimal control formulation, a class of problems whose direct solution is usually rather tedious. In the next section, however, we will present a decomposition algorithm that avoids the direct solution of Problem P and makes the problem much more computationally tractable.

Decomposition Algorithm

There are three main difficulties in directly addressing Problem P:

- The profiles of manipulated variables and uncertain parameter over time, z, $u(t)$, θ, and $\nu(t)$, respectively, represent an infinite number of decision variables; similarly, the number of constraints in Problem P is infinite.
- The objective function involves an expectation term over an optimization problem.
- A max-min-max optimization subproblem representing the feasibility requirements appears as part of the constraint space.

All three difficulties can be effectively overcome based on the following ideas. First, the differential equations in Problem P are converted to algebraic residual equations using orthogonal collocation on finite elements, as analytically shown in Appendix B. This transforms Problem P into a finite-dimensional (stochastic) mixed-integer nonlinear optimization problem. Then, by approximating uncertainty θ and disturbance $\nu(t)$ by a finite number of values (periods/scenarios), (1) expectancy can be replaced by a weighted summation term over the specified set of periods, and (2) the max-min-max operation can in fact be removed, provided that the inequalities in g_k are enforced over all periods. Based on these arguments, Problem P can be rewritten as follows:

$$\min_{\substack{d,X,z^1_{ij}\dots z^P_{ij},y^1_{\text{set}}\dots y^P_{\text{set}}\\ u_o,KC,\tau}} \times \left\{ \sum_p w_p P(d,d_c,x^p_{ij},z^p_{ij},y^p_{\text{set}},\theta^p_i,\nu^p_i,t_{ij}) + C^T X \right\} \quad \text{(P1)}$$

s.t.

$$g_k(X_{nm},d,x^p_{ij},u^p_{ij},z^p_{ij},\theta^p_i,\nu^p_i,t_{ij}) \le 0 \quad k \in K$$

$$\dot{x}^p_{N\text{col}+1}(t_{ij}) - h_l(d,x^p_{ij},u^p_{ij},z^p_{ij},\theta^p_i,\nu^p_i,t_{ij}) = 0 \quad l \in L$$

$$f_q(d,x^p_{ij},u^p_{ij},z^p_{ij},\theta^p_i,\nu^p_i,t_{ij}) = 0 \quad q \in Q$$

$$hc_n(u_o,KC,\tau,x^p_{ij},u^p_{ij},y^p_{\text{set}},\nu^p_i,t_{ij}) = 0 \quad n \in N$$

$$\theta^p_i = \{\theta^p_{i,1},\theta^p_{i,2},\dots,\theta^p_{i,j},\dots,\theta^p_{i,N\text{col}}\}$$

$$\nu^p_i = \{\nu^p_{i,1},\nu^p_{i,2},\dots,\nu^p_{i,j},\dots,\nu^p_{i,N\text{col}}\}$$

$$i \in Nfe, \qquad j \in N\text{col}, \qquad p \in TP,$$

where hc_n is a vector of the equalities in Eq. 6 for the control-structure selection subproblem; p ($p=1,\dots,TP$) is an index for the number of periods; w_p represents weights for each period; Nfe and Ncol denote the number of finite elements and collocation points (within each finite element), respectively.

Note that Problem P1 represents only an approximation (in fact an upper bound) to the solution of Problem P, with the two problems becoming identical at the limit when the number of periods goes to infinity (Grossmann and Sargent, 1978). Instead of arbitrarily selecting periods to determine the sets of uncertainty and disturbances, however, an explicit time-varying feasibility analysis step is introduced after the solution of Problem P1 to identify additional critical parameters/disturbances that may still violate the constraints of Problem P1.

For a fixed design and control scheme [(i.e., for known values of d, X, u_o, KC, τ), such a feasibility analysis step corresponds to the solution of the following problem following an active set strategy, Grossmann and Floudas (1987) and Dimitriadis and Pistikopoulos, (1995)]:

$$\chi(d,t_{ij}) = \max s_{ij} \quad \text{(P2)}$$

s.t.

$$\dot{x}_{N\text{col}+1}(t_{ij}) - h_l(d,x_{ij},z_{ij},u_{ij},\theta_{ij},\nu_{ij},t_{ij}) = 0 \quad l \in L$$

$$f_q(d,x_{ij},z_{ij},u_{ij},\theta_{ij},\nu_{ij},t_{ij}) = 0 \quad q \in Q$$

$$x_{10} = x_o$$

$$q_{k,ij} + g_k(d,x_{ij},z_{ij},u_{ij},\theta_{ij},\nu_{ij},t_{ij}) - s_{ij} = 0 \quad k \in K$$

$$hc_n(u_o,KC,\tau,x_{ij},u_{ij},y_{\text{set}},\nu_{ij},t_{ij}) = 0 \quad n \in N$$

$$\sum_l \mu^T_{l,ij}\frac{\partial h_l(t_{ij})}{\partial x_{ij}} + \sum_q \eta^T_{q,ij}\frac{\partial f_q(t_{ij})}{\partial x_{ij}} + \sum_k \lambda^T_{k,ij}\frac{\partial g_k(t_{ij})}{\partial x_{ij}} + \sum_n \alpha^T_{n,ij}\frac{\partial hc_n(t_{ij})}{\partial x_{ij}} + \dot{\mu}_{N\text{col}+1}(t_{ij}) = 0$$

$$\sum_l \mu^T_{l,ij}\frac{\partial h_l(t_{ij})}{\partial z_{ij}} + \sum_q \eta^T_{q,ij}\frac{\partial f_q(t_{ij})}{\partial z_{ij}} + \sum_k \lambda^T_{k,ij}\frac{\partial g_k(t_{ij})}{\partial z_{ij}} + \sum_n \alpha^T_{n,ij}\frac{\partial hc_n(t_{ij})}{\partial z_{ij}} = 0$$

$$\sum_l \mu^T_{l,ij}\frac{\partial h_l(t_{ij})}{\partial u_{ij}} + \sum_q \eta^T_{q,ij}\frac{\partial f_q(t_{ij})}{\partial u_{ij}} + \sum_k \lambda^T_{k,ij}\frac{\partial g_k(t_{ij})}{\partial u_{ij}} + \sum_n \alpha^T_{n,ij}\frac{\partial hc_n(t_{ij})}{\partial u_{ij}} = 0$$

$$\sum_{k \in K} \lambda_{k,ij} = 1$$

$$\left.\begin{aligned} \lambda_{k,ij} - Y_{k,ij} \le 0 \\ q_{k,ij} - U(1 - Y_{k,ij}) \le 0 \end{aligned}\right\} \qquad k \in K$$

$$\sum_{k \in K} Y_{k,ij} = (n_z + n_u) + 1$$

$$\theta_{ij}^{l} \le \theta_{ij} \le \theta_{ij}^{u} \qquad \nu_{ij}^{l} \le \nu_{ij} \le \nu_{ij}^{u}$$

$$Y_{k,ij} = \{0,1\}, \qquad q_{k,ij}, \lambda_{k,ij} \ge 0, \qquad \alpha_{n,ij}, \eta_{q,ij}, \mu_{l,ij} \in \Re$$

$$i \in [1, Nfe] \qquad j \in [0, N\mathrm{col}],$$

where q_k are (positive) slack variables; μ_l, η_q, α_n, λ_k are the Lagrange multipliers for the equalities h_l, f_q, hc_n and the inequalities g_k, respectively; s is a scalar; the 0–1 variable Y_k indicates whether the feasibility constraint g_k is active or not; n_u and n_z are the number of manipulated variables, $u(t)$ and degrees of freedom z, respectively.

Note that in Problem P2 the optimality conditions for the differential algebraic system were explicitly considered, where the adjoint variable profile was approximated by $\mu_{i,N\mathrm{col}+1}(t)$, a piecewise polynomial function of order $(N\mathrm{col}+1)$; that is, for each element:

$$\mu_{i,N\mathrm{col}+1}(t) = \sum_{j=0}^{N\mathrm{col}} \mu_{ij}\phi_{ij}(t), \tag{9}$$

where ϕ_{ij} is the Lagrange basis polynomial of order $(N\mathrm{col}+1)$ described in Appendix B. A brief discussion of the variational conditions required for the optimal control formulation in Eq. 5 (and feasibility Problem P2) is given in Appendix C.

If the solution of Problem P2 χ has a negative value, then the current design and control structure is feasible for all possible realizations of vector θ and $\nu(t)$, respectively. On the other hand, if χ takes a positive value, then "critical" values of the vectors θ and $\nu(t)$, for which violation of the constraints occur over time, are identified.

Problem P2 corresponds to a mixed-integer optimal control formulation (converted to a set of mixed-integer nonlinear programming problems via orthogonal collocation on finite elements), where no specific knowledge of the uncertainty/disturbance profile is assumed, except that time-dependent parameters are parameterized, assuming a piecewise constant/linear (with or without continuity) or any functional form over the finite elements considered, to make the number of variables finite. Note also that adaptation of manipulated variables is not based on perfect knowledge of the future values of uncertainties and disturbances, since critical periods will be evaluated at each time element by solving the feasibility test problem, Problem P2, in a multistage fashion (as discussed in the preceding section).

Problems P1 and P2 suggest that an iterative decomposition strategy can then be derived for the efficient solution of Problem P, as shown in Figure 2. This decomposition strategy essentially alternates between the solutions of the multiperiod design/control subproblem, Problem P1, providing an optimal set of design variables and control structure, able to accommodate uncertainty and disturbances at specified values/periods, and the feasibility analysis subproblem in Problem P2, providing a new set of critical periods to be further included in Problem P1. Such a strategy will converge to an optimal design and control scheme, being able to cope with the entire specified ranges of uncertainty and disturbances (Gustafson, 1981).

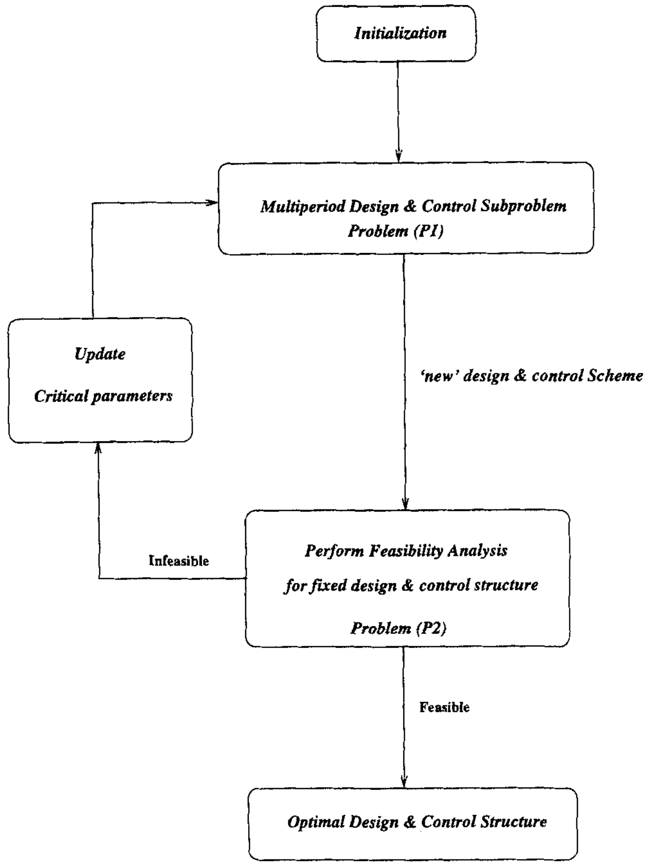

Figure 2. Basic steps of the decomposition algorithm.

The solution of the multiperiod problem, Problem P1, can be further decomposed following generalized Benders decomposition principles. By fixing the vector of discrete decisions X, that is, assuming a control scheme, Problem P1 reduces to a nonlinear programming (NLP) primal subproblem; its solution yields the optimal vector of design variables (d) and controller design parameters (u_o, KC, τ) while providing an upper bound to the solution of Problem P1. Then, a dual mixed-integer linear programming (MILP) master problem is constructed, based on Lagrange multipliers information from the primal problem, the solution of which returns a new control structure and provides a valid lower bound to the overall solution of Problem P1. Figure 3 shows the steps of the solution strategy proposed for the multiperiod design and control subproblem, Problem P1. The detailed analytical steps and formulations are shown in Appendix D.

Based on these developments, the proposed decomposition algorithm for the solution of Problem P, to optimally determine dynamic process design and control structure under uncertainty, involves the following steps (see also Figure 4):

Step 0 (Initialization). Define a time horizon t, $t \in [0, t_f]$. Set the values of uncertainty at their nominal values or define an initial set of periods, θ_i^o, ν_i^o, $k = 0$.

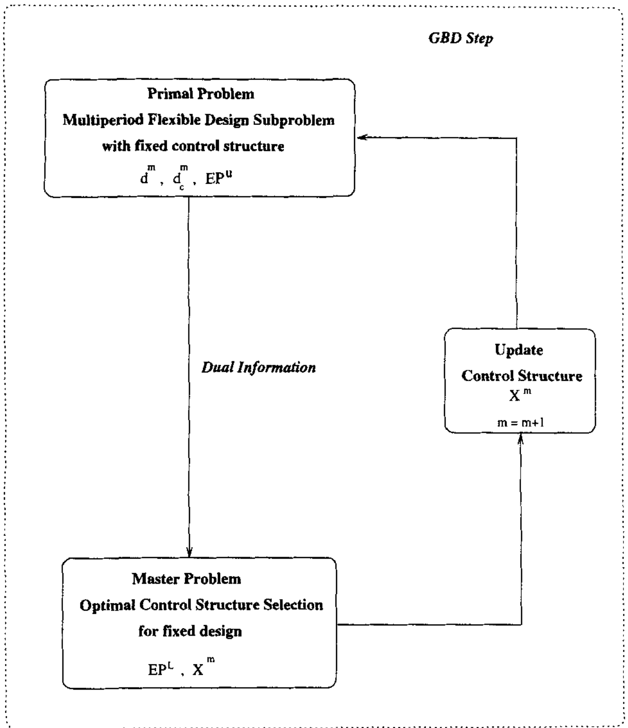

Figure 3. Multiperiod design and control subproblem block.

Step 1 (Multiperiod Design/Control Subproblem)

(i) Assume a control structure, X^k.

Iteration, $k = k + 1$

(ii) Solve the primal NLP problem of Problem P1 with fixed X, to obtain a set of design variables d^k, controller parameters $(u_o, KC, \tau)^k$, and an upper bound on expected cost, $EP^{u,k}$ (see Appendix D).

(iii) From the Lagrange multiplier information, construct and solve a master MILP problem of Problem P1. (With fixed d^k, u_o^k, KC^k, τ^k) to update control structure, X^k and obtain a lower bound of the expected cost, $EP^{l,k}$.

(iv) If $|EP^{u,k} - EP^{l,k}| \leq \epsilon$, Go to **Step 2**; Else, update X and go back to **Step 1(*ii*)**.

Step 2 (Feasibility Analysis). Solve Problem P2 with fixed value of d, X, and (u_o, KC, τ) at the optimal solution of Problem P1 in **Step 1**. If its solution $\chi(d, t)$ is negative, that is, feasibility is ensured, then STOP; an optimal solution has been obtained. Else, obtain new critical profile of uncertainty/disturbances, (θ_i^k, ν_i^k) and go back to **Step 1(*ii*)** (with $X^k = X^{\text{current}}$).

Note that both Steps 1 and 2 involve the solution of mixed-integer optimal-control formulations, which are in fact transformed to standard, albeit large-scale MINLP problems using the collocation technique outlined in Appendix B.

Remarks

While the proposed algorithm offers a useful, systematic framework to address design problems of dynamic systems under uncertainty, a number of issues involved in this development deserve further discussion.

First, from a theoretical viewpoint, it is essential to establish the theoretical properties required to guarantee optimal solutions in each step of the algorithm. For the solution of Problem P1 in step 1, since the 0–1 variables appear linearly (and thus separable) the conditions for convergence of the proposed generalized Benders decomposition scheme to the global optimum (in a finite number of iterations) require the functions g_k and P to be quasi convex in (z, u, d, d_c), and h_l, hc_n to be affine, in step 1(ii); note that the master problem in step 1(iii) will be a MILP for the PI-controller case considered in this work. The variational conditions given in Appendix C are necessary and sufficient for local optimality of Problem P2; furthermore, each square submatrix of dimension $[(n_z + n_u) \times (n_z + n_u)]$ of the partial derivatives of the constraints g_k, $k \in K$; h_l, $l \in L$; f_q, $q \in Q$; hc_n, $n \in N$, with respect to the control/optimization variables (z,u) has to be of full rank to ensure that $(n_z + n_u + 1)$ constraints are active (Madsen and Schjaer-Jacobsen, 1978). It is quite clear that these conditions are rather restrictive for general classes of chemical engineering problems, and in general little can be said regarding the "quality" of the solutions obtained following such an algorithmic approach; here, there is scope and strong incentive for developing rigorous global optimization methods to address general classes of nonlinear dynamic systems under uncertainty.

The use of a collocation technique to transform the mixed-integer optimal control formulations in Problems P1 and P2 to standard mixed-integer nonlinear programs is well known to substantially increase problem size. With the current state of codes available to solve subproblems, a relatively large-scale problem can be tackled (e.g., separators, reactors, heat exchangers). Efficient solution techniques are thus clearly required to ensure the applicability of the proposed framework to large-scale plantwide systems. Here, reduced space techniques coupled with the exploitation of the special banded structure of the equations offer enough hope for further investigation.

Stability is another critical issue. While external system stability (i.e., bounded system output for any bounded disturbance or input) is enforced in our algorithm by the interior point constraints (over the finite time horizon), internal or asymptotic stability (i.e., all the states remain bounded to any bounded disturbance) has not been addressed. Work on the systematic incorporation of robust stability criteria into the proposed design framework is currently under development.

The selection of a general optimal control structure is another issue not fully addressed. Here, we considered multiloop PI-controllers since they are the most widely used industrial controllers; however, optimal multiloop PI structures may not necessarily imply optimal control performance. While in principle one can argue that any general control-structure problem can be incorporated in the proposed algorithm, it is not yet obvious how this general problem should be posed.

In the next section, two example problems will be presented, a mixing tank to present in detail the steps of the proposed algorithmic procedure and a ternary distillation column design problem featuring a tray-by-tray rigorous model.

Example

Simple mixing tank

Consider a mixing tank as shown in Figure 5, where a hot-process stream from another process unit is mixed with a

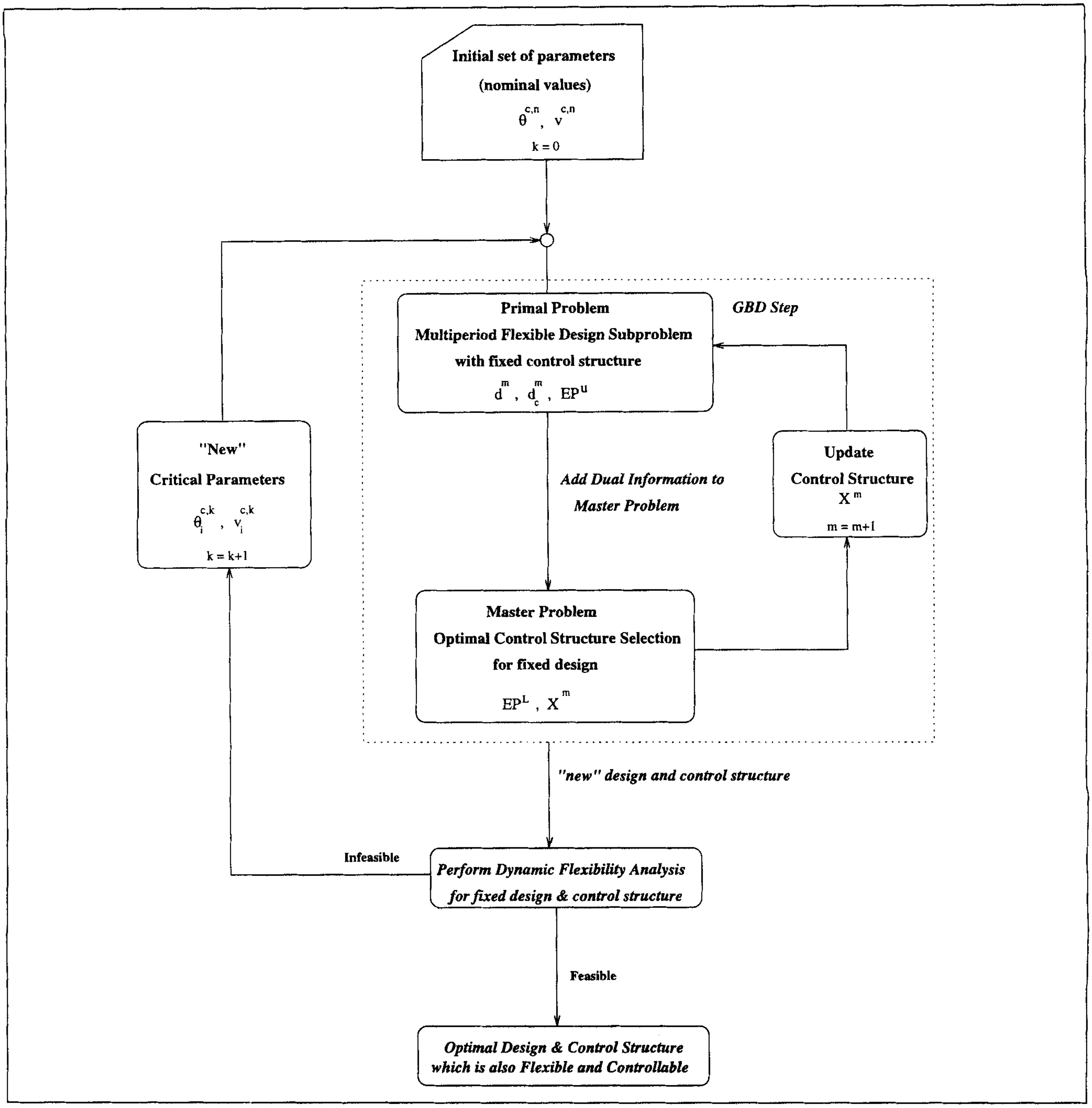

Figure 4. Proposed decomposition algorithm.

cold-process stream. The volume of the liquid in the tank, $V(t)$, and the outlet temperature are state variables that describe the system at time, t. The hot-process stream is faced with varying and changing conditions due to the upstream variations. The hot-feed flow rate, F_h, is a long-term *uncertain* variable, which varies between a lower and an upper bound, whereas the hot-stream temperature, $T_h(t)$, is a short-term *disturbance* described by variations between bounds. The cold feed stream is at constant temperature, T_c, with adjustable flow, F_c. The tank is well stirred and the density of fluid is assumed to be constant. The modeling equations arising from material and energy balances are as follows:

$$\frac{dV}{dt} = F_h + F_c - F(V)$$

$$F(V) = zV^{1/2}$$

$$V\frac{dT}{dt} = F_h(T_h - T) + F_c(T_c - T).$$

Uncertainty, $F_h(t)$, described by a lower and an upper bound:

$$F_h^l(t) \le F_h(t) \le F_h^u(t)$$

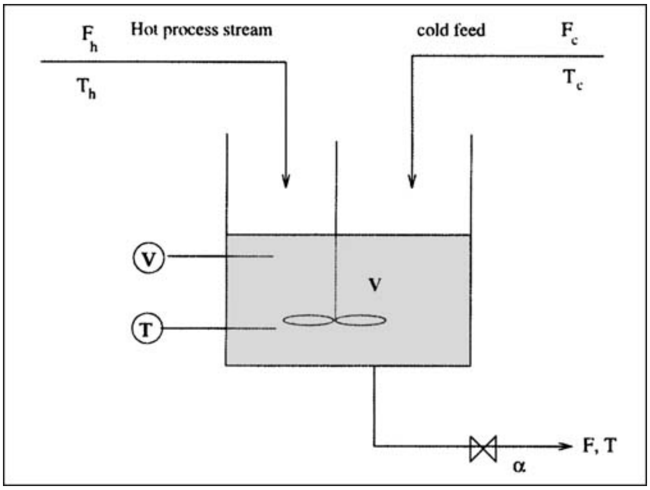

Figure 5. Stirred mixing tank requiring holdup and temperature control.

Disturbance, $T_h(t)$, description:

$$T_h^l(t) \le T_h(t) \le T_h^u(t).$$

Two degrees of freedom exist in this system, the valve constant z and cold feed, F_c. Additional constraints exist to limit the possible values of control variables between lower and upper bounds as follows:

$$z^l(t) \le z(t) \le z^u(t) \qquad F_c^l(t) \le F_c(t) \le F_c^u(t).$$

The initial state of the system can be specified as

$$V(0) = V^o, \qquad T(0) = T^o.$$

For the system to operate normally, both the volume and the temperature of the liquid in the tank should lie between certain limits. This requirement defines a set of inequality constraints that determine the feasibility of the system at any time (dynamic path constraints) as

$$V^l(t) \le V(t) \le V^u(t) \qquad T^l(t) \le T(t) \le T^u(t).$$

There is also an additional feasibility constraint restricting the tank holdup, $V(t)$, from exceeding the design holdup, V_d:

$$V(t) \le V_d.$$

Table 4. Data for Mixing-Tank Motivating Example

Nominal values	$V^o = 1.0$ m^3, $T^o = 360$ K
State variable bounds	$V^l(t) = 0.90$ m^3, $V^u(t) = 1.5$ m^3 $T^l(t) = 350$ K, $T^u(t) = 370$ K
Uncertainty range	$F_h^l(t) = 0.05$, $F_h^u t = 0.15$ (m^3/h)
Disturbance range	$T_h^l(t) = 350$ K, $T_h^u(t) = 390$ K
Manipulated Variable bounds	$z^l(t) = 0.0$, $z^u(t) = 0.30$ $F_c^l(t) = 0.015$, $F_c^u(t) = 0.05$ (m^3/h)

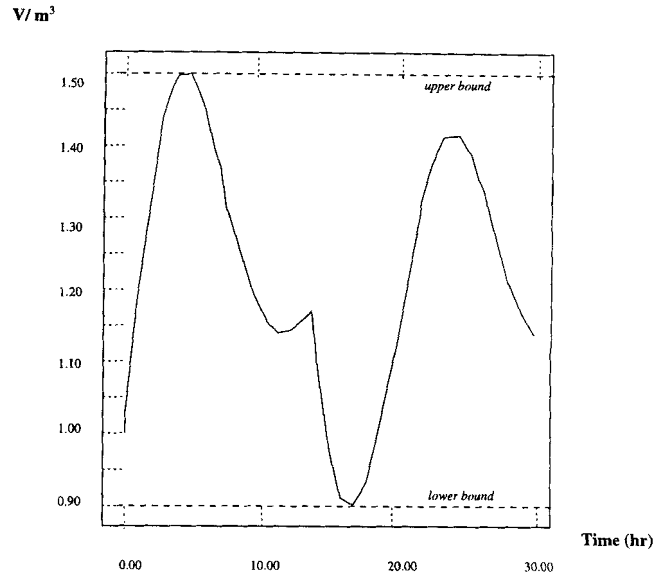

Figure 6. Controlled-tank holdup profile (worst-case design).

Assume that, initially the system is at steady state with the process data given in Table 4. The following cost objective function comprising both design and control structure cost is considered:

$$k_1 + k_2 V_d^{0.7} + C^T X,$$

where $k_1 = \$341$ and $k_2 = \$3,561$ refer to fixed cost (e.g., installation, maintenance costs) and tank capital cost coefficients, respectively, C^T is the control loop costs, and X is the binary variable associated with the control structure. A constant cold-feed temperature ($T_c = 298$ K) and a time horizon of 30 h are considered.

The objective is to determine a design and a control structure of minimum total annualized cost that is able to satisfy

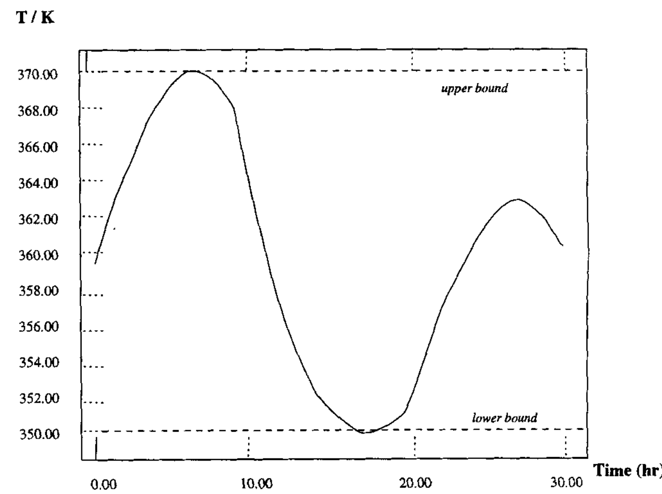

Figure 7. Controlled-tank outlet-temperature profile (worst-case design).

Table 5. Assigning Manipulated Variables to Variations

Variations	Manipulated Variables
Uncertainty	
Hot-process stream flow rate, F_h	Valve constant, z
Disturbance	
Hot-process stream temperature, T_h	Cold-process stream flow rate, F_c

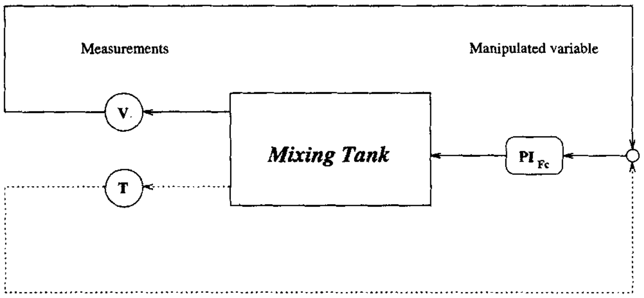

Figure 8. Multiloop PI control superstructure for the mixing tank.

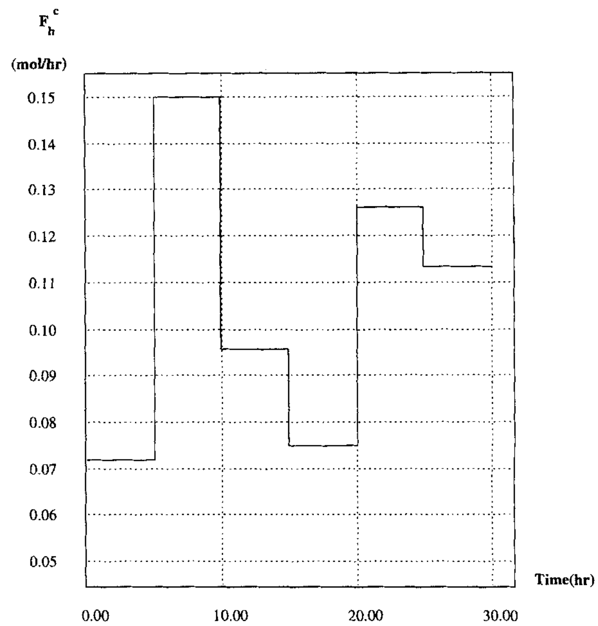

Figure 9. Critical uncertain parameters (hot-process stream flow rate).

the product specification under the variability of feed conditions (in terms of feasible operation and disturbance rejection). Initially we perform a worst-case design optimization by freezing the system inherent degrees of freedom with PI controllers and considering four-step changes between the upper and the lower bounds for T_h and F_h. In this case, there is a tendency to overdesign (see Figures 6 and 7) where the worst-case design holdup, V_d, was found to be the upper bound of the holdup, V.

Next, this mixing-tank problem was solved using the proposed decomposition algorithm. Since there are only two manipulated variables (cold feed, F_c, and valve constant, z), and as shown in Table 5, the cold feed is assigned to reject the hot-feed temperature disturbance, T_h, while the valve constant is manipulated to compensate for the hot-feed flow-rate uncertainty, F_h; that is, only one PI-controller will be included in the multiloop PI-control structure in order to reject the disturbance, T_h, (see Figure 8), with the controller cost data of Table 6. Appendix E presents a brief overview of the resulting mathematical formulation during the steps of the proposed algorithm.

The complete mixed-integer dynamic optimization algorithm was implemented in the modeling system GAMS (Brooke et al., 1988) based on orthogonal collocation on finite elements; the results are illustrated in Table 7. Fifteen

Table 6. Installed Cost Data for Controllers

Measured Variables	Installed Costs
Volumetric flow	\$2,000
Temperature	\$1,500

Table 7. Performance of the New Algorithm for the Motivating Example

Iteration Number	Design V_d (m^3)	Control Structure* X	PI Controller d_c	EP^U (\$)	EP^L (\$)	CPU (s)
0	1.0	X_V	$KC_V = 0.2$ $\tau_V = 10.0$			
1	1.15	X_T	$KC_V = 0.10$ $\tau_V = 16.35$	7,470	5,859	301.16
2	1.0	X_T	$KC_T = 0.005$ $\tau_T = 5.00$	6,120	6,112	255.47
Optimal Solution	1.0	X_T	$KC_T = 0.005$ $\tau_T = 5.00$	6,112		

*Where subscripts T and V represent measurements.

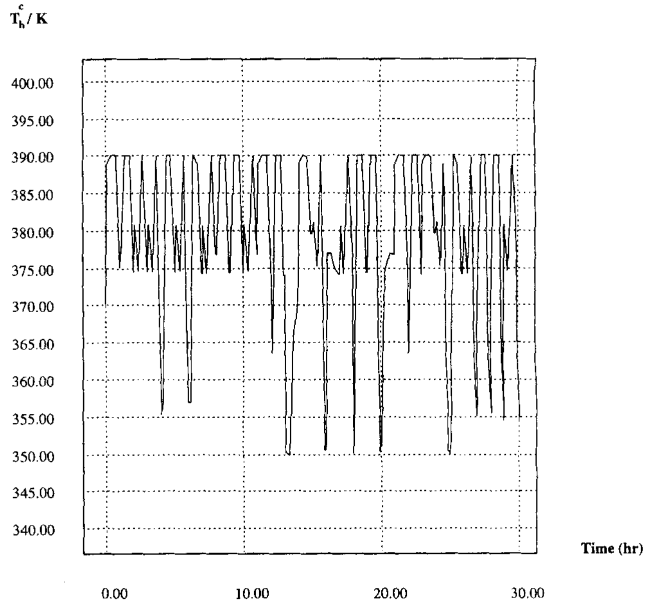

Figure 10. Critical disturbance profile (hot-process stream temperature).

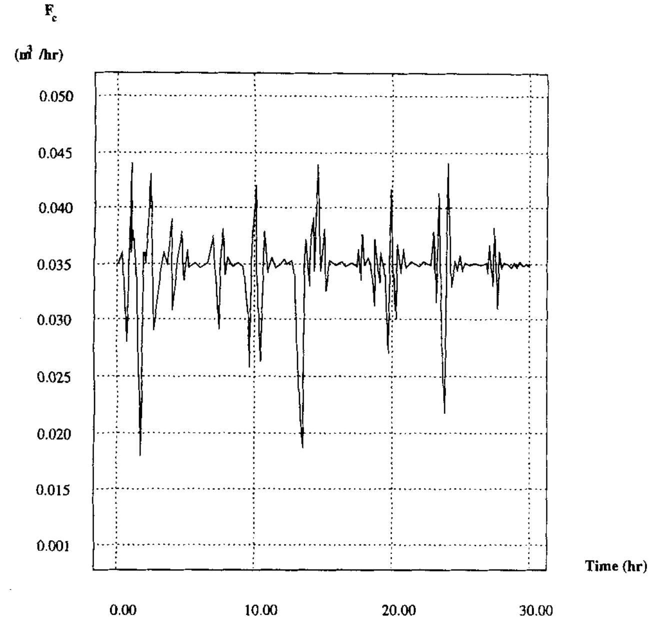

Figure 11. Cold-feed flow-rate control profile (PI controller).

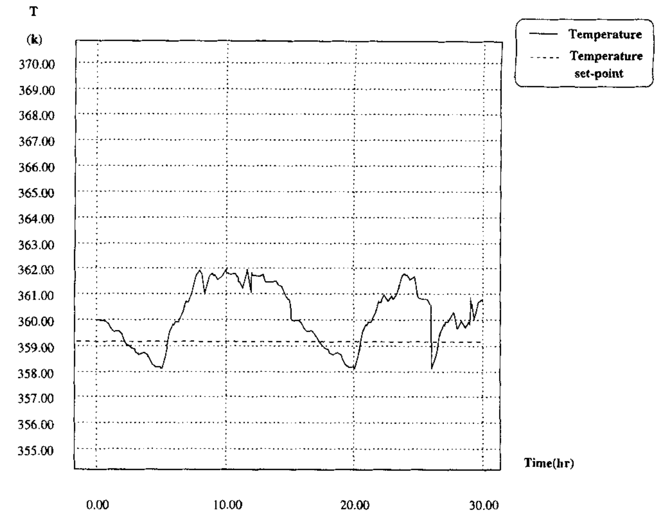

Figure 13. Controlled tank-temperature profile.

finite elements and four collocation points per element were used for the discretization. The design and control subproblem involves 1,067 rows, 671 continuous variables, and 2 binary variables.

The profiles of the critical flow-rate and temperature values are shown in Figures 9 and 10, respectively, for the last iteration. Note that critical parameters do not always lie at the vertex of the uncertainty space, especially for the flow-rate variations. The corresponding profiles of the cold-feed (F_c) PI-control and valve constant are shown in Figures 11 and 12, respectively, whereas the behavior of the controlled tank temperature and holdup constraints are depicted in Figures 13 and 14, respectively. The results are summarized in Table 7. The optimal design and control scheme compares favorably with the worst-case design; note that excessive overdesign has been avoided (an optimal value of 1 m^3 is obtained compared to 1.5 m^3 for the worst-case design). This results in savings of 45% ($6,112 compared to $9,040).

Ternary distillation column design

Here, we consider the *n*-hexane, heptane, toluene distillation problem discussed in the second section. This problem can be briefly stated as follows: Given a single feed of *n*-hexane, heptane, and toluene, which is to be separated into two product streams (predominantly aromatic and nonaromatic) of given specifications, determine the optimum set of design variables and controller structure, so as to minimize total annualized cost under the specified variability.

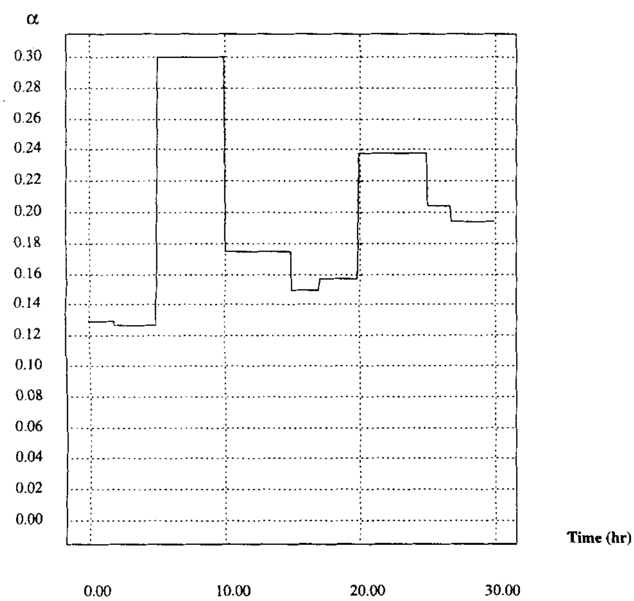

Figure 12. Valve constant-control profile.

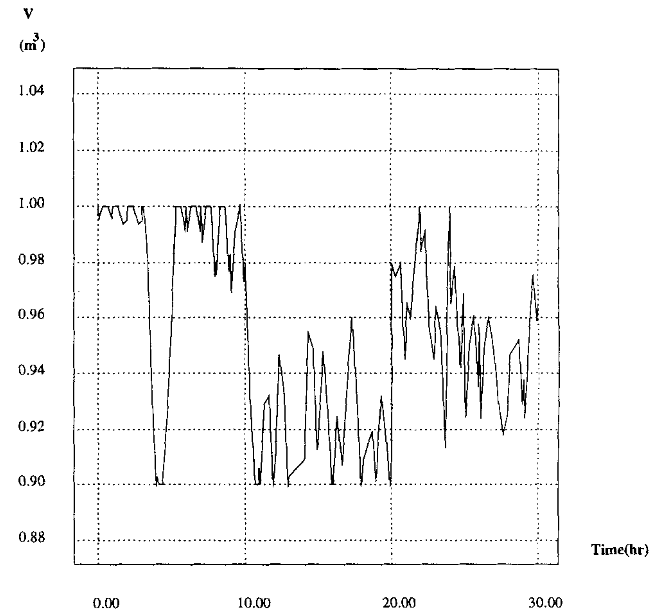

Figure 14. Controlled tank holdup profile.

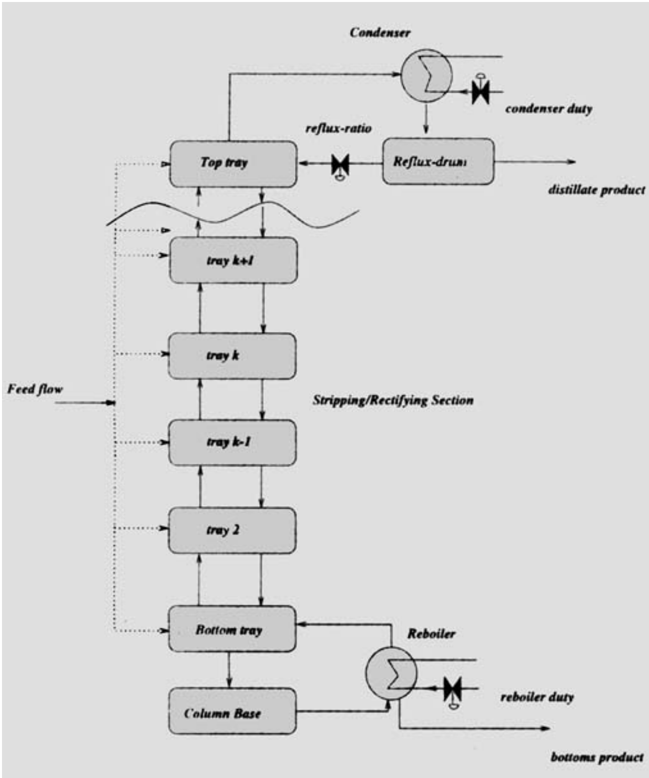

Figure 15. Distillation-column superstructure model.

As stated in the second section, the objective is to design the ternary distillation column and the required control scheme at minimum total annualized cost (comprising investment and operating costs as well as controller costs), and be able to maintain feasible operation in the presence of the involved variability.

Table 9. Optimal Control Structure and Controller Parameters

Controller Outputs	Manipulated Inputs	PI Controller Parameters
Toluene distillate compos. $X_{d_{\text{toluene}}} \leq 0.01$	Reflux ratio, r	$KC = 327.8$ $\tau = 15.7$
Heptane bottom compos. $X_{b_{\text{heptane}}} \leq 0.09$	Reboiler Duty, Q_r	$KC = 15.45$ $\tau = 13.3$
Condenser pressure $0.9 \leq P_c \leq 1.5$ [atm]	Condenser Duty, Q_c	$KC = 0.956$ $\tau = 20.7$

The integrated design framework outlined in the previous subsection is applied to the distillation example with the data given in Tables 1, 2 and 3. A superstructure tray-by-tray model is constructed (see Appendix A), with the number of trays and the location of feed tray and the control structure to be determined as part of the optimization procedure; corresponding sets of 0–1 variables are thus introduced. A one-feed two-product distillation column as shown in Figure 15 is considered, where the overall model consists of three compartments; stripping/rectifying/condenser/reflux-drum, the column base/reboiler and bottom tray sections, respectively.

Four orthogonal collocation points on ten finite elements were used to parameterize the time-varying variables; this results in a large-scale mixed-integer nonlinear programming (MINLP) model. The design and control subproblem involves 10,232 rows, 8,855 continuous variables, and 58 binary variables. The iterative decomposition algorithm, implemented

Table 8. Performance of the Algorithm for the Ternary Distillation Example

Iteration Number	Design Variables	Control Structure	EP^U ($)	EP^L ($)
17	$A_c = 0.69$ m^2 $A_r = 1.14$m^2 $D_t = 2.01$ m $N_f = 15$th tray $N_t = 27$	$X_{d_{\text{heptane}}}$—condenser duty, Q_c $X_{b_{\text{toluene}}}$—reflux ratio, r P_c—reboiler duty, Q_r	144,515	119,659
18	$A_c = 0.80$ $A_r = 1.35$ $D_t = 1.95$ $N_f = 16$th tray $N_t = 25$	$X_{d_{\text{hexane}}}$—Q_c $X_{b_{\text{toluene}}}$—Q_r P_c—r	138,613	122,887
19	$A_c = 0.84$ $A_r = 1.43$ $D_t = 1.97$ $N_f = 11$th tray $N_t = 25$	$X_{d_{\text{toluene}}}$—Q_c $X_{b_{\text{heptane}}}$—Q_r P_c—r	138,613	124,006
20	$A_c = 0.77$ $A_r = 1.28$ $D_t = 1.92$ $N_f = 9$th tray $N_t = 23$	$X_{d_{\text{toluene}}}$—r $X_{b_{\text{heptane}}}$—Q_r P_c—Q_c	133,833	126,876
21 Optimal Solution	$A_c = 0.47$ $A_r = 1.15$ $D_t = 1.90$ $N_f = 10$th tray $N_t = 21$	$X_{d_{\text{toluene}}}$—r $X_{b_{\text{heptane}}}$—Q_r P_c—Q_c	$130,749	$130,228

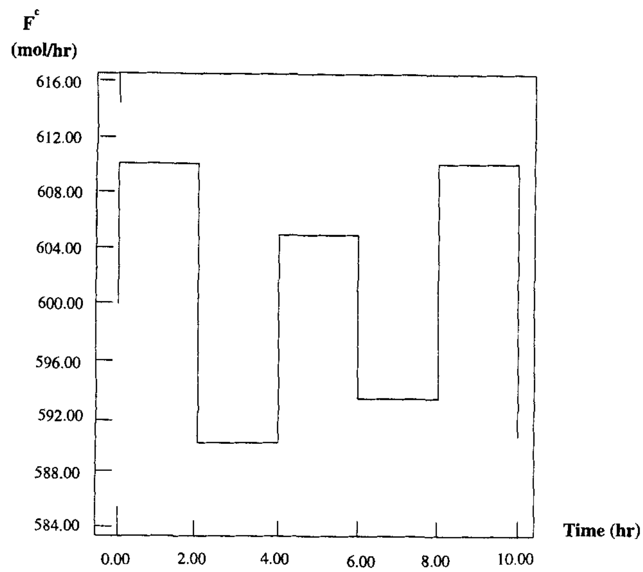

Figure 16. Critical uncertain profile of feed flow rate.

via APROS/GAMS (Paules and Floudas, 1989) with user-provided routines, converged to the optimal design and control structure shown in Tables 8 and 9. Figure 16 depicts the critical profile of the feed flow rate (the slow-varying parametric uncertainty) over a period of 10 h; Figures 17, 18 and 19 depict the optimal profiles of the three controlled (optimization) variables. Note that the critical parameter profile does not always correspond to extreme (vertex) values. Performance of the entire algorithm for this large scale 3×3 dynamic system is shown in Table 8, where the algorithm terminated in 21 iterations requiring approximately 155 min CPU. Note that the optimal distillation column design features 21 trays with the feed entering at the 10th tray with a diameter of 1.90 m; the areas of the condenser and reboiler are 0.47 and 1.15 m^2, respectively. Note also that the optimal control structure corresponds to reflux-ratio control for the distillate specification, reboiler duty for the bottom specification, and condenser duty for the condenser pressure.

The results of the proposed simultaneous design strategy were then compared to a sequential design procedure (Table 10), in which the requirement of controllability was enforced after an economically optimal process design was obtained. Table 11 summarizes the results. Note that the sequential

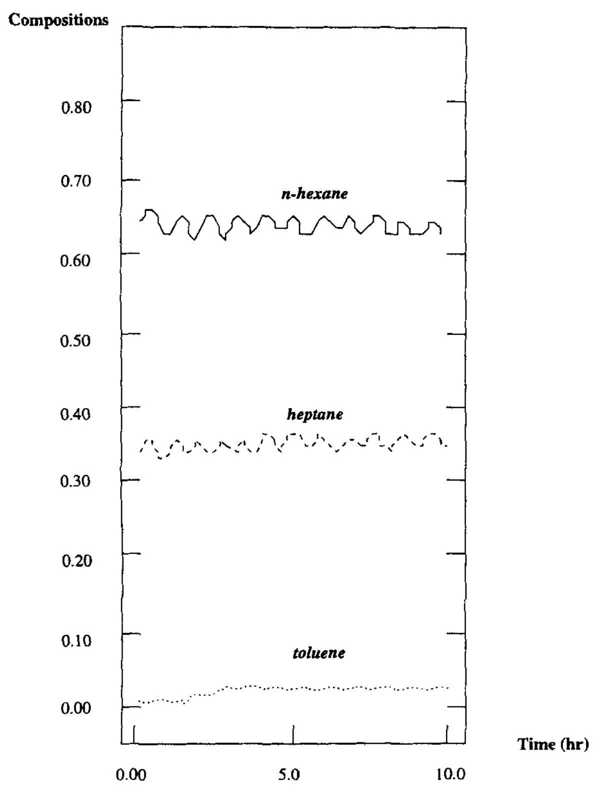

Figure 17. Controlled distillate (P1) composition.

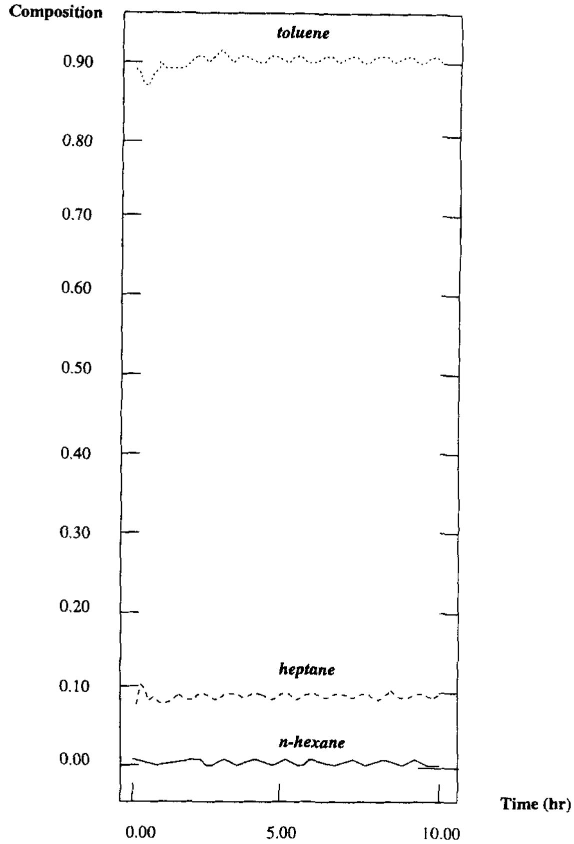

Figure 18. Controlled bottom (P2) composition.

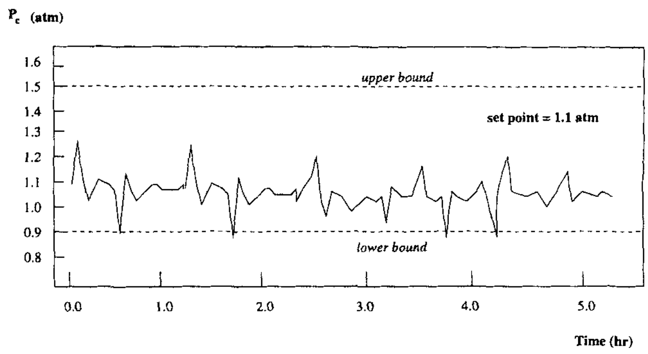

Figure 19. Controlled condenser-pressure profile.

Table 10. Ternary Distillation Column Design and Control using Sequential Procedure

Sequential Procedure	Design Variables	Annualized Costs ($)
Step 1 Flexible Design (steady-state) Only process uncertainties are considered	Number of trays, $N_t = 19$ Reboiler size, $A_r = 0.95\ m^2$ Condenser Size, $A_c = 0.32\ m^2$ Column diameter, $D_t = 1.9$ m	Capital = 73,890 Operating cost = 43,785
Step 2 Control System Design (process design fixed) Process disturbances are considered. If the system is infeasible go to step 3, else, stop	Reflux ratio, r-Cond. pressure, P_c Condenser duty, $Q_c - X_{d_{\text{toluene}}}$ Reboiler duty, $Q_r - X_{b_{\text{heptane}}}$	Cost = 8,450
Step 3 Final Flexible Design (control structure fixed) Feasibility analysis followed by flexible design	$N_t = 27$ trays $A_r = 1.4\ m^2$ $A_c = 0.5\ m^2$ $D_t = 1.96$ m	Capital = 101,356 Operating = 39,213

Table 11. Sequential vs. Integrated Design Procedures for Ternary Distillation Example

Process Design and Control Procedures	Capital Cost	Operating Cost
Sequential	$101,356/yr	$39,213/yr
Integrated	$88,243/yr	$41,985/yr

approach resulted in a 15% more expensive design involving a larger number of trays (27 vs. 21) and a different control scheme. It is also interesting to note that operating costs were higher in the simultaneous approach, whereas capital costs were significantly lower.

Conclusions

We have proposed a conceptual framework for integrated design and control under parametric uncertainty and disturbances. Flexibility aspects were formally incorporated in a multiperiod design subproblem coupled with a feasibility analysis of time-varying systems, while realistic PI-controllers were introduced by a control structure selection subproblem, thereby allowing for the simultaneous determination of the best control structure based on cost/design trade-offs (thus avoiding the use of open-loop indicators). An efficient decomposition-based algorithm was presented for the solution of the resulting mixed-integer stochastic optimal control formulation, which avoids worst-case considerations. The potential of this unified framework was demonstrated through two examples, a mixing tank problem and a ternary distillation design problem, where notable cost savings were made over existing methodologies. Since the proposed algorithm is in principle independent of the uncertainty and controller models, it is envisaged that it can provide the basis for a unified framework toward the integration of process design and control at the synthesis/design stage under considerations of uncertainty.

Notation

d_c = PI-controller design parameters, u_o, KC, and τ
f = algebraic equations
h = differential equations
$i = 1,\ldots,Nfe$ index of finite elements
$j = 1,\ldots,N$col index of collocation points
M = total number of potential measurements
$m = 1,\ldots,M$ index of potential measurements
N = total number of potential inputs, $u(t)$
$n = 1,\ldots,N$ index of potential inputs, $u(t)$
$T(t)$ = continuous uncertainty space with respect to time
TP = total number of periods considered in the multiperiod problem
$V(t)$ = continuous disturbance space with respect to time
α = time step between two finite elements

Literature Cited

Brooke, A., D. Kendrick, and M. Meeraus, *GAMS: A User's Guide*, Scientific Press, Redwood City, CA (1988).

Bahri, P. A., J. A. Bandoni, and J. A. Romagnoli, "Effect of Disturbances in Optimizing Control: Steady-State Open-Loop Back-Off Calculation," *AIChE J.*, **42**(4), 983 (1996).

Ciric, A. R., and D. Gu, "Synthesis of Nonequilibrium Reactive Distillation Processes by MINLP Optimization, *AIChE J.*, **40**(9), 1479 (1994).

Cuthrell, J. E., and L. T. Biegler, "Strategies for Simultaneous Solution and Optimization of Differential-Algebraic Systems," *AIChE J.*, **33**(8), 1257 (1987).

Dimitriadis, V. D., and E. N. Pistikopoulos, "Feasibility and Flexibility Analysis of Dynamic Systems," *Ind. Eng. Chem. Res.*, **34**, 4451 (1995).

Douglas, J. M., *Conceptual Design of Chemical Processes*, McGraw-Hill, New York (1988).

Geoffrion, A. M., "Generalized Benders Decomposition," *JOTA*, **10**, 237 (1972).

Grossmann, I. E., and D. A. Straub, "Recent Development in the Evaluation and Optimization of Flexible Chemical Processes," *Computer-Oriented Proc. Eng.*, L. Puigjaner and A. Espuña, eds., Elsevier, Amsterdam, p. 49 (1991).

Grossmann, I. E., and C. A. Floudas, "Active Constraint Strategy for Flexibility Analysis in Chemical Processes," *Comput. Chem. Eng.*, **11**, 675 (1987).

Grossmann, I. E., and M. Morari, "Operability, Resilience and Flexibility: Process Design Objectives for a Changing World," *Proc. FOCAPD*, Snowmass, CO, p. 931 (1983).

Grossmann, I. E., and K. P. Halemane, "Decomposition Strategies for Designing Flexible Chemical Plants," *AIChE J.*, **28**(4), 686 (1982).

Grossmann, I. E., and R. W. H. Sargent, "Optimum Design of Chemical Plants with Uncertain Parameters," *AIChE J.*, **24**, 1021 (1978).

Gustafson, S. Å., "A Three-Phase Algorithm for Semi-Infinite Programs," *Lecture Notes in Economics and Mathematical Systems: Semi-Infinite Programming and Applications*, A. V. Fiacco and K. O. Kortanek, eds., Springer-Verlag, Berlin, p. 138 (1981).

Heath, J. A., and J. D. Perkins, "Control Structure Selection Based

on Economics., IChemE Research Event 1994," *IChemE Proc.*, Rugby, U.K., p. 841 (1994).
Luyben, M. L., and C. A. Floudas, "Analyzing the Interaction of Design and Control: 1. A Multiobjective Framework and Application to Binary Distillation in Synthesis," *Comput. Chem. Eng.*, **18**, 33 (1994a).
Luyben, M. L., and C. A. Floudas, "Analyzing the Interacting of Design and Control: 2. Reaction-Separator-Recycle System," *Comput. Chem. Eng.*, **18**, 971 (1994b).
Madsen, K., and H. Schjaer-Jacobsen, "Linearly Constrained Minimax Optimization," *Math. Prog.*, **14**, 208 (1978).
Morari, M., and J. D. Perkins, "Design for Operations," *Proc. FOCAPD-94*, Snowmass, CO (1994).
Narraway, L. T., and J. D. Perkins, "Selection of Process Control Structure Based on Economics," *Comp. Chem. Eng.*, **18**, S511 (1993a).
Narraway, L. T., and J. D. Perkins, "Selection of Process Control Structure Based on Linear Dynamic Economics," *Ind. Eng. Chem. Res.*, **32**, 2681 (1993b).
Papalexandri, K. P., and E. N. Pistikopoulos, "Synthesis and Retrofit Design of Operable Heat Exchanger Networks: 1. Flexibility and Structural Controllability Aspects," *Ind. Eng. Chem. Res.*, **33**, 1718 (1994a).
Papalexandri, K. P., and E. N. Pistikopoulos, "Synthesis and Retrofit Design of Operable Heat Exchanger Networks: II. Dynamics and Control Structure Considerations," *Ind. Eng. Chem. Res.*, **33**, 1738 (1994b).
Paules, G. E. IV, and C. A. Floudas, "APROS: Algorithmic Development Methodology for Discrete-Continuous Optimization Problems," *Oper. Res.*, **37**(6), 902 (1989).
Perkins, J. D., and S. P. K. Walsh, "Optimization as a Tool for Design/Control Integration," *Proc. IFAC Workshop on Integration of Process Design and Control*, E. Zafiriou, ed., Pergamon, Oxford, p. 1 (1994).
Pistikopoulos, E. N., "Uncertainty in Process Design and Operation," *Comp. Chem. Eng.*, **18**, S553 (1995).
Sounders, M., and G. G. Brown, "Design of Fractionating Columns Entrainment and Capacity," *Ind. Eng. Chem.*, **26**, 98 (1934).
Tanarkit, P., and L. T. Biegler, "Boundary Value Approach for Dynamic Optimization," *EDRC 06-170-94 Tech. Rep.*, Carnegie Mellon Univ., Pittsburgh (1993).
Varvarezos, D. K., I. E. Grossmann, and L. T. Biegler, "Multiperiod Design Optimization with SQP Decomposition," *Comput. Chem. Eng.*, **18**(7), 579 (1994).
Walsh, S. P. K., and J. D. Perkins, "Integrated Process and Control System Design to Waste Water Neutralization," *Comp. Chem. Eng.*, **18**, S183 (1994).
Zangwill, W. I., *Nonlinear Programming: A Unified Approach*, Prentice-Hall, Englewood Cliffs, N.J. (1969).

Appendix A: Mixed-Integer Dynamic Model of Distillation Column

The overall distillation model consists of three units: a stripping/rectifying/condenser/reflux-drum unit, a bottom tray unit, and a column base-reboiler unit (see Figure 15). Since the number of trays and the location of feed tray are treated as 0–1 variables, the resulting model is a mixed-integer dynamic model. The overall model developed here has some similarities to the synthesis model presented by Ciric and Gu (1994) for reactive distillation (but their work was based on relatively simple tray-by-tray steady-state models).

The liquid holdup on each tray, M_k, is assumed to be constant, therefore we ignore tray hydraulics. The holdup of the vapor is assumed to be negligible throughout the system. We also assume that the vapor boilup and reflux enter tray $k=1$ and the top tray, respectively. Here, the number of trays is accounted for by introducing a set of binary variables, Z_k, where $Z_k = 1$ represent the existence of the kth tray from the bottom of the column. The process model describing the distillation column design and operation is given by a set of differential algebraic equations (DAEs) for mass, composition, energy, and equilibrium relationships on a tray-by-tray basis for the three column compartments, the rectifying/stripping/condenser/reflux-drum, the column-base/reboiler, and bottom tray sections, respectively.

Stripping/rectifying/condenser/reflux-drum lumped model

Here we express a general model to denote stripping, rectifying, condenser, and reflux-drum compartments.

$$(F_k + L_{k+1} + V_{K-1} - L_k - V_k - D_k) = 0 \qquad k \in 2,\dots,N$$

$$M_k \frac{dx_{k,i}}{dt} = (F_k xf_{k,i} + L_{k+1}x_{k+1,i} + V_{k-1}K_{k-1,i}x_{k-1,i} - L_k x_{k,i} - V_k K_{k,i} x_{k,i} - D_k x_{k,i}) \qquad k \in 2,\dots,N$$

$$M_k \frac{dhl_k}{dt} = (F_k hlf_k + L_{k+1} hl_{k+1} + V_{k-1} h\nu_{k-1} - L_k hl_k - V_k h\nu_k - D_k hl_k - Q_{ck}) \qquad k \in 2,\dots,N$$

where L_k and V_k are liquid and vapor flow off tray k, respectively; $x_{k,i}$ and $xf_{k,i}$ are liquid mole fractions of component i on tray k and feed, respectively; $K_{k,i}$ vapor–liquid equilibrium constant of component i on tray k; hl_k and $h\nu_k$ are molar enthalpies of liquid and vapor on tray k; hlf_k is the enthalpy of feed entering tray k.

In each section, it simplifies into the respective forms, for example, in the case of the rectifying section feed flow, F, distillate, D, and condenser duty, Q_c, disappear from the preceding equations. In this model, we treat the condenser-reflux drum section as though it is a tray with a heat sink and product removal.

Reflux rate

$$R_k = L_k(Z_k - Z_{K+1}) \qquad k \in 2,\dots,N,$$

where the term $(Z_k - Z_{K+1})$ is one only at the top of the column (i.e., condenser-reflux drum).

Bottom tray (tray k = 1)

The set of equations below describe the bottom tray. This tray is modeled separately to allow the column base-reboiler compartment to be connected to the tray section just described.

$$L_2 + V_B - V_1 - L_1 = 0$$

$$M_1 \frac{dx_{1,i}}{dt} = L_2 x_{2,i} + V_B K_{B,i} x_{B,i} - V_1 K_{1,i} x_{1,i} - L_1 x_{1,i}$$

$$M_1 \frac{dhl_1}{dt} = L_2 hl_2 + V_B h\nu_B - V_1 h\nu_1 - L_1 hl_1,$$

where V_B is the vapor flow off column base/reboiler section and $h\nu_B$ is the enthalpy of that stream.

Column base and reboiler

The column base and reboiler are lumped together to give a single general model:

$$L_1 - V_B - B = 0$$

$$M_B \frac{dx_{B,i}}{dt} = L_1 x_{1,i} - V_B K_{B,i} x_{B,i} - Bx_{B,i}$$

$$M_B \frac{dhl_B}{dt} = L_1 hl_1 + Q_r - V_B h\nu_B - Bhl_B,$$

where B is the bottom product flow and Q_r is the reboiler duty.

The earlier differential algebraic equations are expressed for all the components $i \in nc$. The inherent restriction on the mole fractions can be expressed as follows:

$$\sum_i x_{k,i} = 1 \qquad k \in 1,\ldots,N$$

$$\sum_i K_{k,i} x_{k,i} = 1 \qquad k \in 1,\ldots,N.$$

Physical properties

Vapor–liquid equilibrium constant of component i on tray k, given by

$$K_{k,i} = \frac{P_{k,i}^{\text{vap}}(T_k)}{P}.$$

Liquid enthalpy on tray k

$$hl_k = \sum_i x_{k,i} hl_{k,i}(T_k).$$

Vapor enthalpy on tray k

$$h\nu_k = \sum_i K_{k,i} x_{k,i} h\nu_{k,i}(T_k).$$

Here the operating path constraints considered are the flooding velocity (Sounders and Brown, 1934), minimum column diameter, and design equations for reboiler and total condenser.

Logical constraints

These constraints are needed to link flow onto and off a tray, with the existence of the tray due to the presence of binary variables:

$$M_k - M_{\max} Z_k \le 0 \qquad \text{(A1)}$$

$$V_k - V_{\max} Z_k \le 0 \qquad \text{(A2)}$$

$$L_k - L_{\max} Z_k \le 0 \qquad \text{(A3)}$$

$$Z_{k+1} \le Z_k. \qquad \text{(A4)}$$

Equation A4 ensures that the bottom tray, k, should exist for the top tray, $k+1$, to exist. For a single feed stream:

$$F_k - F_{\max} ZF_k \le 0 \qquad \text{(A5)}$$

$$\sum_{k \in K} F_k = F \qquad \text{(A6)}$$

$$\sum_k ZF_k = 1 \qquad \text{(A7)}$$

$$ZF_k \le Z_k, \qquad \text{(A8)}$$

where ZF_k is the binary variable denoting the existence of the feed tray.

Here, Eqs. A5, A6, and A7 ensure that feed stream F is fed to only one tray in the column, and Eq. A8 is an integer cut specifying that the feed tray must be assigned to existing trays:

$$ZT_k = (Z_k - Z_{k+1}) \qquad \text{(A9)}$$

$$ZT_k \le Z_k. \qquad \text{(A10)}$$

Equation A9 is the definition of integer variable ZT_k, where the term $Z_k - Z_{k+1}$ is one only at the top tray.

$$L_{k+1} - L_{\max}(1 - ZT_k) \le 0 \qquad \text{(A11)}$$

$$V_k - V_{\max}(1 - ZT_k) \le 0 \qquad \text{(A12)}$$

$$D_k - F_{\max} ZT_k \le 0 \qquad \text{(A13)}$$

$$Q_{c_k} - Q_{\max} ZT_k \le 0 \qquad \text{(A14)}$$

$$F_k - F_{\max}(1 - ZT_k) \le 0, \qquad \text{(A15)}$$

where $L_{\max}$, $F_{\max}$, and $V_{\max}$ are upper bounds on liquid and vapor flow rates, respectively; $Q_{\max}$ is the upper bound on condenser duty.

Equations A11, A12, A13, and A14 ensure the change of models from stripping/rectifying section models to condenser/reflux-drum when Z_k reaches top tray, and Eq. A15 is an integer cut specifying that the feed tray must not be assigned to the top tray (i.e., condenser/reflux-drum section).

Number of trays

The total number of trays N_t in the column including the condenser and the reboiler is given by

$$N_t = 1 + \sum_k k(Z_k - Z_{k+1}), \qquad \text{(A16)}$$

where one represents the partial reboiler, and the rest represent all the other trays including the total condenser.

Objective function

The objective function P is composed of capital and operating costs. The annualized investment cost is determined by the cost of the column, its internals, and reboiler and condenser.

Column Shell Capital Cost. The overall column shell cost correlation given by Douglas (1988) was transformed into a form where the binary variables appear linearly (Ciric and Gu, 1994) as follows:

$$C_{\text{shell}} = \frac{1}{3}\left(\frac{M\&S}{280}\right)(101.9 D_t)(2.18 + F_C)\sum_k \times\left(H_o + \sum_{k'<k} 2A_{k'}\right)^{0.802}(Z_k - Z_{k+1}), \quad \text{(A17)}$$

where $M\&S$ is the Marshal and Swift index; H is the height of the column; F_c is the material of construction factor; H_o is the sum of the spacing at the top and bottom of the column; D_t is the column diameter; $A_{k'}$ is a dummy variable that is a function of tray spacing and is set to 1 for a tray spacing of 2 feet.

Column Tray and Tower Internals Capital Cost.

$$C_{\text{tray}} = \left(\frac{M\&S}{280}\right)4.7 D_t^{1.55} F_c' \sum_k (2Z_k), \quad \text{(A18)}$$

where F_c' is the material of construction factor.

Heat-Exchanger Capital Costs.

$$C_{hx} = \frac{1}{3}\left(\frac{M\&S}{280}\right)101.3(2.29 + F_{cc})(A_c^{0.65} + A_r^{0.65}) \quad \text{(A19)}$$

where F_{cc} is the material of construction factor for heat exchanger; A_c and A_r are condenser and reboiler sizes, respectively.

Operating Cost. We can compute the cost of steam and cooling water directly:

$$C_{op} = Q_c C_{\text{water}} + Q_r C_{\text{steam}}, \quad \text{(A20)}$$

where C_{water} is the cost of cooling water and C_{steam} is the cost of steam.

Appendix B: Dynamic Optimization using the Collocation Technique

All collocation techniques reduce an optimal control problem to a finite-dimensional optimization problem by the discretization of both controls and state variables, using some approximating functions involving a finite set of parameters. Cuthrell and Biegler (1987) proposed the use of finite-element collocation for both state and control variables using Lagrange polynomials to convert the DAEs involved to algebraic equations with unknown coefficients, evaluated at each point.

For the optimal control problems under uncertainty, state variables, control variables, critical uncertain parameters, and critical disturbance profiles are approximated by Lagrange polynomials (piecewise) over each finite element. The number of finite elements is taken to be *Nfe*. The number of collocation points within each element is *N*col and is taken to be the same for every element. The length of each element will be denoted by α_i. It is convenient to map each finite element into the domain τ using the following transformation:

$$t_{ij} = \alpha_i + \tau_j(\alpha_{i+1} - \alpha_i) \quad \text{(A21)}$$
$$0 \le \tau \le 1,$$

The definition of the Lagrange basis polynomials used are:

$$\alpha_i \le t \le \alpha_{i+1} \qquad (t \text{ in element } i)$$

$$\phi_j(t) = \prod_{\substack{n=0\\ n\neq j}}^{N\text{col}} \frac{(t - t_{in})}{(t_{ij} - t_{in})} \quad \text{(A22)}$$

$$\psi_j(t) = \prod_{\substack{n=1\\ n\neq j}}^{N\text{col}} \frac{(t - t_{in})}{(t_{ij} - t_{in})}. \quad \text{(A23)}$$

The property of the Lagrange basis polynomials can be expressed as follows:

$$\phi_j(t_{ij}) = \phi_j(\tau_j) = 1; \qquad \phi_n(t_{ij}) = \phi_n(\tau_j) = 0 \qquad n \neq j$$

$$x(t_{ij}) = \sum_{n=0}^{N\text{col}} x_{in}\phi_n(\tau_j) = x_{ij}.$$

The polynomial approximation for the state variables and the control variables can then be expressed as

$$x_i(t) = \sum_{j=0}^{N\text{col}} x_{ij}\phi_j(t), \qquad u_i(t) = \sum_{j=1}^{N\text{col}} u_{ij}\psi_j(t). \quad \text{(A24)}$$

Here, we discretize both the critical uncertainty and disturbance. The corresponding polynomial approximations are

$$\theta_i^c(t) = \sum_{j=1}^{N\text{col}} \theta_{ij}\psi_j(t), \qquad \nu_i^c(t) = \sum_{j=1}^{N\text{col}} \nu_{ij}\psi_j(t)$$
$$\theta_i^c(t) \in [\theta_l(t), \theta_u(t)], \qquad \nu_i^c(t) \in [\nu_l(t), \nu_u(t)]. \quad \text{(A25)}$$

We obtain the following expression for the time derivatives of state variables $x(t)$ at a collocation point (i, j):

$$\dot{x}_{N\text{col}+1}(t_{ij}) = \frac{1}{\alpha_i}\sum_{n=0}^{N\text{col}} x_{in}\dot{\phi}_{jn}. \quad \text{(A26)}$$

In addition, continuity of the state profiles is enforced by the following equations. This defines the state variables at the beginning of element i, by extrapolating to $\tau = 1$ as follows:

$$x_{i+1,0} - \sum_{j=0}^{N\text{col}} x_{i,j}\phi_j(\tau = 1) = 0. \quad \text{(A27)}$$

Similarly, we could extrapolate state, control, critical disturbance, and uncertain variables to final time $(Nfe + 1)$.

In order to estimate and bound the discretized and round-off errors, a wide spectrum of element placement constraints can be used, ranging from highly nonlinear constraints based on the residual at noncollocation points to simple ad hoc bounds on elements. In this study, we incorporate the following relation:

$$-\epsilon_m \le C\xi_{im}(\tau_{\text{nonc}}) \le \epsilon_m, \quad \text{(A28)}$$

where ξ_{im} refers to the interpolated residual for equation, m, at element, i; C is a constant depending on τ_{nonc} and the order of the collocating polynomial. Error control may be achieved by introducing the constraint just given in the optimization by bounding the residual for each equation, including algebraic equations at noncollocation points τ_{nonc}.

Element placement plays a crucial role on the final result and efficiency of this method, and the optimal element placement has significant impact on both the solution and the computational time. The constraint, Eq. A28, makes the problem nonlinear and very sensitive to initialization. To overcome this difficulty, we use the framework proposed by Tanarkit and Biegler (1993), which accommodates the element placement with bilevel programming. The outer problem of the bilevel optimization determines the finite-element lengths, and the fixed-mesh (inner) problem determines the control and state variables once the element sizes are fixed.

Appendix C: On the Optimality Conditions

The corresponding variational conditions derived for the feasibility test optimal control problem Eq. 5, based on orthogonal collocation on finite elements, can be shown as follows.

Adjoint Condition.

$$\sum_k \lambda_{k,ij}^T \frac{\partial g_k(t_{ij})}{\partial x_{ij}} + \sum_q \eta_{q,ij}^T \frac{\partial f_q(t_{ij})}{\partial x_{ij}} + \sum_l \mu_{l,ij}^T \frac{\partial h_l(t_{ij})}{\partial x_{ij}} + \dot{\mu}_{N\text{col}+1}(t_{ij}) = 0 \quad \text{(A29)}$$

where

$$\dot{\mu}_{N\text{col}+1}(t_{ij}) = \sum_{j=1}^{N\text{col}} \mu_{ij}\dot{\phi}_{ij}(t).$$

Hamiltonian Condition.

$$\sum_k \lambda_{k,ij}^T \frac{\partial g_k(t_{ij})}{\partial z_{ij}} + \sum_q \eta_{q,ij}^T \frac{\partial f_q(t_{ij})}{\partial z_{ij}} + \sum_l \mu_{l,ij}^T \frac{\partial h_l(t_{ij})}{\partial z_{ij}} = 0 \quad \text{(A30)}$$

$$\sum_k \lambda_{k,ij}^T \frac{\partial g_k(t_{ij})}{\partial u_{ij}} + \sum_q \eta_{q,ij}^T \frac{\partial f_q(t_{ij})}{\partial u_{ij}} + \sum_l \mu_{l,ij}^T \frac{\partial h_l(t_{ij})}{\partial u_{ij}} = 0 \quad \text{(A31)}$$

$$\dot{x}_{N\text{col}+1}(t_{ij}) - h_l(d,x_{ij},z_{ij},u_{ij},\theta_{ij},\nu_{ij},t_{ij}) = 0 \quad l \in L \quad \text{(A32)}$$

$$f_q(d,x_{ij},z_{ij},u_{ij},\theta_{ij},\nu_{ij},t_{ij}) = 0 \quad q \in Q \quad \text{(A33)}$$

$$g_k(d,x_{ij},z_{ij},u_{ij},\theta_{ij},\nu_{ij},t_{ij}) \le 0 \quad k \in K. \quad \text{(A34)}$$

Complementarity Condition.

$$q_{k,ij} = s_{ij} - g_k(d,x_{ij},z_{ij},u_{ij},\theta_{ij},\nu_{ij},t_{ij}) \quad \text{(A35)}$$

$$\lambda_{k,ij}q_{k,ij} = 0 \qquad \lambda_{k,ij} \ge 0 \quad \text{(A36)}$$

for

$$i = 1,\ldots,Nfe \qquad j = 0,\ldots,N\text{col}$$

We now see that Eq. A29 is a discrete analog of the adjoint equations that can easily be derived from standard optimal control theory. They can also be obtained by applying orthogonal collocation on finite elements to the adjoint equation. Similarly, Eqs. A30 and A31 are discrete analogs of the variational condition on the control profiles. Finally, Eqs. A32–A34 are simply feasibility conditions for differential–algebraic equations and the remaining expressions relate to the optimality condition for the inequality constraints.

The Hamiltonian function L_{ij} at time t_{ij} for feasibility problem, Eq. 5, can be defined as

$$L_{ij}(\mu_{l,ij},\eta_{q,ij},\lambda_{k,ij},d,x_{ij},z_{ij},u_{ij},\theta_{ij},\nu_{ij},t_{ij}) = \sum_l \mu_{l,ij}^T h_l(t_{ij}) + \sum_q \eta_{q,ij}^T f_q(t_{ij}) + \sum_k \lambda_{k,ij}^T \partial g_k(t_{ij}) + x_{ij}^T \dot{\mu}_{N\text{col}+1}(t_{ij}). \quad \text{(A37)}$$

Observe that the adjoint conditions, Eq. A29, require that the gradient of the Hamiltonian w.r.t. the state variables x_{ij} be zero, while the Hamiltonian condition, Eqs. A30 and A31, relate to the gradient w.r.t. the control variables z_{ij} and u_{ij} being zero.

Minimum principle

Suppose each Hamiltonian function $L_{ij}(\mu_{l,ij}, \eta_{q,ij}, \lambda_{k,ij}, d, x_{ij}, z_{ij}, u_{ij}, \theta_{ij}, \nu_{ij}, t_{ij})$ were a convex function in z_{ij}, u_{ij} for each fixed, $x_{ij}, \theta_{ij}, \nu_{ij}$ and $\mu_{l,ij}, \eta_{q,ij}, \lambda_{k,ij}$. Then the Hamiltonian condition just stated is equivalent to the following minimum principle. The Hamiltonian satisfies the minimum principle if for each $i = 1,\ldots,Nfe$, $j = 0,\ldots,N\text{col}$

$$L_{ij}(\mu_{l,ij},\eta_{q,ij},\lambda_{k,ij},d,x_{ij},z_{ij},u_{ij},\theta_{ij},\nu_{ij},t_{ij}) = \min_{z,u} L_{ij}(\mu_{l,ij},\eta_{q,ij},\lambda_{k,ij},d,x_{ij},z,u,\theta_{ij},\nu_{ij},t_{ij}), \quad \text{(A38)}$$

where the minimum is over all $z = (z_1, z_2, z_3, \ldots, z_a)$, $u = (u_1, u_2, u_3, \ldots, u_N)$, and $\mu_{l,10} = 0$; and N and a are dimensions of u and z, respectively.

Under this convexity assumption the necessary conditions for a feasible (x, z, u) to be optimal are the existence of multipliers λ, η, and μ that satisfy the optimality conditions Eqs. A29–A36 (Zangwill, 1969).

Appendix D: Multiperiod Design and Control Subproblem

Here, we decompose the multiperiod design and control problem, Problem P1, into two subproblems as shown in Figure 4:

(1) A multiperiod flexible design *primal problem*

(2) An optimal multiloop PI control structure selection *master problem*.

The primal problem generates an upper bound of the expected cost, whereas the master problem generates a lower bound of the expected cost. Therefore the algorithm alternates between these two steps until both the expected costs are within a required tolerance.

Primal problem (multiperiod design)

This step determines both an optimal design and control design parameters, which are flexible over the entire critical parameter space, for a fixed control structure X. The expected cost obtained from this subproblem represents an upper bound EP^u of the original problem. This is because the overall design is suboptimal, since the control structure $\hat{X}$ is fixed during the optimization of the primal problem. Hence, the multiperiod design problem for fixed control structure, $\hat{X}$, is

$$\min_{\substack{d,z_{ij}^1,\ldots,z_{ij}^p,y_{\text{set}}^1,\ldots,y_{\text{set}}^p\\ u_o,KC,\tau}} \times\left\{\sum_p w_p\left[P(d,d_c,x_{ij}^p,z_{ij}^p,y_{\text{set}}^p,\theta_i^p,\nu_i^p,t_{ij})+C^T\hat{X}_{nm}\right]\right\} \tag{A39}$$

s.t.

$$\begin{aligned} g_k\left(\hat{X}_{nm},d,x_{ij}^p,u_{ij}^p,z_{ij}^p,\theta_i^p,\nu_i^p,t_{ij}\right)&\le 0 && k\in K\\ x_{N\text{col}+1}^p(t_{ij})-h_l(d,x_{ij}^p,u_{ij}^p,z_{ij}^p,\theta_i^p,\nu_i^p,t_{ij})&=0 && l\in L\\ f_q(d,x_{ij}^p,u_{ij}^p,z_{ij}^p,\theta_i^p,\nu_i^p,t_{ij})&=0 && q\in Q\\ hc_n(u_o,KC,\tau,x_{ij}^p,u_{ij}^p,y_{\text{set}}^p,\nu_i^p,t_{ij})&=0 && n\in N \end{aligned}$$

Critical Parameters.

$$\theta_i^p=\{\theta_{i,1}^p,\theta_{i,2}^p,\ldots,\theta_{i,j}^p,\ldots,\theta_{i,N\text{col}}^p\}$$

$$\nu_i^p=\{\nu_{i,1}^p,\nu_{i,2}^p,\ldots,\nu_{i,j}^p,\ldots,\nu_{i,N\text{col}}^p\}$$

$$i\in[1,Nfe],\qquad j\in[0,N\text{col}],\qquad p\in[1,TP].$$

Generalized Benders decomposition requires Lagrange multiplier information at each iteration from the nonlinear subproblem with respect to all the linking constraints to formulate the master problem. For the type of problems we are concerned with, the dual information obtained with respect to a fixed control structure is weak. This weak duality arises from the strong interaction between the two problems (i.e., multiperiod design and the control structure selection), which results in weak supporting hyperplanes. Thus, once the convergence of the NLP *primal* problem is reached, all the constraints are moved into a single, complete representation of the *overall* problem, containing the optimal design values.

This *overall* problem is constructed to obtain strong dual information. Solution of this problem with design variables and the control structure at the optimal solutions, d^k, d_c^k, X^{k-1}, (kth iteration), will then provide the needed multiplier information. Optimal multipliers of all the constraints and the optimal values of the objective function are used in constructing the outer master problem. Although we fix the control structure, X, the Lagrangian function generated from the overall problem would be a function of control structure, X, since it is assumed to be dual adequate and includes all the control superstructure constraints explicitly.

Master problem (optimal control structure selection)

The master problem is a min-max problem consisting of a scalar variable μ_B that is to be minimized, plus a growing collection of Lagrangian functions and multiplier data that are generated from the overall problem. Solution of the master problem will provide a new set of values for the control structure X to be used for the next iteration of the algorithm and a lower bound for the expected cost, EP^L. The form of the master problem is

$$\min_{X_{nm},\mu_B} \mu_B \tag{A40}$$

s.t.

$$\mu_B\ge\xi(X_{nm},\alpha_{n,ij}^{*,a},\mu_{l,ij}^{*,a},\eta_{q,ij}^{*,a},\lambda_{k,ij}^{*,a})\qquad a=1,2,\ldots,A\quad\text{(feasible)}$$

$$0\ge\bar{\xi}\left(X_{nm},\bar{\alpha}_{n,ij}^{*,b},\bar{\mu}_{l,ij}^{*,b},\bar{\eta}_{q,ij}^{*,a},\bar{\lambda}_{k,ij}^{*,b}\right)\qquad b=1,2,\ldots,B\quad\text{(infeasible)}$$

$$\sum_{n\in N^*}X_{nm}\le 1$$

$$\sum_{m\in M^*}X_{nm}\le 1$$

$$\forall m=1,2,\ldots,M;\qquad\forall n=1,2,\ldots,N;\qquad X_{nm}=[0,1]^{N\times M}$$

$$i\in[1,Nfe],\qquad j\in[0,N\text{col}]$$

where

$$\xi(X_{nm},\alpha_{n,ij}^*,\mu_{l,ij}^*,\eta_{q,ij}^*,\lambda_{k,ij}^*)=\inf_{d,d_c,y_{\text{set}},z}L(X_{nm},d^*,d_c^*,z_{ij},y_{\text{set}},\lambda_{k,ij}^*,\alpha_{n,ij}^*,\eta_{q,ij}^*,\mu_{l,ij}^*)$$

$$\bar{\xi}\left(X_{nm},\bar{\alpha}_{n,ij}^*,\bar{\mu}_{l,ij}^*,\bar{\eta}_{q,ij}^*,\bar{\lambda}_{k,ij}^*\right)=\inf_{d,d_c,y_{\text{set}},z}\bar{L}\left(X_{nm},d^*,d_c^*,z_{ij},y_{\text{set}},\bar{\lambda}_{k,ij}^*,\bar{\alpha}_{n,ij}^*,\bar{\eta}_{q,ij}^*,\bar{\mu}_{l,ij}^*\right).$$

From the Overall Problem.

$$\begin{aligned} L(X_{nm},d^*,d_c^*,z_{ij},y_{\text{set}},\lambda_{k,ij}^*,\alpha_{n,ij}^*,\eta_{q,ij}^*,\mu_{l,ij}^*)&=P(d^*,d_c^*)+C^TX+\sum_l(\mu_{l,ij}^*)^Th_l(d^*,z_{ij})\\ &\quad+\sum_q(\eta_{q,ij}^*)^Tf_q(d^*,z_{ij})\\ &\quad+\sum_k(\lambda_{k,ij}^*)^Tg_k(X_{nm},d^*,d_c^*,z_{ij})+\sum_n(\alpha_{n,ij}^*)^Thc_n(d_c^*,y_{\text{set}}). \end{aligned}$$

If infeasible primal problems are encountered, the form of the master problem would be modified to include *infeasibility* *cuts*, which are added constraints derived from Lagrangian functions generated by solution of an alternative subproblem that minimizes infeasibilities (see Geoffrion, 1972).

From the Infeasibility Minimization Problem.

$$\bar{L}\Big(X_{nm}, d^*, d_c^*, z_{ij}, y_{\text{set}}, \bar{\lambda}_{k,ij}^*, \bar{\alpha}_{n,ij}^*, \bar{\eta}_{q,ij}^*, \bar{\mu}_{l,ij}^*\Big)$$

$$= \sum_l (\bar{\mu}_{l,ij}^*)^T h_l(d^*, z_{ij}) + \sum_k \left(\bar{\lambda}_{k,ij}^*\right)^T g_k(X_{nm}, d^*, d_c^*, z_{ij})$$

$$+ \sum_q (\bar{\eta}_{q,ij}^*)^T f_q(d^*, z_{ij}) + \sum_n (\bar{\alpha}_{n,ij}^*)^T hc_n(d_c^*, y_{\text{set}})$$

$$\bar{\lambda}_{k,ij}^* \geq 0 \qquad \sum_k \bar{\lambda}_{k,ij}^* = 1 \qquad \bar{\mu}_{l,ij}^*, \bar{\eta}_{q,ij}^*, \bar{\alpha}_{n,ij}^* \in R.$$

Since nonlinearities are not present in the preceding master problem, it can be solved using a standard branch-and-bound algorithm for solution of mixed-integer linear programming (MILP) problems.

Appendix E: Decomposition Algorithm—Mixing Tank

Here, we briefly illustrate how the first iteration progresses for the mixing-tank example. The steps of the decomposition algorithm are as follows:

Step 0 (Initialization):

Iteration, $k = 0$

Set the nominal values of uncertainty F_h^o and disturbance T_h^o. The time horizon of interest is set to 30 h.

Step 1 (Multiperiod Design/Control Subproblem):

(i) Select an initial control structure X_V. Let us say this control structure represents a PI-controller connecting input F_c with the tank holdup V (measurement). Next, perform the multiperiod flexible design.

Iteration, $k = k + 1$

(ii) Solve the multiperiod flexible design problem for the critical parameters obtained. Store the optimal flexible design V_d^m, controller parameters, d_c^m, and an upper bound of the expected cost EP^U.

Multiperiod flexible design problem

We solve the multiperiod flexible design problem for a fixed control structure, X_V:

$$\min_{V_d, d_c, z, V_{\text{set}}} \left\{ \sum_p w_p \big[P(V_d, d_c, V_{ij}^p, T_{ij}^p, z_{ij}^p, F_{c,ij}^p, F_{h,ij}^{c,p}, T_{h,ij}^{c,p}, t_{ij}) + C^T X_V \big] \right\} \quad \text{(A41)}$$

s.t.

$$\dot{V}_{N\text{col}+1}^p(t_{ij}) - F_{h,ij}^p - F_{c,ij}^p + z_{ij}^p V_{ij}^{p0.5} = 0$$

$$V_{ij}^p \dot{T}_{N\text{col}+1}^p(t_{ij}) - F_{h,ij}^p(T_{h,ij}^p - T_{ij}^p) - F_{c,ij}^p(T_c - T_{ij}^p) = 0.$$

Critical Parameters

Uncertainty

$$F_{h,i}^p = \{F_{h,i,j}^{c,p}, F_{h,i,2}^{c,p}, \ldots, F_{h,i,j}^{c,p}, \ldots, F_{h,i,N\text{col}}^{c,p}\}.$$

Disturbance

$$T_{h,i}^p = \{T_{h,i,j}^{c,p}, T_{h,i,2}^{c,p}, \ldots, T_{h,i,j}^{c,p}, \ldots, T_{h,i,N\text{col}}^{c,p}\}.$$

Feasibility Constraints

$$V_{ij}^p \leq V_d$$

$$V_{ij}^p \leq V_{ij}^u$$

$$V_{ij}^p \geq V_{ij}^l$$

$$T_{ij}^p \leq T_{ij}^u$$

$$T_{ij}^p \geq T_{ij}^l.$$

Control Scheme

$$F_{c,ij}^p = F_{c,o} + KC_V \left(e_{V,ij}^p + \sum_i \sum_j wt_{ij} \frac{e_{V,ij}^p}{\tau_V} \right)$$

$$e_{V,ij}^p = V_{ij}^p - V_{\text{set}}^p$$

$$KC_V \geq KC_V^l X_V$$

$$KC_V \leq KC_V^u X_V$$

$$i \in Nfe, \qquad j \in N\text{col}, \qquad p \in TP,$$

where wt_{ij} represent Gaussian quadrature weights.

This multiperiod flexible design problem yields an optimal design V_d^*, controller parameters $d_c^* = \{KC_V = 0.10,\ \tau_V = 16.35\}$, and an upper bound of the expected cost ($EP^U =$ \$7,470). Next, we evaluate the necessary Lagrangian information to construct the control structure selection master problem.

$$L(X_V, X_T, V_d^*, d_c^*, z_{ij}, V_{\text{set}}, T_{\text{set}}, \lambda_{k,ij}^*, \alpha_{n,ij}^*, \mu_{l,ij}^*) = P(V_d^*, d_c^*)$$

$$+ C^T X + \sum_{l=1}^{2} (\mu_{l,ij}^*)^T h_l(V_d^*, z_{ij})$$

$$+ \sum_{k=1}^{5} (\lambda_{k,ij}^*)^T g_k(X_V, X_T, V_d^*, z_{ij})$$

$$+ \sum_{n=1}^{1} (\alpha_{n,ij}^*)^T hc_n(d_c^*, V_{\text{set}}, T_{\text{set}})$$

$$\lambda_{k,ij}^* \geq 0 \qquad \sum_{k=1}^{5} \lambda_{k,ij}^* = 1 \qquad \alpha_{n,ij}^*, \mu_{l,ij}^* \in R,$$

where h_l, g_k, and hc_n refer to tank model differential equations, feasibility constraints, and control superstructure equality constraints, respectively. Store the necessary Lagrange multiplier information to formulate the *master problem.*

(iii) Generate and solve the optimal control structure selection–*master problem* that is a mixed-integer linear programming (MILP) problem.

Optimal control structure selection – master problem

$$\min_{X_V, X_T, \mu_B} \mu_B \tag{A42}$$

s.t.

$$\mu_B \geq \xi(X_V, X_T, \lambda^{*,a}_{k,ij}, \alpha^{*,a}_{n,ij}, \mu^{*,a}_{l,ij})$$

$$a = 1,2,\ldots,A \text{ (feasible)}$$

$$0 \geq \bar{\xi}\left(X_V, X_T, \bar{\lambda}^{*,b}_{k,ij}, \bar{\alpha}^{*,b}_{n,ij}, \bar{\mu}^{*,b}_{l,ij}\right)$$

$$b = 1,2,\ldots,B \text{ (infeasible)}$$

$$X_V + X_T = 1$$

$$X_T, X_V = \{0,1\}, \qquad i \in Nfe, \qquad j \in N\text{col},$$

where

$$\xi(X_V, X_T, \lambda^{*,a}_{k,ij}, \alpha^{*,a}_{n,ij}, \mu^{*,a}_{l,ij})$$

$$= \inf_{V_d, d_c, V_{\text{set}}, T_{\text{set}}} L(X_V, X_T, V^*_d, d^*_c, z_{ij}, V_{\text{set}}, T_{\text{set}}, \lambda^*_{k,ij}, \alpha^*_{n,ij}, \mu^*_{l,ij})$$

$$\bar{\xi}\left(X_V, X_T, \bar{\lambda}^{*,b}_{k,ij}, \bar{\alpha}^{*,b}_{n,ij}, \bar{\mu}^{*,b}_{l,ij}\right)$$

$$\inf_{V_d, d_c, V_{\text{set}}, T_{\text{set}}} \bar{L}\left(X_V, X_T, V^*_d, d^*_c, z_{ij}, V_{\text{set}}, T_{\text{set}}, \bar{\lambda}^*_{k,ij}, \bar{\alpha}^*_{n,ij}, \bar{\mu}^*_{l,ij}\right).$$

Solution of the above master problem provided a new control structure, $X^{*,m}_T$, and a lower bound for the expected cost, $EP^L = \$5{,}859$.

(iv) Bounds are compared according to GBD and $|EP^{U,m} - EP^{L,m}| \geq \epsilon$. Therefore, update X and go back to **Step 1** (ii). Once the inner loop is converged, Go to **Step 2** for feasibility analysis of this optimal design and control structure.

Step 2 (Feasibility Analysis)

Feasibility analysis is performed to identify the critical parameters that would drive the system infeasible.

Feasibility analysis of dynamic system

$$\chi(V_d, t_{ij}) = \max_{s, F_h, T_h, z, q, \lambda, \mu, \alpha, Y} s_{ij} \tag{A43}$$

s.t.

$$\dot{V}_{N\text{col}+1}(t_{ij}) - F_{h,ij} - F_{c,ij} + z_{ij} V^{0.5}_{ij} = 0 \quad \rightarrow \mu_1$$

$$V_{ij} \dot{T}_{N\text{col}+1}(t_{ij}) - F_{h,ij}(T_{h,ij} - T_{ij}) - F_{c,ij}(T_c - T_{ij}) = 0 \quad \rightarrow \mu_2.$$

Feasibility Constraints

$$q_{1,ij} + V_{ij} - V_d = s_{ij} \quad \rightarrow \lambda_1$$

$$q_{2,ij} + V_{ij} - V^u_{ij} = s_{ij} \quad \rightarrow \lambda_2$$

$$q_{3,ij} + V^l_{ij} - V_{ij} = s_{ij} \quad \rightarrow \lambda_3$$

$$q_{4,ij} + T_{ij} - T^u_{ij} = s_{ij} \quad \rightarrow \lambda_4$$

$$q_{5,ij} + T^l_{ij} - T_{ij} = s_{ij} \quad \rightarrow \lambda_5.$$

Control Scheme

$$F_{c,ij} = F_{c,o} + KC_T\left(e_{T,ij} + \sum_i \sum_j w_{ij} \frac{e_{T,ij}}{\tau_T}\right) \quad \rightarrow \alpha_1.$$

$$e_{T,ij} = T_{ij} - T_{\text{set}}$$

From Optimality Conditions

$$\frac{\partial}{\partial z} \qquad -\mu_{1,ij}\left(V^{0.5}_{ij}\right) = 0$$

$$\frac{\partial}{\partial F_c} \qquad +\mu_{1,ij} + \mu_{2,ij}(T_c - T_{ij}) + \alpha_{1,ij} = 0$$

$$\frac{\partial}{\partial V} \qquad -\mu_{1,ij}\left(\frac{1}{2} z_{ij} V^{-0.5}_{ij}\right) + \lambda_{1,ij} + \lambda_{2,ij} - \lambda_{3,ij} + \dot{\mu}_{1,N\text{col}+1}(t_{ij}) = 0$$

$$\frac{\partial}{\partial T} \qquad -\mu_{2,ij}(F_{h,ij} + F_{c,ij}) + \alpha_{1,ij}\left\{-KC_{Fc}\left(1 + \sum_i \sum_j \frac{wt_{ij}}{\tau_T}\right)\right\} + \lambda_{4,ij} - \lambda_{5,ij} + \dot{\mu}_{2,N\text{col}+1}(t_{ij}) = 0$$

$$\lambda_{1,ij} + \lambda_{2,ij} + \lambda_{3,ij} + \lambda_{4,ij} + \lambda_{5,ij} = 1$$

$$\lambda_{1,ij} - Y_{1,ij} \leq 0$$

$$\lambda_{2,ij} - Y_{2,ij} \leq 0$$

$$\lambda_{3,ij} - Y_{3,ij} \leq 0$$

$$\lambda_{4,ij} - Y_{4,ij} \leq 0$$

$$\lambda_{5,ij} - Y_{5,ij} \leq 0$$

$$q_{1,ij} - 1{,}000(1 - Y_{1,ij}) \leq 0$$

$$q_{2,ij} - 1{,}000(1 - Y_{2,ij}) \leq 0$$

$$q_{3,ij} - 1{,}000(1 - Y_{3,ij}) \leq 0$$

$$q_{4,ij} - 1{,}000(1 - Y_{4,ij}) \leq 0$$

$$q_{5,ij} - 1{,}000(1 - Y_{5,ij}) \leq 0$$

$$Y_{1,ij} + Y_{2,ij} + Y_{3,ij} + Y_{4,ij} + Y_{5,ij} \leq (n_u + n_z) + 1$$

Uncertainty

$$F^l_{h,ij} \le F_{h,ij} \le F^u_{h,ij}.$$

Disturbance

$$T^l_{h,ij} \le T_{h,ij} \le T^u_{h,ij}.$$

$$Y_{k,ij} = [0,1]; \qquad q_{k,ij}, \lambda_{k,ij} \ge 0; \qquad \mu_{l,ij}, \alpha_{n,ij} \in R$$

$$i \in [1, Nfe]; \qquad j \in [0, N\text{col}].$$

The optimal design is found to be infeasible (i.e., $\chi > 0$). Obtain the critical uncertainty and disturbance profiles (F^c_h, T^c_h) for this infeasible design:

$$F^c_h = \{F^c_{h,1,j}, F^c_{h,1,2}, \ldots, F^c_{h,1,j}, \ldots, F^c_{h,1,N\text{col}}, \ldots, F^c_{h,Nfe,j}, \ldots, F^c_{h,Nfe+1,0}\}$$

$$T^c_h = \{T^c_{h,1,j}, T^c_{h,1,2}, \ldots, T^c_{h,1,j}, \ldots, T^c_{h,1,N\text{col}}, \ldots, T^c_{h,Nfe,j}, \ldots, T^c_{h,Nfe+1,0}\}$$

and go back to **Step 1** (ii) (with $X^k_{\text{current}} = X^k_T$).

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