PROCESS SYNTHESIS, DESIGN, AND CONTROL: A MIXED-INTEGER OPTIMAL CONTROL FRAMEWORK

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Abstract: A mixed-integer optimal control framework for analyzing the interaction of process synthesis, design, and control is presented in this paper. The approach integrates the economic design and dynamic controllability into a multiobjective Mixed-Integer Optimal Control Problem (MIOCP). The problem formulation includes dynamic models and incorporates both discrete and continuous decisions. An algorithm for the solution of the MIOCP is developed based on the principles of Generalized Benders Decomposition for mixed-integer nonlinear optimization. The algorithm is used to determine the trade-offs between the economic design and dynamic controllability of a reactor-separator-recycle system.

Keywords: Mixed-Integer Nonlinear Optimization, Optimal Control

1. INTRODUCTION

An important issue in the area of process synthesis, design, and control is the solution of optimization problems which involve dynamic models along with discrete decisions. This type of problem arises in analyzing the interaction of the design and control of a process. Discrete decisions are used to indicate the existence of units in the process while dynamic modeling is necessary for the design of the control system.

Traditional approaches to process design and control separate the two by handling them sequentially. First, an optimal steady-state process design is determined and then a control strategies are applied to maintain the process at the specified stead-state. This neglects the well-established notion that the controllability of the process is an inherent characteristic of its design.

In order to address this limitation, the controllability of the process should be considered at the early stages of the design of the process. This is handled by using an integrated approach to design and control with the the following features:

- simultaneous consideration of controllability and economic criteria of the process at the early stages
- incorporation of the dynamic operation of the process

The interaction of design and control has been addressed in previous work, and Morari and Perkins (1994) provide a review of the various design/control methodologies. Noting that a great amount of effort has been placed on the assessment of controllability, particularly for linear dynamic models, they indicate that very little has been published on algorithmic approaches for determination of process designs where economics and controllability are traded off systematically. Control structure selection issues are addressed in Narraway and Perkins (1993*b*) and Narraway and Perkins (1993*a*) to assess the economics associated with the process dynamics. A multiobjective approach was presented by Luyben and Floudas (1994*a*) and Luyben and Floudas (1994*b*) where

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both design and control aspects are incorporated into a process synthesis framework. The work of Bahri *et al.* (1996) and Figueroa *et al.* (1996) proposed a method for determining the economic penalty associated with maintaining feasible operation for a given set of uncertainties and disturbances. The problem of optimal design of dynamic systems under uncertainty is addressed in Mohideen *et al.* (1996) where both flexibility and controllability issues are considered.

The previous work either did not include the process synthesis issues or did not include the dynamic operation of the process. This work focuses on a process synthesis framework where both structural decisions and dynamic models are included.

2. INTERACTION OF PROCESS SYNTHESIS, DESIGN, AND CONTROL

The objective is to determine the process structure, operating conditions, controller structure, and tuning parameters which optimize both the economics and controllability of the process and guarantee feasible operation.

The problem is formulated by modeling the postulated superstructure of process alternatives of interest. Since the dynamic operation of the process is being considered the process is modeled dynamically which gives rise to a system of differential and algebraic equations (DAEs).

The problem considered has the following general formulation:

$$\begin{aligned}
\min \quad & \boldsymbol{J}(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{u}(t_i), \boldsymbol{x}, \boldsymbol{y}) \\
\text{s.t.} \quad \boldsymbol{f}_1(\dot{\boldsymbol{z}}_1(t), \boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{u}(t), \boldsymbol{x}, \boldsymbol{y}, t) &= \boldsymbol{0} \\
\boldsymbol{f}_2(\boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{u}(t), \boldsymbol{x}, \boldsymbol{y}, t) &= \boldsymbol{0} \\
\boldsymbol{z}_1(t_0) &= \boldsymbol{z}_1^0 \\
\boldsymbol{z}_2(t_0) &= \boldsymbol{z}_2^0 \\
\boldsymbol{h}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{u}(t_i), \boldsymbol{x}, \boldsymbol{y}) &= \boldsymbol{0} \\
\boldsymbol{g}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{u}(t_i), \boldsymbol{x}, \boldsymbol{y}) &\leq \boldsymbol{0} \\
\boldsymbol{h}''(\boldsymbol{x}, \boldsymbol{y}) &= \boldsymbol{0} \\
\boldsymbol{g}''(\boldsymbol{x}, \boldsymbol{y}) &\leq \boldsymbol{0} \\
\boldsymbol{x} &\in \mathcal{X} \subseteq \mathbb{R}^p \\
\boldsymbol{y} &\in \{0,1\}^q \\
t_i &\in [t_0, t_N] \\
i &= 0 \ldots N
\end{aligned} \tag{1}$$

where $\boldsymbol{z}_1(t)$ is a vector of n dynamic variables whose time derivatives, $\dot{\boldsymbol{z}}_1(t)$, appear explicitly, and $\boldsymbol{z}_2(t)$ is a vector of m dynamic variables whose time derivatives do not appear explicitly, $\boldsymbol{x}$ is a vector of p time invariant continuous variables, $\boldsymbol{y}$ is a vector of q binary variables, and $\boldsymbol{u}(t)$ is a vector of r control variables. Time t is the independent variable for the DAE system where t_0 is the fixed initial time, t_i are time instances, and t_N is the final time. The DAE system is represented by $\boldsymbol{f}_1$, the n differential equations, and $\boldsymbol{f}_2$, the m dynamic algebraic equations. The constraints $\boldsymbol{h}'$ and $\boldsymbol{g}'$ are point constraints where t_i represents the time instance at which the constraint is enforced and $\boldsymbol{h}''$ and $\boldsymbol{g}''$ are general constraints.

The initial condition for the above system is determined by specifying n of the $2n+m$ variables $\boldsymbol{z}_1(t_0), \dot{\boldsymbol{z}}_1(t_0), \boldsymbol{z}_2(t_0)$. For DAE systems with index 0 or 1, the remaining $n+m$ values can be determined. In this work, DAE systems of index 0 or 1 are considered and the initial conditions for $\boldsymbol{z}_1(t)$ and $\boldsymbol{z}_2(t)$ are $\boldsymbol{z}_1^0$ and $\boldsymbol{z}_2^0$ respectively.

Two points about this formulation should be noted. First the $\boldsymbol{y}$ variables appear in the DAE system as well as in the point constraints and general constraints. Second, the objective function $\boldsymbol{J}$ is a vector of two objectives representing the economic and controllability objectives. The formulation is classified as a multiobjective Mixed Integer Optimal Control Problem (MIOCP).

3. ALGORITHMIC FRAMEWORK FOR THE INTERACTION OF SYNTHESIS, DESIGN, AND CONTROL

There are three characteristics which complicate the solution of the Multiobjective MIOCP formulation: the multiobjective nature, the optimal control problem, and the mixed integer aspects. By addressing each aspect, subproblems that are easier to solve than the original problem are formulated.

3.1 *Multiobjective Optimization*

In order to handle the multiobjective nature in this problem, the ϵ-constraint method is used to generate a pareto-optimal solution. This noninferior solution set is the set of solutions where one objective can be improved only at the expense of the other. thus indicate the trade-offs between the two objectives.

The use of the ϵ-constraint method reduces the multiobjective problem to successive solutions of single objective problems. Consider the vector of objective functions $\boldsymbol{J} = (J_1, J_2)$ where J_1 represents a design objective and J_2 a controllability objective. The application of the ϵ constraint method to this two objective problem leads to the following formulation:

The ϵ constraint involving J_2 becomes a point constraint in the problem and is included in the constraints $\boldsymbol{h}'$. Thus the original problem formulation has been reduced to a single objective problem which must be solved multiple times with varying values of ϵ to generate the noninferior solution set.

3.2 *Solution of the Optimal Control Problem*

The solution of the optimal control problem can be handled in several ways: complete discretization, solution of the necessary conditions, dynamic programming, and control parameterization. The current practice for solving the optimal control problem when it is part of a mixed-integer problem is to use complete discretization to convert the problem to a large scale MINLP. The problem with this method is that the size of the problem grows dramatically with the number of DAEs in the problem.

This work focuses on the control parameterization techniques which parameterize only the control variables $\boldsymbol{u}(t)$ in terms of time invariant parameters. At each step of the optimization procedure, the DAEs are solved for given values of the decision variables and a feasible path for $\boldsymbol{z}(t)$ is obtained. This solution is used to evaluate the objective function and remaining constraints. The control parameterization can either be open loop as described in Vassiliadis *et al.* (1994) or closed-loop such as that described in Narraway and Perkins (1993*b*) and Narraway and Perkins (1993*a*) which also includes the control structure selection. By applying the control parameterization, the control variables $\boldsymbol{u}(t)$ are converted to dynamic state variables $\boldsymbol{z}(t)$ and the parameters for the control are added to the set of time invariant decision variable $\boldsymbol{x}$. The following problem results:

$$\begin{aligned}
\min \quad & J(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}, \boldsymbol{y}) \\
\text{s.t.} \quad \boldsymbol{f}_1(\dot{\boldsymbol{z}}_1(t), \boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{x}, \boldsymbol{y}, t) &= \boldsymbol{0} \\
\boldsymbol{f}_2(\boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{x}, \boldsymbol{y}, t) &= \boldsymbol{0} \\
\boldsymbol{z}_1(t_0) &= \boldsymbol{z}_1^0 \\
\boldsymbol{z}_2(t_0) &= \boldsymbol{z}_2^0 \\
\boldsymbol{h}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}, \boldsymbol{y}) &= \boldsymbol{0} \\
\boldsymbol{g}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}, \boldsymbol{y}) &\leq \boldsymbol{0} \\
\boldsymbol{h}''(\boldsymbol{x}, \boldsymbol{y}) &= \boldsymbol{0} \\
\boldsymbol{g}''(\boldsymbol{x}, \boldsymbol{y}) &\leq \boldsymbol{0} \\
\boldsymbol{x} &\in \mathcal{X} \subseteq \mathbb{R}^p \\
\boldsymbol{y} &\in \{0,1\}^q \\
t_i &\in [t_0, t_N] \\
i &= 0 \ldots N
\end{aligned} \tag{2}$$

3.3 *MINLP/DAE Solution Algorithm*

The strategy for solving the MINLP/DAE is to apply iterative decomposition strategies similar to standard MINLP algorithms. An overview of MINLP algorithms and extensive theoretical, algorithmic, and applications-oriented descriptions of these algorithms are found in Floudas (1995). The MINLP/DAE algorithmic development closely follows the developments of Generalized Benders Decomposition with appropriate extensions for the DAE system.

3.3.1. *Primal Problem*

The primal problem is obtained by fixing the $\boldsymbol{y}$ variables and its solution provides an upper bound on the solution of the MINLP/DAE. For fixed values of $\boldsymbol{y} = \boldsymbol{y}^k$, the MINLP/DAE becomes an NLP/DAE.

The NLP/DAE problem is solved using a parametric method where the DAE system is solved as a function of the $\boldsymbol{x}$ variables. The solution of the DAE system is achieved through an integration routine which returns the values of the $\boldsymbol{z}$ variables at the time instances, $\boldsymbol{z}(t_i)$, along with their sensitivities with respect to the parameters, $\frac{d\boldsymbol{z}}{d\boldsymbol{x}}(t_i)$. The resulting problem is an NLP optimization over the space of $\boldsymbol{x}$ variables which has the form:

$$\begin{aligned}
\min \quad & J(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}, \boldsymbol{y}^k) \\
\text{s.t.} \quad \boldsymbol{h}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}, \boldsymbol{y}^k) &= \boldsymbol{0} \\
\boldsymbol{g}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}, \boldsymbol{y}^k) &\leq \boldsymbol{0} \\
\boldsymbol{h}''(\boldsymbol{x}, \boldsymbol{y}^k) &= \boldsymbol{0} \\
\boldsymbol{g}''(\boldsymbol{x}, \boldsymbol{y}^k) &\leq \boldsymbol{0} \\
\boldsymbol{x} &\in \mathcal{X} \\
t_i &\in [t_0, \ldots, t_N] \\
i &= 0 \ldots N
\end{aligned} \tag{3}$$

where the variables $\dot{\boldsymbol{z}}_1(t_i)$, $\boldsymbol{z}_1(t_i)$, and $\boldsymbol{z}_2(t_i)$ are determined through the solution of the DAE system by integration:

$$\begin{aligned}
\boldsymbol{f}_1(\dot{\boldsymbol{z}}_1(t), \boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{x}, \boldsymbol{y}^k, t) &= \boldsymbol{0} \\
\boldsymbol{f}_2(\boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{x}, \boldsymbol{y}^k, t) &= \boldsymbol{0} \\
\boldsymbol{z}_1(t_0) &= \boldsymbol{z}_1^0 \\
\boldsymbol{z}_2(t_0) &= \boldsymbol{z}_2^0
\end{aligned} \tag{4}$$

The functions $J(\cdot)$, $\boldsymbol{g}'(\cdot)$, and $\boldsymbol{h}'(\cdot)$ are functions of $\boldsymbol{z}(t_i)$ which are implicit functions of the $\boldsymbol{x}$ variables through the integration of the DAE system. For the solution of the NLP the objective and constraints evaluations along with their gradients with respect to $\boldsymbol{x}$.are required. These are evaluated directly for the constraints $\boldsymbol{g}''(\boldsymbol{x})$ and $\boldsymbol{h}''(\boldsymbol{x})$. However, for the functions $J(\cdot)$, $\boldsymbol{g}'(\cdot)$, and $\boldsymbol{h}'(\cdot)$, the values $\boldsymbol{z}(t_i)$, and the gradients $\frac{d\boldsymbol{z}}{d\boldsymbol{x}}(t_i)$ returned from the integration are used. The functions $J(\cdot)$, $\boldsymbol{g}'(\cdot)$, and $\boldsymbol{h}'(\cdot)$ are evaluated directly and the gradients $\frac{dJ}{d\boldsymbol{x}}$, $\frac{d\boldsymbol{g}_i'}{d\boldsymbol{x}}$, and $\frac{d\boldsymbol{h}'}{d\boldsymbol{x}}$ are evaluated by using the chain rule:

$$\begin{aligned}
\frac{dJ}{d\boldsymbol{x}} &= \left(\frac{\partial J}{\partial \boldsymbol{z}}\right)\left(\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}}\right) + \left(\frac{\partial J}{\partial \boldsymbol{x}}\right) \\
\frac{d\boldsymbol{h}_i'}{d\boldsymbol{x}} &= \left(\frac{\partial \boldsymbol{h}_i'}{\partial \boldsymbol{z}}\right)\left(\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}}\right) + \left(\frac{\partial \boldsymbol{h}_i'}{\partial \boldsymbol{x}}\right) \\
\frac{d\boldsymbol{g}_i'}{d\boldsymbol{x}} &= \left(\frac{\partial \boldsymbol{g}_i'}{\partial \boldsymbol{z}}\right)\left(\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}}\right) + \left(\frac{\partial \boldsymbol{g}_i'}{\partial \boldsymbol{x}}\right)
\end{aligned} \tag{5}$$

Standard gradient based optimization techniques can be applied to solve this problem as an NLP. The solution of this problem provides values of the $\boldsymbol{x}$ variables and trajectories for $\boldsymbol{z}(t)$.

Table 1. Primal constraints and corresponding dual variables

constraint	dual variable
$\boldsymbol{f}_1$	$\boldsymbol{\nu}_1(t)$
$\boldsymbol{f}_2$	$\boldsymbol{\nu}_2(t)$
$\boldsymbol{g}'$	$\boldsymbol{\mu}'$
$\boldsymbol{h}'$	$\boldsymbol{\lambda}'$
$\boldsymbol{g}''$	$\boldsymbol{\mu}''$
$\boldsymbol{h}''$	$\boldsymbol{\lambda}''$

3.3.2. *Master Problem*

The master problem is formulated using dual information and the solution of the primal problem. Provided that the $\boldsymbol{y}$ variables participate linearly, the problem is an MILP whose solution provides a lower bound and $\boldsymbol{y}$ variables for the next primal problem. Dual information is required from all of the constraints including the DAEs whose dual variables, or adjoint variables, are dynamic. The constraints and their corresponding dual variables are listed in Table 1.

The dual variables $\boldsymbol{\mu}'$, $\boldsymbol{\lambda}'$, $\boldsymbol{\mu}''$, and $\boldsymbol{\lambda}''$ are generally obtained from the solution technique for the primal problem. Dual information from the DAE system is obtained by solving the adjoint problem for the DAE system which has the following formulation:

$$\begin{aligned} \boldsymbol{p} &= \left(\frac{d\boldsymbol{f}_1}{d\dot{\boldsymbol{z}}_1}\right)^T \boldsymbol{\nu}_1(t) \\ \dot{\boldsymbol{p}} &= \left(\frac{d\boldsymbol{f}_1}{d\boldsymbol{z}_1}\right)^T \boldsymbol{\nu}_1(t) + \left(\frac{d\boldsymbol{f}_2}{d\boldsymbol{z}_1}\right)^T \boldsymbol{\nu}_2(t) \\ \boldsymbol{0} &= \left(\frac{d\boldsymbol{f}_1}{d\boldsymbol{z}_2}\right)^T \boldsymbol{\nu}_1(t) + \left(\frac{d\boldsymbol{f}_2}{d\boldsymbol{z}_2}\right)^T \boldsymbol{\nu}_2(t) \end{aligned} \tag{6}$$

This is a set of DAEs where the solutions for $\frac{d\boldsymbol{f}_1}{d\dot{\boldsymbol{z}}_1}$, $\frac{d\boldsymbol{f}_1}{d\boldsymbol{z}_1}$, $\frac{d\boldsymbol{f}_2}{d\boldsymbol{z}_1}$, $\frac{d\boldsymbol{f}_1}{d\boldsymbol{z}_2}$, and $\frac{d\boldsymbol{f}_2}{d\boldsymbol{z}_2}$ are known functions of time obtained from the solution of the primal problem. The variables $\boldsymbol{\nu}_1(t)$ and $\boldsymbol{\nu}_2(t)$ are the adjoint variables and the solution of this problem is a backward integration in time with the following final time conditions:

$$\begin{aligned} &\left.\left(\frac{d\boldsymbol{f}_1}{d\dot{\boldsymbol{z}}_1}\right)^T\right|_{t_N} \boldsymbol{\nu}_1(t_N) = \\ &\qquad -\left(\frac{d\boldsymbol{J}}{d\boldsymbol{z}_1}\right) - \left(\frac{d\boldsymbol{g}'}{d\boldsymbol{z}_1}\right)^T \boldsymbol{\mu}' - \left(\frac{d\boldsymbol{h}'}{d\boldsymbol{z}_1}\right)^T \boldsymbol{\lambda}' \end{aligned} \tag{7}$$

Thus, the Lagrange multipliers for the end-time constraints are used as the final time conditions for the adjoint problem and are not included in the master problem formulation.

The master problem is formulated using the solution of the primal problem, $\boldsymbol{x}^k$ and $\boldsymbol{z}^k(t)$ along with the dual information, $\boldsymbol{\mu}''^k$, $\boldsymbol{\lambda}''^k$, and $\boldsymbol{\nu}^k(t)$. The master problem has the following form:

$$\begin{aligned} \min_{\boldsymbol{y},\boldsymbol{\mu}_b}\ & \boldsymbol{\mu}_b \\ \text{s.t. } & \boldsymbol{\mu}_b \geq J(\boldsymbol{x}^k, \boldsymbol{y}) \\ & + \int_{t_0}^{t_N} \boldsymbol{\nu}_1^k(t) \boldsymbol{f}_1(\dot{\boldsymbol{z}}_1^k(t), \boldsymbol{z}_1^k(t), \boldsymbol{z}_2^k(t), \boldsymbol{x}^k, \boldsymbol{y}, t)dt \\ & + \int_{t_0}^{t_N} \boldsymbol{\nu}_2^k(t) \boldsymbol{f}_2(\boldsymbol{z}_1^k(t), \boldsymbol{z}_2^k(t), \boldsymbol{x}^k, \boldsymbol{y}, t)dt \\ & + \boldsymbol{\mu}''^k \boldsymbol{g}''(\boldsymbol{x}^k, \boldsymbol{y}) + \boldsymbol{\lambda}''^k \boldsymbol{h}''(\boldsymbol{x}^k, \boldsymbol{y}) \\ & \qquad k \in K_{\text{feas}} \\ \boldsymbol{0} \geq & \int_{t_0}^{t_N} \boldsymbol{\nu}_1^k(t) \boldsymbol{f}_1(\dot{\boldsymbol{z}}_1^k(t), \boldsymbol{z}_1^k(t), \boldsymbol{z}_2^k(t), \boldsymbol{x}^k, \boldsymbol{y}, t)dt \\ & + \int_{t_0}^{t_N} \boldsymbol{\nu}_2^k(t) \boldsymbol{f}_2(\boldsymbol{z}_1^k(t), \boldsymbol{z}_2^k(t), \boldsymbol{x}^k, \boldsymbol{y}, t)dt \\ & + \boldsymbol{\mu}''^k \boldsymbol{g}''(\boldsymbol{x}^k, \boldsymbol{y}) + \boldsymbol{\lambda}''^k \boldsymbol{h}''(\boldsymbol{x}^k, \boldsymbol{y}) \\ & \qquad k \in K_{\text{infeas}} \\ & \boldsymbol{y} \in \{0, 1\}^q \end{aligned} \tag{8}$$

The integral term can be evaluated since the profiles for $\boldsymbol{z}^k(t)$ and $\boldsymbol{\nu}^k(t)$ both are fixed and known. Note that this formulation has no restrictions on whether or not $\boldsymbol{y}$ variables participate in the the DAE system.

4. NUMERICAL PROCEDURE

The solution algorithm for the MINLP/DAE has been implemented in the program MINOPT (Schweiger and Floudas, 1997) (Mixed Integer Nonlinear OPTimizer) which has been developed as a unified framework for the solution of various classes of optimization problems. MINOPT features a front-end parser which allows for the concise problem representation. MINOPT implements a broad range of solution algorithms for handling linear programs, mixed integer linear programs, nonlinear programs, mixed integer nonlinear programs, and problems involving dynamic models. For the solution of the NLP/DAE problems, MINOPT incorporates NPSOL (Gill *et al.*, 1986) (SQP). For the solution of the DAE system and sensitivity analysis, MINOPT uses DASOLV (Jarvis and Pantelides, 1992) which is an implementation of a backwards difference formula algorithm for large sparse DAEs. For the solution of the MILP problems, CPLEX (CPL, 1995) is used.

5. EXAMPLE: REACTOR-SEPARATOR-RECYCLE SYSTEM

The example problem considered here is the design of a process involving a reaction step, a separation step, and a recycle loop is considered. Fresh feed containing A and B flow into a an isothermal

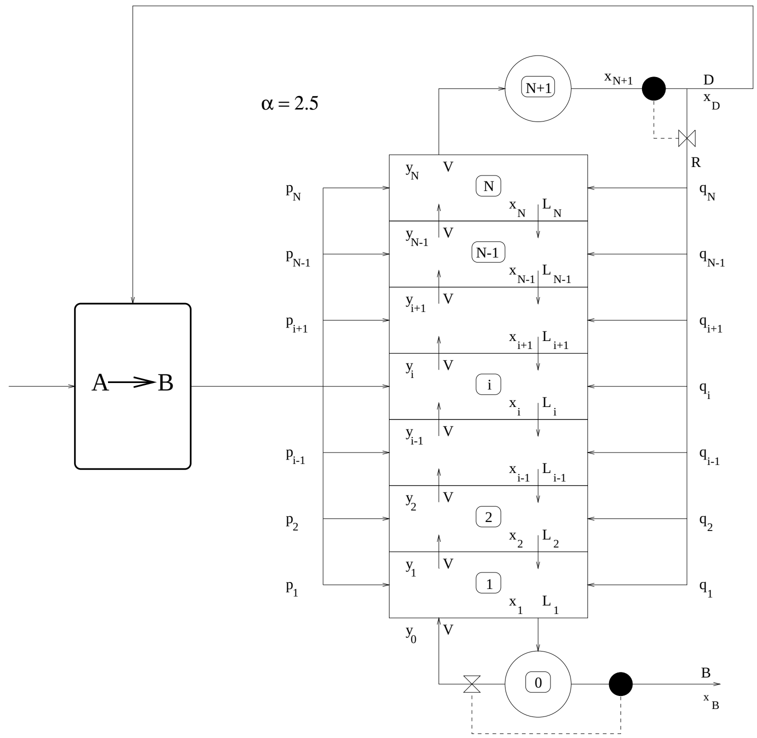

Fig. 1. Superstructure for Reactor-Separator-Recycle system

reactor where the first order irreversible reaction $A \rightarrow B$ takes place. The product is from the reactor is sent to a distillation column where the unreacted A is separated from the product B and sent back to the reactor. The superstructure is shown in Figure 1.

The model equations for the reactor (CSTR) and the separator (ideal binary distillation column) can be found in Luyben (1990). The specific problem design follows the work in Luyben and Floudas (1994*b*).

For this problem, the single output is the product composition. The bottoms (product) composition is controlled by the vapor boil-up and the distillate composition is controlled by the reflux rate. Since only the product composition is specified, the distillate composition set-point is free and left to be determined through the optimization.

The cost function includes column and reactor capital and utility costs.

$$\text{cost}_{\text{reactor}} = 17639 D_r^{1.066} (2D_r)^{0.802}$$

$$\begin{aligned}\text{cost}_{\text{column}} = \; & 6802 D_c^{1.066} (2.4 N_t)^{0.802} \\ & + 548.8 D_c^{1.55} N_t\end{aligned}$$

$$\text{cost}_{\text{exchangers}} = 193023 V_{ss}^{0.65}$$

$$\text{cost}_{\text{utilities}} = 72420 V_{ss}$$

$$\begin{aligned}\text{cost}_{\text{total}} = \; & \frac{1}{\beta_{\text{pay}}} [\text{cost}_{\text{reactor}} + \text{cost}_{\text{column}} \\ & + \text{cost}_{\text{exchangers}}] \quad + \beta_{\text{tax}} [\text{cost}_{\text{utilities}}]\end{aligned}$$

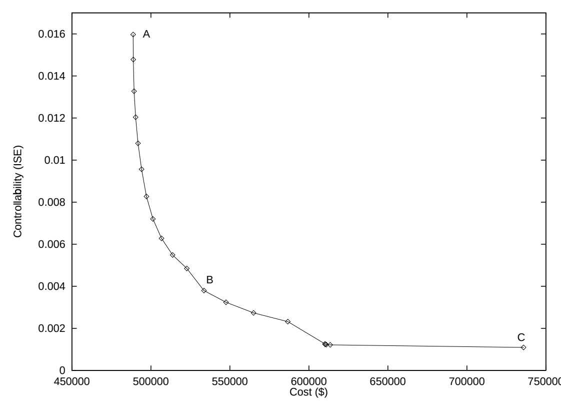

Fig. 2. Noninferior solution set for the Reactor–Separator–Recycle System

Table 2. Results for three designs

Solution	A	B	C
Cost ($)	489,000	534,000	736,000
Capital Cost ($)	321,000	364,000	726,000
Utility Cost ($)	168,000	170,000	10,000
ISE	0.0160	0.00379	0.0011
Trays	19	8	1
Feed	19	8	1
$V_r(kmol)$	2057.9	3601.2	15000
$V(kmol/hr)$	138.94	141.25	85.473
K_V	90.94	80.68	87.40
$\tau_V(hr)$	0.295	0.0898	0.0156

The controllability measure is the time weighted ISE of the product composition:

$$\frac{d\boldsymbol{\mu}}{dt} = t(x_B - x_B^\star)^2$$

The noninferior solution set is shown in Figure 2 and the results for three of the designs are shown

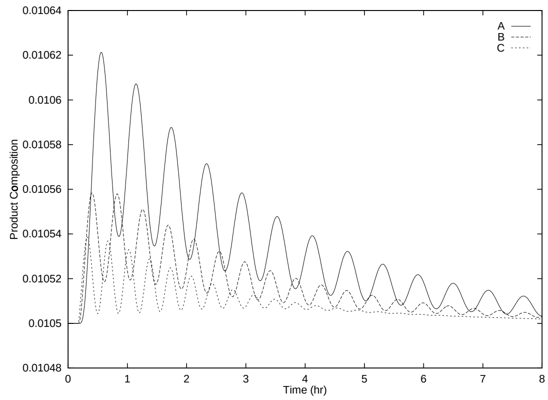

Fig. 3. Dynamic responses of product compositions for three designs

in Table 2. All of the designs in the noninferior solution set are strippers. Since the feed enters at the top of the column, there is no reflux and thus no control loop for the distillate composition. The controllability of the process is increased by increasing the size of the reactor and decreasing the size of the column. The most controllable design has a large reactor and a single flash unit. The dynamic responses for the three designs are shown in Figure 3. The most economic design (A) has more prominent oscillations in comparison to the most controllable design.

6. CONCLUSIONS

This work presents a method for systematically analyzing the interaction of process synthesis, design, and control. The principal characteristic of the problem is the existence of both discrete decisions and dynamic models. The application of the process synthesis framework leads to multi-objective mixed-integer optimal control problem. By applying the proposed solution algorithm, the trade-offs between economic design and dynamic controllability are determined. This is demonstrated in the reactor-separator-recycle design example.

The proposed approach has been applied by considering a single disturbance. Although the feedback control can be robust, the resulting solution is likely to be specific to the proposed disturbance. The approach also does not consider uncertainty in the process that may arise due to variation in external variables or internal parameters. Further work should address both of these issues involving the ideas of robust control and flexibility analysis.

7. ACKNOWLEDGMENTS

The authors gratefully acknowledge financial support from the National Science Foundation and Mobil Technology Company.

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