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Interaction of Design and Control: Optimization with Dynamic Models *

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Abstract

Process design is usually approached by considering the steady-state performance of the process based on an economic objective. Only after the process design is determined are the operability aspects of the process considered. This sequential treatment of the process design problem neglects the fact that the dynamic controllability of the process is an inherent property of its design. This work considers a systematic approach where the interaction between the steady-state design and the dynamic controllability is analyzed by simultaneously considering both economic and controllability criteria. This method follows a process synthesis approach where a process superstructure is used to represent the set of structural alternatives. This superstructure is modeled mathematically by a set of differential and algebraic equations which contains both continuous and integer variables. Two objectives representing the steady-state design and dynamic controllability of the process are considered. The problem formulation thus is a multiobjective Mixed Integer Optimal Control Problem (MIOCP). The multiobjective problem is solved using an ϵ-constraint method to determine the noninferior solution set which indicates the trade-offs

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between the design and controllability of the process. The (MIOCP) is transformed to a Mixed Integer Nonlinear Program with Differential and Algebraic Constraints (MINLP/DAE) by applying a control parameterization technique. An algorithm which extends the concepts of MINLP algorithms to handle dynamic systems is presented for the solution of the MINLP/DAE problem. The MINLP/DAE solution algorithm decomposes the problem into a NLP/DAE primal and MILP master problems which provide upper and lower bounds on the solution of the problem. The MINLP/DAE algorithm is implemented in the framework MINOPT which is used as the computational tool for the analysis of the interaction of design and control. The solution of the MINLP/DAE problems is repeated with varying values of ϵ to generated the noninferior solution set. The proposed approach is applied to three design/control examples: a reactor network involving two CSTRs, an ideal binary distillation column, and a reactor/separator/recycle system. The results of these design examples quantitatively illustrate the trade-offs between the steady-state economic and dynamic controllability objectives.

Keywords: Mixed Integer Nonlinear Optimization, Parametric Optimal Control.

1 Introduction

Chemical processes are generally designed to operate at a steady-state which has been determined to be economically optimal. The ever-changing environment tends to drive the operation of the process away from this steady-state design thus having an adverse effect on the economic operation of the process. A process design which is optimal at steady-state may not be optimal in light of the changes it may face. Therefore, the operability of the process or its ability to adapt to a changing environment is an important quality of the process which must be considered.

The traditional approach to handling operational issues is to deal with them sequentially with the process design. First, the process is designed to be economically optimal using a fully specified nominal case. Then, after the process is designed, the operability aspects are considered which may include control system design, reliability, and flexibility design issues.

The sequential design approach leads to problems when the economics are based solely on the steady-state operation of the process. The steady-state design does not reflect the impact of the control system on the economic operation nor the trade-offs between design and controllability. Thus, a particular design may appear to be optimal with respect to its steady-state economic operation, but due to poor operability characteristics, the plant may not exhibit good economic operation over time. This may be due to the production of material that is off specification or increased utility consumption necessary to adapt to the changes in the process. Since operability issues are ignored during the steady-state design of the process, the fact that the operability issues affect the economics of the plant is neglected. Poor operability is reflected in the economics of the process over time.

There are other incentives for including dynamic controllability aspects of the process during the design phase. The operation of the process must adhere to strict operational constraints due to tight restrictions on product quality and strict environmental regulations. The process design must be able to handle a fluctuating economy characterized by varying customer demands. Industrial trends towards more highly integrated and complex plants are leading to processes with interacting process units. For these reasons, the dynamic effects of the process become more dominant and the dynamic operation more important. Thus, a simultaneous design approach which considers the operability and dynamic aspects of the process along with economic aspects is necessary.

This work focuses on the integration of controllability into the design phase of a process at the early stages of the design. This integrated approach to design and control has 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 need for assessing operability issues during the design phase has been known for some time, but quantitative approaches for addressing the problem are rather new. Morari and Perkins [17] provide a review of the various design/control methodologies. Their work describes the process synthesis problem and the concept of controllability emphasizing that the design of a control system for a process is part of the overall design of the process. They also state that the design of a process can effect the control performance. They describe a number of techniques that address the assessment of the controllability of a process. 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.

In order to deal with the controllabilty issues on a economic level, Narraway *et al.* [19] presented the back-off method which determines the economics associated with the process dynamics. In this method the optimal steady-state is determined and then the economic penalty associated with backing away from this point to maintain feasible operation and accommodate disturbances is determined. The method is further developed by Narraway and Perkins [20] where the control structure selection problem is analyzed. Perfect control assumptions are used along with a linearized model to formulate a mixed integer linear program where the integer variables indicate the pairings between the manipulated and controlled variables.

Brengel and Seider [2] present an approach for determining process designs which are both steady-state and operationally optimal. The controllability of potential designs are evaluated along with their economic performance by incorporating a model predictive control algorithm into the process design optimization algorithm. This coordinated approach uses an objective function which is a weighted sum of economic and controllability measures.

Luyben and Floudas [14, 15] used a multiobjective approach to simultaneously consider both controllability and economic aspects of the design. In this framework, the tradeoffs between various open-loop controllability measures and the economics of the process can be observed. This approach incorporates both design and control aspects into a process synthesis framework and is the only approach which addresses the synthesis issues. Through the application of multiobjective techniques, a process design which is both economic and controllable is determined.

A screening approach was proposed by Elliott and Luyben [6] where the variability in the product quality is used to compare different steady-state process designs. The dynamic controllability is measured economically by calculating the amount of material produced that is off-specification and on-specification. The on-specification material leads to profits while the off-spec material results in costs for reworking or disposal.

Bahri *et al.* [1] also developed a backoff technique for the design of steady-state and open-loop dynamic processes. Both uncertainties and disturbances are considered for determining the amount of back-off. The ideas are further developed by Figueroa *et al.* [7] where a recovery factor is defined as the ratio of the amount of penalty recovered with control to the penalty with no control. This ratio is then used to rank different control strategies.

The advantage of the back-off approaches is that they determine the cost increase associated with moving to the back-off position which is attributed to the uncertainties and disturbances. A limitation of this approach is that it can lead to rather conservative designs since the worst case uncertainty scenario is considered. Although the probability of the worst case uncertainty occurring may not be high, this is the basis for the final design. Also, the method has not been applied to the design/synthesis problem. A fixed design is considered and then the back-off is considered as a modification of this design.

Mohideen *et al.* [16] address the problem of optimal design of dynamic systems under uncertainty. They incorporate flexibility aspects as well as control design considerations simultaneously with the process design. The algorithm is used to find the economic optimum which satisfies all of the constraints for a given set of uncertainties and disturbances when the control system is included.

Walsh and Perkins [25] outline the use of optimization as a tool for the design/control problem. They note that the advances in computational hardware and optimization tools has made it possible to solve the complex problems that arise in design/control. Their assessment focuses on the control structure selection problem where the economic cost of a disturbance is balanced against the performance of the controller.

This article presents a framework for analyzing the interaction of design and control. In the following section, the problem statement is given which outlines the characteristics of the problem. Section 3 discusses the mathematical formulation for the interaction of design and control problem and describes the types of variables and constraints employed in the problem. In Section 4, the algorithmic framework for the solution of the interaction of design and control problem is proposed. The various aspects of the framework are addressed separately and an algorithmic procedure is presented. Section 5 presents the framework, MINOPT, which is used as a computational tool for the solution of the design and control problem. Section 6 discusses the application of the proposed procedure to three example problems: a simple reactor network problem, a binary distillation problem, and a reactor-separator-recycle problem.

2 Problem Statement

The interaction of design and control problem is posed within the process synthesis framework. The following information is assumed to be given:

- A process superstructure indicating the set of design alternatives
- A mathematical model describing the process superstructure
- The sets of potential manipulated and controlled variables
- Desired levels for process outputs
- Set of control structure alternatives (control superstructure)
- Set of Disturbances
- Feasibility Constraints (path, point, etc.)
- Cost data (Capital and operating)
- Finite time horizon

The goal 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 has two objectives which measure the design and controllability of the process. Economic criteria are typically used to measure the design of the process. These take the form of cost or profit expressions which are functions of the variables of the design. The controllability measure for the process is not as concrete nor as easy to ascertain. Although many measures exist for the controllability of linear systems (singular value, condition number, relative gain array, and disturbance condition number), chemical systems are generally nonlinear and there is a deficiency in controllability measures for nonlinear systems. The traditional choice for a controllability measure is the Integral Square Error (ISE); however, there are a number of drawbacks in using such a measure. First, ISE is not of direct interest in practice. It only reflects the dynamics of the measured variables and neglects the dynamics of the unmeasured state variables. The ISE only contains information about the area magnitude of the violations of the measured variables but neglects the magnitude of the violation of the outputs along the trajectory. This drawback can be handled by incorporating path constraints into the problem formulation.

Another drawback related to ISE as a controllability measure and the control structure selection has to do with the selection of the control parameters. First, the search for optimal control parameters based on the ISE objective exhibits multiple local optima. Second, there is no one to one correspondence between the control structure and the ISE measure. Thus, similar ISE measures may be obtained for entirely different structures by adjusting the controller parameters. Therefore, different dynamic characteristics of the process may not be reflected in the ISE.

Despite the problems associated with ISE, its usage does have a number of positive aspects and meets the requirements of a controllability measure for this work. First, it is easy to calculate and it can be determined directly as part of the process model. It does reflect the dynamic performance of the process in terms of the outputs of the process. Designs that exhibit poor dynamic characteristics have larger ISE measures whereas better designs are characterized by smaller ISE measures. As a dynamic performance criterion, ISE encompasses the entire response of the process and not just an isolated characteristic. Finally, ISE is a differentiable function which facilitates it use in gradient based methods.

In the following section, the mathematical formulation is described. The central point in this formulation is the inclusion of dynamic models.

3 General Mathematical Formulation of the Interaction of Design and Control Problem

The interaction of process synthesis and control problem is formulated by first modeling the postulated superstructure of process alternatives of interest. The controllabilty of the process deals with the dynamic operation of the process, and this requires the introduction of dynamic models. The dynamic modeling leads to a system of differential and algebraic equations referred to as DAEs. The differential equations are used to model material and energy balances while algebraic relations are used for relations such as equilibrium expressions.

The mathematical formulation for this problem is characterized by different types of variables and constraints. The variables (listed in Table 1) are divided into two categories: continuous and integer. The continuous variables represent the flow rates, compositions, temperatures, equipment sizes, etc. The integer variables ($\boldsymbol{y}$) are used to represent the existence of process units. The continuous variables are further categorized as design

Table 1: Variable definitions for problem formulation

$\boldsymbol{v}$:	Time Invariant Continuous Variables
$\boldsymbol{y}$:	Integer Variables
$\boldsymbol{z}(t)$:	Dynamic State Variables
$\boldsymbol{u}(t)$:	Dynamic Control Variables
t:	Time
t_i:	Time instant

variables or time invariant decision variables ($\boldsymbol{v}$), dynamic state variables ($\boldsymbol{z}(t)$), and control variables or time varying decision variables ($\boldsymbol{u}(t)$). The time invariant variables are those that represent design parameters such as equipment size. The dynamic variables are those such as composition and temperature which vary with time. The control variables represent quantities that can be manipulated over time to maintain controlled variables at prespecified levels. The controlled variables are a subset of the dynamic variables which have a desired value or set-point.

The dynamic model for the process structure is modeled using DAEs:

$$\boldsymbol{f}_1(\dot{\boldsymbol{z}}_1(t), \boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{u}(t), \boldsymbol{v}, \boldsymbol{y}, t) = \boldsymbol{0} \tag{1}$$

$$\boldsymbol{f}_2(\boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{u}(t), \boldsymbol{v}, \boldsymbol{y}, t) = \boldsymbol{0} \tag{2}$$

$$\boldsymbol{z}_1(t_0) = \boldsymbol{z}_1^0 \tag{3}$$

$$\boldsymbol{z}_2(t_0) = \boldsymbol{z}_2^0 \tag{4}$$

where $\boldsymbol{f}_1$ represents the n differential equations, $\boldsymbol{f}_2$ represents the m dynamic algebraic equations, $\boldsymbol{z}_1(t)$ 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. The variables $\boldsymbol{v}$ and $\boldsymbol{y}$ are parameters for the DAE system and variables for the optimization where $\boldsymbol{v}$ is a vector of p time invariant continuous variables and $\boldsymbol{y}$ is a vector of q binary variables. The control variables are represented by $\boldsymbol{u}(t)$ which is a vector of r variables. Time t is the independent variable for the DAE system and t_0 is the fixed initial time. 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.

The point constraints are the constraints involving the dynamic variables at a specific time instance. They have the form

$$\boldsymbol{h}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{u}(t_i), \boldsymbol{v}, \boldsymbol{y}) = \mathbf{0} \tag{5}$$

$$\boldsymbol{g}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{u}(t_i), \boldsymbol{v}, \boldsymbol{y}) \leq \mathbf{0} \tag{6}$$

where t_i represents the time instance at which the constraint is enforced. The index i can have values from 0 to N where N is the number of time instances necessary in the problem and t_N is the final time.

There are also constraints which involve only the $\boldsymbol{v}$ and $\boldsymbol{y}$ variables:

$$\boldsymbol{h}''(\boldsymbol{v}, \boldsymbol{y}) = \mathbf{0} \tag{7}$$

$$\boldsymbol{g}''(\boldsymbol{v}, \boldsymbol{y}) \leq \mathbf{0} \tag{8}$$

With the constraint and variable definitions given, the interaction of process synthesis and control problem has the following mathematical formulation:

$$\begin{array}{rrcl}
\min & \boldsymbol{J}(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{u}(t_i), \boldsymbol{v}, \boldsymbol{y}) & & \\
\text{s.t.} & \boldsymbol{f}_1(\dot{\boldsymbol{z}}_1(t), \boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{u}(t), \boldsymbol{v}, \boldsymbol{y}, t) & = & \mathbf{0} \\
 & \boldsymbol{f}_2(\boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{u}(t), \boldsymbol{v}, \boldsymbol{y}, t) & = & \mathbf{0} \\
 & \boldsymbol{z}_1(t_0) & = & \boldsymbol{z}_1^0 \\
 & \boldsymbol{z}_2(t_0) & = & \boldsymbol{z}_2^0 \\
 & \boldsymbol{h}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{u}(t_i), \boldsymbol{v}, \boldsymbol{y}) & = & \mathbf{0} \\
 & \boldsymbol{g}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{u}(t_i), \boldsymbol{v}, \boldsymbol{y}) & \leq & \mathbf{0} \\
 & \boldsymbol{h}''(\boldsymbol{v}, \boldsymbol{y}) & = & \mathbf{0} \\
 & \boldsymbol{g}''(\boldsymbol{v}, \boldsymbol{y}) & \leq & \mathbf{0} \\
 & \boldsymbol{v} & \in & \mathcal{V} \subseteq \Re^p \\
 & \boldsymbol{y} & \in & \{0,1\}^q \\
 & t_i & \in & [t_0, t_N] \\
 & i & = & 0 \ldots N
\end{array} \tag{9}$$

In this formulation the objective function $\boldsymbol{J}$ is a vector and therefore the problem is a multiobjective Mixed Integer Optimal Control Problem (MIOCP). The next section discusses the development of an algorithmic framework for addressing the solution of this problem.

4 Interaction of Design and Control Algorithmic Framework

There are three characteristics which complicate the solution of the Multiobjective Mixed Integer Optimal Control problem formulation. These are the multiobjective nature, the optimal control problem, and the mixed integer aspects. The algorithmic framework can be decomposed into three steps which address each of these issues. First, the multiobjective nature is addressed by applying the ϵ-constraint technique which reduces the problem to a single objective optimization problem. The second step addresses the optimal control aspects of the problem and involves the application of control parameterization to the problem to reduce the infinite dimensional programming problem to a finite dimensional programming problem. The third step involves the solution of the mixed integer optimization problem where the theoretical concepts for the solution of Mixed Integer Nonlinear Programming problems are extended to the solution of problems involving dynamic models.

4.1 Multiobjective Optimization

The most straightforward method for handling multiobjective optimization is to measure both objectives on the same basis. If this is possible, the problem can be reduced to a single objective and this would obviate the need for any further consideration. However, this is usually not the case as the two objectives are not always easily measured by some common basis. For the design and control problem the two objectives are used to measure the economic design and dynamic controllability of the process.

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. This pareto-optimal solution can thus be used to indicate the trade-offs between the two objectives achieved by using alternative designs.

Through the use of the ϵ-constraint method, the multiobjective problem is reduced to the successive solution 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:

$$
\begin{array}{lrcl}
\min & J_1(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{u}(t_i), \boldsymbol{v}, \boldsymbol{y}) & & \\
\text{s.t.} & J_2(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{u}(t_i), \boldsymbol{v}, \boldsymbol{y}) & \leq & \epsilon \\
& \boldsymbol{f}_1(\dot{\boldsymbol{z}}_1(t), \boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{u}(t), \boldsymbol{v}, \boldsymbol{y}, t) & = & \mathbf{0} \\
& \boldsymbol{f}_2(\boldsymbol{z}_1(t), \boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{u}(t), \boldsymbol{v}, \boldsymbol{y}, t) & = & \mathbf{0} \\
& \boldsymbol{z}_1(t_0) & = & \boldsymbol{z}_1^0 \\
& \boldsymbol{z}_2(t_0) & = & \boldsymbol{z}_2^0 \\
& \boldsymbol{h}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{u}(t_i), \boldsymbol{v}, \boldsymbol{y}) & = & \mathbf{0} \\
& \boldsymbol{g}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{u}(t_i), \boldsymbol{v}, \boldsymbol{y}) & \leq & \mathbf{0} \\
& \boldsymbol{h}''(\boldsymbol{v}, \boldsymbol{y}) & = & \mathbf{0} \\
& \boldsymbol{g}''(\boldsymbol{v}, \boldsymbol{y}) & \leq & \mathbf{0} \\
& \boldsymbol{v} & \in & \mathcal{V} \subseteq \Re^p \\
& \boldsymbol{y} & \in & \{0,1\}^q \\
& t_i & \in & [t_0, t_N] \\
& i & = & 0 \ldots N
\end{array}
\tag{10}
$$

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.

4.2 Parameterization of Optimal Control Problem

There are a number of different approaches to the solution of this optimal control problem. These include dynamic programming, solution of the necessary conditions, complete discretization, and control parameterization. Complete discretization techniques discretize both the state variables, $\boldsymbol{z}(t)$ and the control variables $\boldsymbol{u}(t)$ and convert the problem to a finite dimensional nonlinear program (NLP) where the optimization is carried out over the full space of discretized variables (parameters for $\boldsymbol{z}(t)$ and $\boldsymbol{u}(t)$) and the design variables $\boldsymbol{v}$. This work focuses on the control parameterization techniques which parameterize only the control variables $\boldsymbol{u}(t)$ in terms of time invariant parameters. In these methods the optimization of carried out in the space of the decision variables only (parameters $\boldsymbol{u}(t)$ and the design variables $\boldsymbol{v}$). 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. These techniques make use of well-established integration techniques which efficiently control the discretization error through the size and order of the integration steps.

The two control parameterization approaches discussed here are open loop and closed loop parameterization. In the open loop parameterization, the control variables are expressed as polynomial functions in the independent variable, time t, whereas in the closed loop parameterization they are expressed as functions of the state variables, $\boldsymbol{z}(t)$.

One possible method for open loop control parameterization is the technique described in [23]. The parameterization is done through collocation where the control variables are approximated by piecewise continuous Lagrange polynomials in t. This control parameterization is done in each of the time intervals which are defined by the time instances. The number of parameters for each control variable depends on the number of intervals, indexed by i, as well as the number of collocation points (order of the approximating polynomial), indexed by j. Through the parameterization, the control variables $\boldsymbol{u}(t)$ become polynomial functions with time invariant parameters $\boldsymbol{w}_{ij}$:

$$\boldsymbol{u}(t) = \phi(\boldsymbol{w}_{ij}, t)$$

When this control parameterization is applied to the MIOCP formulation, the set of time invariant variables is expanded to include the parameters $\boldsymbol{w}_{ij}$ along with $\boldsymbol{v}$.

Open loop control laws are generally applicable only to the situation for which they were computed and are less robust than closed loop control laws. Moreover, closed loop control laws are generally easier to compute and implement. For these reasons, this work focuses on the closed loop parameterization.

For closed loop control parameterization, the control is formulated as a function of the state variables instead of the independent variable time. The control law has the form

$$\boldsymbol{u}(t) = \psi(\boldsymbol{w}, \boldsymbol{z}(t))$$

where $\boldsymbol{w}$ is the set of control parameters. The application of this control parameterization again leads to augmenting the set of time invariant decision variables to include the control parameters, $\boldsymbol{w}$. This provides a general formulation for the feedback control, but the specific control law which determines the function $\psi(\boldsymbol{w}, \boldsymbol{z}(t))$ needs to be specified.

The control structure can also be included within the optimization framework of the design and control problem. The control structure selection is formulated by using binary variables to represent the alternative control structures. In this case, both the control parameters and the control structure are determined through the optimization.

As a particular definition of the control scheme to be included in the design and control framework, the multi-loop Proportional Integral control structure as outlined in [20, 21] is considered. This control structure selection problem involves determining the pairings between the manipulated and controlled variables as well as the control parameter tuning values. Binary variables are used to indicate the pairings between manipulated and controlled variables and continuous variables are used for the control parameters.

The control parameterization and control structure selection is appended to the problem by adding an appropriate set of constraints. The control law ($\boldsymbol{u}(t) = \psi(\boldsymbol{w}, \boldsymbol{z}(t))$) is represented by the following:

$$\begin{array}{ll} u_r(t) = u_{0,r} + \sum_{s\in S}\{\kappa_r s[(z_{meas,s}(t) - z_{set,s}) & \\ \quad + \frac{1}{\tau_{rs}} \int_0^t (z_{meas,s}(t) - z_{set,s})]\} & \forall r \in R \end{array} \tag{11}$$

and the additional constraints for the control structure selection are the following:

$$\begin{array}{ll} \kappa_{rs}^L \bar{y}_{rs} \le \kappa_{rs} \le \kappa_{rs}^U \bar{y}_{rs} & \forall r \in R, \forall s \in S \\ \tau_{rs}^L \le \tau_{rs} \le \tau_{rs}^U & \forall r \in R, \forall s \in S \\ \sum_{s\in S} \bar{y}_{rs} \le 1 & \forall r \in R \\ \sum_{r\in R} \bar{y}_{rs} \le 1 & \forall s \in S \end{array} \tag{12}$$

where the set of manipulated and controlled variables are denoted by R and S respectively.

The control parameters $\boldsymbol{w}$ are the variables κ_{rs} and τ_{rs} which are the gain and integral time constant for the controllers. The variables $z_{meas,s}(t)$ are the measured variables and $z_{set,s}$ are the respective set-points. The variables $\bar{y}_{rs}$ are binary variables which have been added to the problem to indicate the matches between manipulated variable r and controlled variable s. The last two inequalities are logical constraints which enforce that at most one pairing exists for each manipulated and controlled variable.

Through the application of the control parameterization and control structure selection, the following problem results:

$$
\begin{array}{llcl}
\min & J(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{v}, \boldsymbol{y}) & & \\
\text{s.t.} & \boldsymbol{f}_1(\dot{\boldsymbol{z}}_1(t), \boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{v}, \boldsymbol{y}, t) & = & \mathbf{0} \\
& \boldsymbol{f}_2(\boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{v}, \boldsymbol{y}, t) & = & \mathbf{0} \\
& u_r(t) - u_{0,r} - \sum_{s\in S}\{\kappa_r s[(z_{meas,s}(t) - z_{set,s}) & & \\
& \quad + \frac{1}{\tau_{rs}} \int_0^t (z_{meas,s}(t) - z_{set,s})]\} & = & 0 \quad \forall r \in R \\
& \boldsymbol{z}_1(t_0) & = & \boldsymbol{z}_1^0 \\
& \boldsymbol{z}_2(t_0) & = & \boldsymbol{z}_2^0 \\
& \boldsymbol{h}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{v}, \boldsymbol{y}) & = & \mathbf{0} \\
& \boldsymbol{g}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{v}, \boldsymbol{y}) & \leq & \mathbf{0} \\
& \boldsymbol{h}''(\boldsymbol{v}, \boldsymbol{y}) & = & \mathbf{0} \\
& \boldsymbol{g}''(\boldsymbol{v}, \boldsymbol{y}) & \leq & \mathbf{0} \\
& \kappa_{rs}^L \bar{y}_{rs} \leq \kappa_{rs} \leq \kappa_{rs}^U \bar{y}_{rs} \quad \forall r \in R, \forall s \in S & & \\
& \tau_{rs}^L \leq \tau_{rs} \leq \tau_{rs}^U \quad \forall r \in R, \forall s \in S & & \\
& \sum_{s\in S} \bar{y}_{rs} & \leq & 1 \quad \forall r \in R \\
& \sum_{r\in R} \bar{y}_{rs} & \leq & 1 \quad \forall s \in S \\
& \boldsymbol{v} & \in & \mathcal{V} \subseteq \Re^p \\
& \boldsymbol{y} & \in & \{0,1\}^q \\
& t_i & \in & [t_0, t_N] \\
& i & = & 0 \ldots N
\end{array} \tag{13}
$$

This problem is classified as a Mixed Integer Nonlinear Program with Differential and Algebraic Constraints (MINLP/DAE).

This formulation can be simplified notationally by combining some of the sets of variables. Since the sets of variables $\boldsymbol{v}$ and $\boldsymbol{w}$ are both sets of time invariant decision variables, they can be combined into a single set

$$\boldsymbol{x} = \{\boldsymbol{v}, \boldsymbol{w}\}$$

where $\boldsymbol{w}$ are the control parameters

$$\boldsymbol{w} = \{\kappa_{rs}, \tau_{rs}\}$$

The vector $\boldsymbol{x}$ is now used to represent the complete set of time invariant continuous variables.

The control parameterization results in the conversion of the control variables to state variables. Thus, the set of dynamic variables can be augmented to include the control variables:

$$\boldsymbol{z}_2 = \{\boldsymbol{z}_2(t), \boldsymbol{u}(t)\}$$

The control parameterization equations, $\psi(\boldsymbol{w}, \boldsymbol{z}(t))$, are algebraic equations that are added to the DAE system and can be included in the set of equations $\boldsymbol{f}_2$. An equal number of variables and equations are added to the DAE system thus maintaining a consistent set of equations.

The binary variables introduced for the control structure selection problem can be added to the original set of binary variables:

$$\boldsymbol{y} = \{\boldsymbol{y}, \bar{\boldsymbol{y}}\}$$

Since the constraints for the control structure selection involve the control parameters and binary variables, these constraints can be included in the set of constraints $\boldsymbol{g}''(\boldsymbol{x}, \boldsymbol{y})$

Applying these notational simplifications, the following MINLP/DAE problem results:

$$\begin{array}{rrcl}
\min & J(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}, \boldsymbol{y}) & & \\
\text{s.t.} & \boldsymbol{f}_1(\dot{\boldsymbol{z}}_1(t), \boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{x}, \boldsymbol{y}, t) & = & \boldsymbol{0} \\
& \boldsymbol{f}_2(\boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{x}, \boldsymbol{y}, t) & = & \boldsymbol{0} \\
& \boldsymbol{z}_1(t_0) & = & \boldsymbol{z}_1^0 \\
& \boldsymbol{z}_2(t_0) & = & \boldsymbol{z}_2^0 \\
& \boldsymbol{h}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}, \boldsymbol{y}) & = & \boldsymbol{0} \\
& \boldsymbol{g}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}, \boldsymbol{y}) & \leq & \boldsymbol{0} \\
& \boldsymbol{h}''(\boldsymbol{x}, \boldsymbol{y}) & = & \boldsymbol{0} \\
& \boldsymbol{g}''(\boldsymbol{x}, \boldsymbol{y}) & \leq & \boldsymbol{0} \\
& \boldsymbol{x} & \in & \mathcal{X} \\
& \boldsymbol{y} & \in & \{0,1\}^q \\
& t_i & \in & [t_0, \ldots, t_N] \\
& i & = & 0 \ldots N
\end{array} \tag{14}$$

4.3 MINLP/DAE Solution Algorithm

The algorithmic development for the MINLP/DAE problem closely follows the developments of MINLP algorithms with appropriate extensions for the DAE system. An overview of MINLP algorithms and extensive theoretical, algorithmic, and applications-oriented descriptions of these algorithms are found in [9]. The two classes of algorithms that are addressed here are the Generalized Benders Decomposition (GBD) [10, 8] and the Outer Approximation (OA) [5] and its variants, Outer Approximation/Equality Relaxation (OA/ER) [13], and outer Approximation/Equality Relaxation/Augmented Penalty (OA/ER/AP) [24]. These algorithms solve

MINLP problems through iterations of NLP primal problems and MILP master problems which provide upper and lower bounds on the solution of the original problem. In the following sections, the application of GBD and OA/ER to the solution of the MINLP/DAE is discussed. The primal and master problems are described as extensions of the MINLP algorithms to the solution of the MINLP/DAE formulation. The formulation of the primal problem is the same for both algorithms but the master problems are formulated differently.

4.3.1 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 MIOCP becomes an optimal control problem which has the following form:

$$
\begin{array}{lrcl}
\min & J(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}, \boldsymbol{y}^k) & & \\
\text{s.t.} & \boldsymbol{f}_1(\dot{\boldsymbol{z}}_1(t), \boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{x}, \boldsymbol{y}^k, t) & = & \mathbf{0} \\
 & \boldsymbol{f}_2(\boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{x}, \boldsymbol{y}^k, t) & = & \mathbf{0} \\
 & \boldsymbol{z}_1(t_0) & = & \boldsymbol{z}_1^0 \\
 & \boldsymbol{z}_2(t_0) & = & \boldsymbol{z}_2^0 \\
 & \boldsymbol{h}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}, \boldsymbol{y}^k) & = & \mathbf{0} \\
 & \boldsymbol{g}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}, \boldsymbol{y}^k) & \leq & \mathbf{0} \\
 & \boldsymbol{h}''(\boldsymbol{x}, \boldsymbol{y}^k) & = & \mathbf{0} \\
 & \boldsymbol{g}''(\boldsymbol{x}, \boldsymbol{y}^k) & \leq & \mathbf{0} \\
 & \boldsymbol{x} & \in & \mathcal{X} \subseteq \Re^p \\
 & t_i & \in & [t_0, \ldots, t_N] \\
 & i & = & 0 \ldots N
\end{array}
\tag{15}
$$

NLP/DAE Solution Algorithm: 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 constraints that are implicit functions of the $\boldsymbol{x}$ variables through the integration. The NLP problem has the form:

$$\begin{array}{lrcl} \min & J(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}, \boldsymbol{y}^k) & & \\ \text{s.t.} & \boldsymbol{h}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}, \boldsymbol{y}^k) & = & \mathbf{0} \\ & \boldsymbol{g}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}, \boldsymbol{y}^k) & \leq & \mathbf{0} \\ & \boldsymbol{h}''(\boldsymbol{x}, \boldsymbol{y}^k) & = & \mathbf{0} \\ & \boldsymbol{g}''(\boldsymbol{x}, \boldsymbol{y}^k) & \leq & \mathbf{0} \\ & \boldsymbol{x} & \in & \mathcal{X} \\ & t_i & \in & [t_0, \ldots, t_N] \\ & i & = & 0 \ldots N \end{array} \tag{16}$$

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:

$$\begin{array}{rcl} \boldsymbol{f}_1(\dot{\boldsymbol{z}}_1(t), \boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{x}, \boldsymbol{y}^k, t) & = & \mathbf{0} \\ \boldsymbol{f}_2(\boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{x}, \boldsymbol{y}^k, t) & = & \mathbf{0} \\ \boldsymbol{z}_1(t_0) & = & \boldsymbol{z}_1^0 \\ \boldsymbol{z}_2(t_0) & = & \boldsymbol{z}_2^0 \end{array} \tag{17}$$

This reformulated problem is an optimization over the space of $\boldsymbol{x}$ variables where the variables $z(t_i)$ are implicit functions of the $\boldsymbol{x}$ variables through the integration of the DAE system. Since the functions $J(\cdot)$, $\boldsymbol{g}'(\cdot)$, and $\boldsymbol{h}'(\cdot)$ include $\boldsymbol{z}(t_i)$, they are also implicit functions of $\boldsymbol{x}$. The solution algorithms for the NLP require the evaluation of the objective and constraints and their gradients with respect to $\boldsymbol{x}$. 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:

$$\begin{array}{rcl} \frac{dJ}{d\boldsymbol{x}} & = & \left(\frac{\partial J}{\partial \boldsymbol{z}}\right)\left(\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}}\right) + \left(\frac{\partial J}{\partial \boldsymbol{x}}\right) \\ \frac{d\boldsymbol{h}'_i}{d\boldsymbol{x}} & = & \left(\frac{\partial \boldsymbol{h}'_i}{\partial \boldsymbol{z}}\right)\left(\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}}\right) + \left(\frac{\partial \boldsymbol{h}'_i}{\partial \boldsymbol{x}}\right) \\ \frac{d\boldsymbol{g}'_i}{d\boldsymbol{x}} & = & \left(\frac{\partial \boldsymbol{g}'_i}{\partial \boldsymbol{z}}\right)\left(\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}}\right) + \left(\frac{\partial \boldsymbol{g}'_i}{\partial \boldsymbol{x}}\right) \end{array} \tag{18}$$

With the function and gradient evaluations calculable, standard gradient based optimization techniques can be applied to solve this problem as an NLP. The solution of this problem provides values of the x variables and trajectories for $z(t)$.

4.3.2 Outer Approximation/Equality Relaxation Master Problem

The Outer Approximation based algorithms were developed for the solution of a class of MINLP problems whose objective function and constraints are separable in the $\boldsymbol{x}$ and $\boldsymbol{y}$ variables and linear in the $\boldsymbol{y}$ variables. Therefore, the class of MINLP/DAE problems that are addressed by these algorithm have the following form:

$$
\begin{array}{lrcl}
\min & J(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}) + \boldsymbol{c}^T \boldsymbol{y} & & \\
\text{s.t.} & \boldsymbol{f}_1(\dot{\boldsymbol{z}}_1(t), \boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{x}, t) & = & \mathbf{0} \\
& \boldsymbol{f}_2(\boldsymbol{z}_1(t), \boldsymbol{z}_2(t), \boldsymbol{x}, t) & = & \mathbf{0} \\
& \boldsymbol{z}_1(t_0) & = & \boldsymbol{z}_1^0 \\
& \boldsymbol{z}_2(t_0) & = & \boldsymbol{z}_2^0 \\
& \boldsymbol{h}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}) + \boldsymbol{B}'\boldsymbol{y} & = & \mathbf{0} \\
& \boldsymbol{g}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}) + \boldsymbol{A}'\boldsymbol{y} & \leq & \mathbf{0} \\
& \boldsymbol{h}''(\boldsymbol{x}) + \boldsymbol{B}''\boldsymbol{y} & = & \mathbf{0} \\
& \boldsymbol{g}''(\boldsymbol{x}) + \boldsymbol{A}''\boldsymbol{y} & \leq & \mathbf{0} \\
& \boldsymbol{x} & \in & \mathcal{X} \\
& \boldsymbol{y} & \in & \{0,1\}^q \\
& t_i & \in & [t_0, t_N] \\
& i & = & 0 \ldots N
\end{array}
\tag{19}
$$

Note that in this formulation, not only must the binary variables participate in a linear and separable fashion, but they also can not participate in the DAE system. Since the general problem includes equality constraints, the algorithm which applied here is the Outer Approximation with Equality Relaxation (OA/ER).

The basic idea behind the OA/ER master problem is the linearization of the objective function and constraints. The linearization is done in the $\boldsymbol{x}$ space and results in a MILP problem whose solution provides a lower bound on the solution to the MINLP problem and values of the $\boldsymbol{y}$ variables for the next primal iteration.

The OA/ER master problem for the MINLP/DAE problem is formulated in a similar way. The problem is again linearized in the $\boldsymbol{x}$ space, but the DAE system is not directly included. The implicit functionality of the point constraints is utilized to include the DAE information in the master problem. The point constraints are implicit functions of the $\boldsymbol{x}$ variables and are viewed as general nonlinear constraints in $\boldsymbol{x}$ with possible explicit $\boldsymbol{y}$ functionality. These constraints are linearized about the solution to the primal problem using the known gradient information with respect to the $\boldsymbol{x}$ variables from the solution of the primal problem. These point constraints contain the necessary information about the DAE system which is not explicitly part of the master problem formulation. The resulting master problem formulation is a MILP.

The master problem is expressed mathematically as the following:

$$
\begin{array}{llll}
\min\limits_{\boldsymbol{x},\boldsymbol{y}} & & & \boldsymbol{c}^T\boldsymbol{y}+\mu \\[2ex]
\text{s.t.} & \mu & \geq & J(\dot{\boldsymbol{z}}_1^k(t_i),\boldsymbol{z}_1^k(t_i),\boldsymbol{z}_2^k(t_i),\boldsymbol{x}^k) \\
& & & +\left[\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)\right]_{\boldsymbol{x}^k,\boldsymbol{z}^k(t_i)}(\boldsymbol{x}-\boldsymbol{x}^k) \\[2ex]
& \mathbf{0} & \geq & \boldsymbol{T}'^k\left\{\boldsymbol{h}'(\dot{\boldsymbol{z}}_1^k(t_i),\boldsymbol{z}_1^k(t_i),\boldsymbol{z}_2^k(t_i),\boldsymbol{x}^k)\right. \\
& & & \left.+\left[\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)\right]_{\boldsymbol{x}^k,\boldsymbol{z}^k(t_i)}(\boldsymbol{x}-\boldsymbol{x}^k)+\boldsymbol{B}'\boldsymbol{y}\right\} \\[2ex]
& \mathbf{0} & \geq & \boldsymbol{g}'(\dot{\boldsymbol{z}}_1^k(t_i),\boldsymbol{z}_1^k(t_i),\boldsymbol{z}_2^k(t_i),\boldsymbol{x}^k) \\
& & & +\left[\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)\right]_{\boldsymbol{x}^k,\boldsymbol{z}^k(t_i)}(\boldsymbol{x}-\boldsymbol{x}^k)+\boldsymbol{A}'\boldsymbol{y} \\[2ex]
& \mathbf{0} & \geq & \boldsymbol{T}''^k\left\{\boldsymbol{h}''(\boldsymbol{x}^k)+\left(\frac{\partial \boldsymbol{h}''}{\partial \boldsymbol{x}}\right)(\boldsymbol{x}-\boldsymbol{x}^k)+\boldsymbol{A}''\boldsymbol{y}\right\} \\[2ex]
& \mathbf{0} & \geq & \boldsymbol{g}''(\boldsymbol{x}^k)+\left(\frac{\partial \boldsymbol{g}''}{\partial \boldsymbol{x}}\right)(\boldsymbol{x}-\boldsymbol{x}^k)+\boldsymbol{B}''\boldsymbol{y} \\[2ex]
& \boldsymbol{x} & \in & \mathcal{X} \\
& \boldsymbol{y} & \in & \{0,1\}^q \\
& & & \sum_{j\in B^k} y_j-\sum_{j\in N^k} y_j \leq |B^k|-1 \\
& & & B^k=\{j|y_j^k=1\} \\
& & & N^k=\{j|y_j^k=0\} \\
& & & k=0,1,2,\ldots,K
\end{array}
\tag{20}
$$

Table 2: Primal constraints and corresponding dual variables.

constraint	dual variable
$\boldsymbol{f}_1(\cdot)$	$\nu_1(t)$
$\boldsymbol{f}_2(\cdot)$	$\nu_2(t)$
$\boldsymbol{g}'$	μ'
$\boldsymbol{h}'$	λ'
$\boldsymbol{g}''$	μ''
$\boldsymbol{h}''$	λ''

where K is the set of solutions to the primal problem. The matrices $\boldsymbol{T}'^k$ and $\boldsymbol{T}''^k$ are diagonal matrices used to relax the equality constraints. These matrices are defined by

$$\boldsymbol{T}'^k = \mathrm{diag}(t_{ii}'^k) \quad t_{ii}'^k = \mathrm{sign}(\lambda_i'^k)$$

$$\boldsymbol{T}''^k = \mathrm{diag}(t_{ii}''^k) \quad t_{ii}''^k = \mathrm{sign}(\lambda_i''^k)$$

where $\lambda_i'^k$ and $\lambda_i''^k$ are the Lagrange multipliers for the equality constraints.

If the $\boldsymbol{y}$ variables had participated in the DAE system, the point constraints would also be implicit functions of the $\boldsymbol{y}$ variables. The formulation would not longer be valid as the DAE system would need to be included in the master problem formulation.

4.3.3 Generalized Benders Decomposition Master Problem

The master problem for GBD 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.

In applying the GBD algorithm to the general MINLP/DAE formulation, dual information is required from all of the constraints including the DAEs. The dual variables for the DAEs, or adjoint variables, are analogous to the Lagrange multipliers for the other constraints with the difference that they are dynamic. The constraints and their corresponding dual variables are listed in Table 2.

Dual information from the DAE system is obtained by solving the adjoint problem for the DAE system which has the following formulation:

$$\begin{aligned} \left(\frac{d\boldsymbol{f}_1}{d\dot{\boldsymbol{z}}_1}\right)^T \dot{\nu}_1(t) - \left(\frac{d\boldsymbol{f}_1}{d\boldsymbol{z}_1}\right)^T \nu_1(t) - \left(\frac{d\boldsymbol{f}_2}{d\boldsymbol{z}_1}\right)^T \nu_2(t) &= \mathbf{0} \\ - \left(\frac{d\boldsymbol{f}_1}{d\boldsymbol{z}_2}\right)^T \nu_1(t) - \left(\frac{d\boldsymbol{f}_2}{d\boldsymbol{z}_2}\right)^T \nu_2(t) &= \mathbf{0} \end{aligned} \tag{21}$$

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 solution of the primal problem. The variables $\nu_1(t)$ and $\nu_2(t)$ are the adjoint variables and the solution of this problem is a backward integration in time with the following final time conditions:

$$\left.\left(\frac{d\boldsymbol{f}_1}{d\dot{\boldsymbol{z}}_1}\right)^T\right|_{t_N} \nu_1(t_N) + \left(\frac{d\boldsymbol{g}'}{d\boldsymbol{z}_1}\right)^T \mu' + \left(\frac{d\boldsymbol{h}'}{d\boldsymbol{z}_1}\right)^T \lambda' = \mathbf{0} \tag{22}$$

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, μ''^k, λ''^k, and $\nu^k(t)$. The relaxed master problem has the following form:

$$\begin{array}{lrcll}
\min\limits_{\boldsymbol{y},\mu_b} & \mu_b & & & \\
\text{s.t.} & \mu_b & \geq & J(\boldsymbol{x}^k, \boldsymbol{y}) & \\
& & & + \int_{t_0}^{t_N} \nu_1^k(t) \boldsymbol{f}_1(\dot{\boldsymbol{z}}_1^k(t), \boldsymbol{z}_1^k(t), \boldsymbol{z}_2^k(t), \boldsymbol{x}^k, \boldsymbol{y}, t) dt & \\
& & & + \int_{t_0}^{t_N} \nu_2^k(t) \boldsymbol{f}_2(\boldsymbol{z}_1^k(t), \boldsymbol{z}_2^k(t), \boldsymbol{x}^k, \boldsymbol{y}, t) dt & \\
& & & + \mu''^k \boldsymbol{g}''(\boldsymbol{x}^k, \boldsymbol{y}) + \lambda''^k \boldsymbol{h}''(\boldsymbol{x}^k, \boldsymbol{y}) & k \in K_{\text{feas}} \\
& \mathbf{0} & \geq & \int_{t_0}^{t_N} \nu_1^k(t) \boldsymbol{f}_1(\dot{\boldsymbol{z}}_1^k(t), \boldsymbol{z}_1^k(t), \boldsymbol{z}_2^k(t), \boldsymbol{x}^k, \boldsymbol{y}, t) dt & \\
& & & + \int_{t_0}^{t_N} \nu_2^k(t) \boldsymbol{f}_2(\boldsymbol{z}_1^k(t), \boldsymbol{z}_2^k(t), \boldsymbol{x}^k, \boldsymbol{y}, t) dt & \\
& & & + \mu''^k \boldsymbol{g}''(\boldsymbol{x}^k, \boldsymbol{y}) + \lambda''^k \boldsymbol{h}''(\boldsymbol{x}^k, \boldsymbol{y}) & k \in K_{\text{infeas}} \\
& & & \boldsymbol{y} \in \{0, 1\}^q &
\end{array} \tag{23}$$

The integral term can be evaluated since the profiles for $\boldsymbol{z}^k(t)$ and $\nu^k(t)$ 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.

An alternate solution method which does not use the adjoint problem can be used if the $\boldsymbol{y}$ variables do not participate in the DAEs. The point constraints are implicit functions of the $\boldsymbol{x}$ variables and can be viewed as general nonlinear constraints in $\boldsymbol{x}$ with possible explicit $\boldsymbol{y}$ functionality. For this formulation, the Lagrange multipliers for the point constraints are used in the master problem formulation instead of the final time conditions for the adjoint problem. Thus, it is not necessary to solve the adjoint problem and obtain $\nu(t)$ since the dual information for the DAE system is contained in the Lagrange multipliers for the point constraints. For this situation, the master problem has the following form:

$$
\begin{aligned}
\min_{\boldsymbol{y},\mu_b} \quad & \mu_b \\
\text{s.t.} \quad \mu_b \geq\; & J(\dot{\boldsymbol{z}}_1^k(t_i), \boldsymbol{z}_1^k(t_i), \boldsymbol{z}_2^k(t_i), \boldsymbol{x}^k, \boldsymbol{y}) \\
& +\mu'^k \boldsymbol{g}'(\dot{\boldsymbol{z}}_1^k(t_i), \boldsymbol{z}_1^k(t_i), \boldsymbol{z}_2^k(t_i), \boldsymbol{x}^k, \boldsymbol{y}) \\
& +\lambda'^k \boldsymbol{h}'^k(\dot{\boldsymbol{z}}_1^k(t_i), \boldsymbol{z}_1^k(t_i), \boldsymbol{z}_2^k(t_i), \boldsymbol{x}^k, \boldsymbol{y}) \\
& +\mu''^k \boldsymbol{g}''(\boldsymbol{x}^k, \boldsymbol{y}) + \lambda''^k \boldsymbol{h}''(\boldsymbol{x}^k, \boldsymbol{y}) \qquad k \in K_{\text{feas}} \\
\mathbf{0} \geq\; & \mu'^k \boldsymbol{g}'(\dot{\boldsymbol{z}}_1(t_i), \boldsymbol{z}_1^k(t_i), \boldsymbol{z}_2(t_i), \boldsymbol{x}^k, \boldsymbol{y}) \\
& +\lambda'^k \boldsymbol{h}'(\dot{\boldsymbol{z}}_1^k(t_i), \boldsymbol{z}_1^k(t_i), \boldsymbol{z}_2^k(t_i), \boldsymbol{x}^k, \boldsymbol{y}) \\
& +\mu''^k \boldsymbol{g}''(\boldsymbol{x}^k, \boldsymbol{y}) + \lambda''^k \boldsymbol{h}''(\boldsymbol{x}^k, \boldsymbol{y}) \qquad k \in K_{\text{infeas}} \\
& \boldsymbol{y} \in \{0,1\}^q
\end{aligned}
\tag{24}
$$

If the $\boldsymbol{y}$ variables do not participate in the DAEs, the second form of the master problem is preferred since it does not require the solution of the adjoint problem.

4.4 MINLP/DAE Algorithmic Statement

The algorithmic statement for the solution of the MINLP can be stated as follows:

Step 1 (Initialization): Set the counter k to zero. Obtain initial values for the $\boldsymbol{y}$ variables $\boldsymbol{y} = \boldsymbol{y}^k$.

Step 2 (Primal Problem): Solve the primal problem for the fixed values of $\boldsymbol{y} = \boldsymbol{y}^k$. Obtain the optimal solution, optimal $\boldsymbol{x}^k$, optimal state profiles,$\boldsymbol{z}(t)$, optimal Lagrange multipliers λ^k and μ^k, and gradients $\frac{d\boldsymbol{g}}{d\boldsymbol{x}}$ and $\frac{d\boldsymbol{h}}{d\boldsymbol{x}}$. If the primal is not feasible solve an infeasibility problem for fixed values of $\boldsymbol{y} = \boldsymbol{y}^k$. Obtain the optimal $\boldsymbol{x}^k$ and the Lagrange multipliers λ^k and μ^k. Update the upper bound.

Step 3 (Adjoint Problem): If necessary, solve the adjoint problem. From the solution of the adjoint problem, obtain the $\nu(t)$.

Step 4 (Master Problem): Solve the master problem using the fixed solutions of the previous primal problems. Obtain optimal values of $\boldsymbol{y}$ and μ_b, update the lower bound, and set $\boldsymbol{y}^{k+1} = \boldsymbol{y}$.

Step 5 (Convergence): If the difference between the upper and lower bound is less than some specified tolerance, terminate. Otherwise update the counter: $k = k + 1$ and go to step 2.

A schematic of the general solution algorithm is given in Figure 4.4.

Note that problems that have $\boldsymbol{y}$ variables in the DAEs can be reformulated so that these variables are replaced by $\boldsymbol{x}$ variables. This eliminates the complications caused by having $\boldsymbol{y}$ variables in the DAEs but creates a new problem. The $\boldsymbol{x}$ variables used to replace the $\boldsymbol{y}$ variables are decision variables for NLP/DAE optimization, yet they have fixed values. Experience has shown that due to the nature of the NLP/DAE solution algorithm, these fixed values tend to cause numerical difficulties when solving the NLP/DAE problem.

5 Implementation

The solution algorithm for the MINLP/DAE has been implemented in the program MINOPT [22] (Mixed Integer Nonlinear OPTimizer) which has been developed as a unified framework for the solution of various classes of optimization problems. MINOPT is capable of solving problems including continuous and integer variables in the presence of steady-state and dynamic models. 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. MINOPT implements OA, OA/ER, OA/ER/AP,

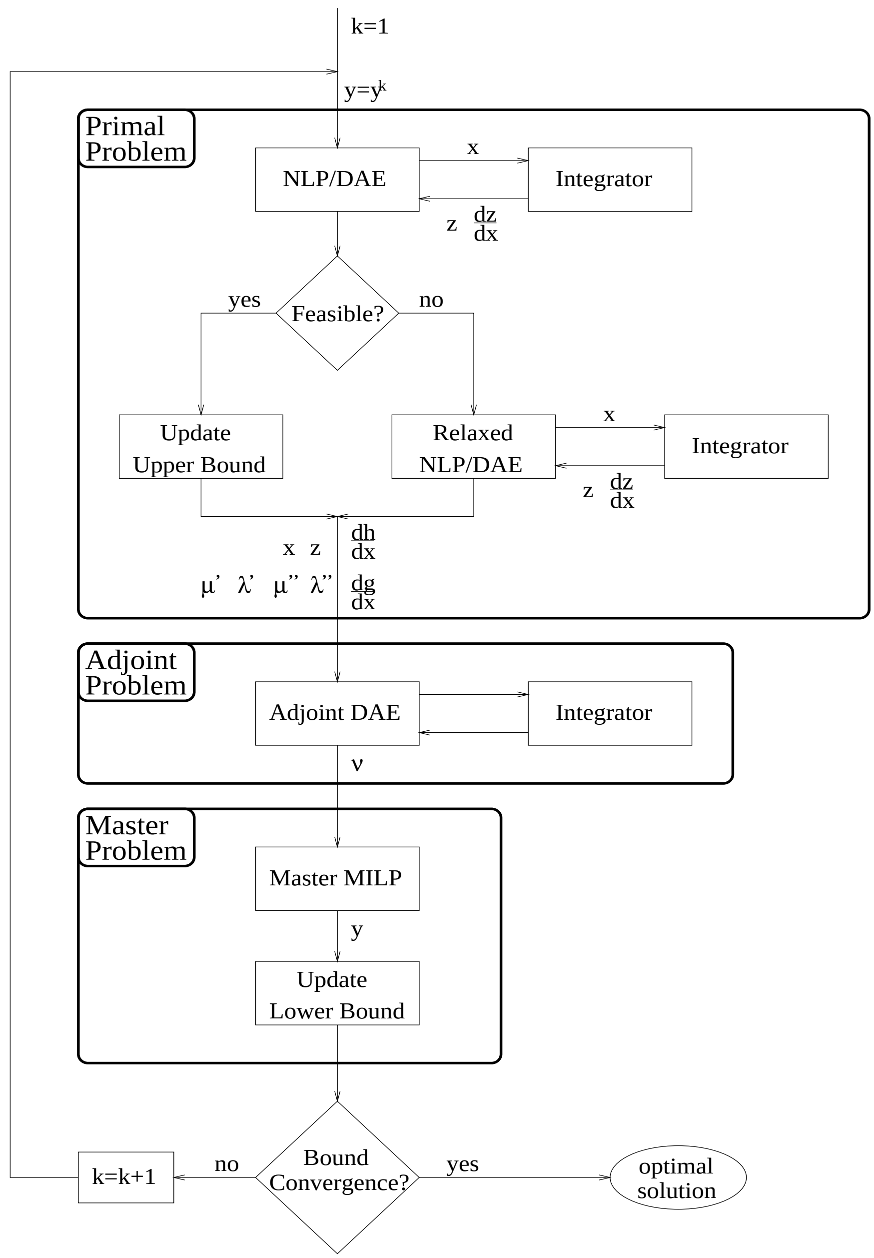

Figure 1: Schematic flowsheet for the MINLP/DAE algorithm

and GBD algorithms for the solution of the MINLPs. For the solution of the LP, MILP, NLP, and DAE subproblems, MINOPT connects to existing software packages.

For the solution of the NLP/DAE problems, any appropriate gradient based solver can be used. However, the function evaluations are expensive since they involve the solution of the DAE system. For this reason, sequential quadratic programming methods are preferable to augmented Lagrangian methods since they generally require fewer function evaluations. MINOPT incorporates both NPSOL [11] (SQP) and MINOS [18] (augmented Lagrangian) for the solution of the NLPs, but NPSOL is generally used for the NLP/DAE problems.

For the solution of the DAE system and sensitivity analysis, MINOPT uses DASOLV [12] which is an implementation of a backwards difference formula algorithm for large sparse DAEs and features efficient sensitivity evaluation and discontinuity handling. For the solution of the LP and MILP problems, CPLEX [3] is used.

6 Examples

6.1 Example 1—Reactor Network

The first example is a reactor network synthesis problem which considers a single, first-order, exothermic, irreversible reaction ($A \rightarrow B$). The superstructure has two Continuous Stirred Tank Reactors (CSTRs) arranged as shown in Figure 2. The reactor is cooled by a perfectly mixed cooling jacket which surrounds the vertical walls of the reactor. Constant density and constant volume reactors are assumed for this problem.

The temperature in each reactor is selected as the controlled variable, and the jacket flow rate is used as the manipulated variable. Although the desired output for the problem is the single product stream, both reactor outputs are considered for the controllability analysis, since both need to be controlled. As part of the design and control analysis, the set-points for the reactor temperatures are variables for the problem. The controllability measure used in this problem is the integral square error of the reactor temperatures and their respective set-points. The set-points or nominal values for the reactor temperature affects both the economic design and the controllability of the process.

The variables in the problem are the flow rates, compositions, temperatures, dimensions of the reactors, and number of reactors. The variables

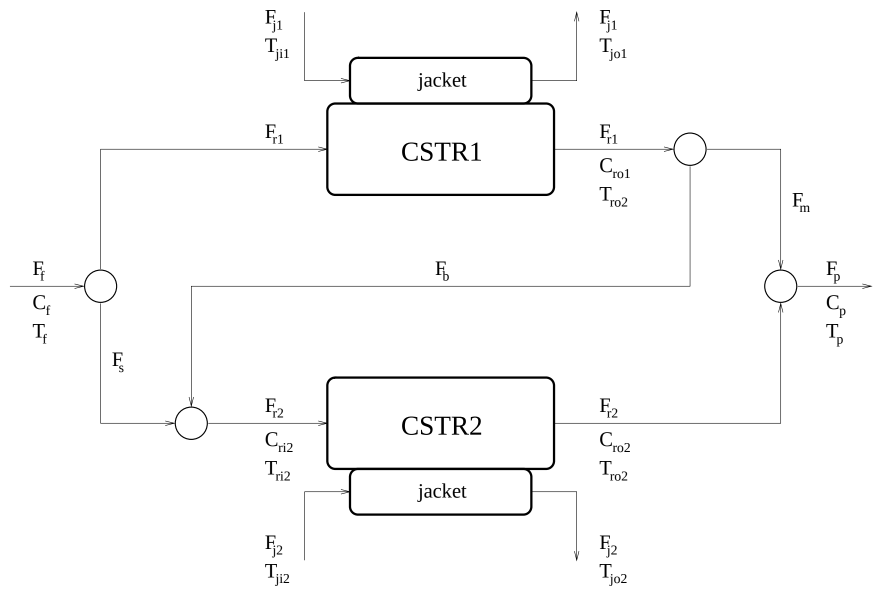

Figure 2: Reactor Network Superstructure for Example 1

used in the problem are outlined in Table 3 and the parameters and values are listed in Table 4.

The two objectives for this problem are the total cost for the economic design and the Integral Square Error (ISE) for the dynamic controllability. The capital cost is determined from the diameter and height of the reactors using the cost correlation in [4]:

$$\text{cost}_{\text{cap}} = 1916.9 D_{r1}^{1.066} (H_{r1})^{0.802} + 1916.9 D_{r2}^{1.066} (H_{r2})^{0.802}$$

The utility cost is determined from the flow rate of the cooling water.

$$\text{cost}_{\text{util}} = 32.77 (F_{jn1} + F_{jn2})$$

The total cost of the process is determined by assuming a operating period of four years

$$\text{cost}_{\text{tot}} = \text{cost}_{\text{cap}} + 4yr \times \text{cost}_{\text{util}}$$

The integral square error of the reactor temperatures and their set-points is represented by the following differential equation:

$$\frac{d\mu}{dt} = (T_{ro1} - T_{ro1}^{\star})^2 + (T_{ro2} - T_{ro2}^{\star})^2$$

Table 3: Variables used for the reactor network problem

z variable	description
C_{ri2}	inlet concentration to reactor 2
T_{ri2}	inlet temperature to reactor 2
C_{ro1}, C_{ro2}	outlet concentrations in reactors 1,2
T_{ro1}, T_{ro2}	outlet temperatures in reactors 1,2
F_{j1}, F_{j2}	jacket coolant flow rate
T_{ji1}, T_{ji2}	jacket coolant inlet temperature
T_{jo1}, T_{jo2}	jacket coolant outlet temperature
C_p	product composition
T_p	product temperature
k_1, k_2	reaction rates
I_{tro1}, I_{tro2}	Integral term for the PI controllers
μ	Integral square error controllability objective
x variable	**description**
$T^{\star}_{r1}, T^{\star}_{r2}$	set-points for outlet temperatures
V_{r1}, V_{r2}	volume of reactors 1, 2
A_1, A_2	heat exchange area for reactors 1, 2
D_{r1}, D_{r2}	diameter of reactors 1, 2
H_{r1}, H_{r2}	height of reactors 1, 2
V_{j1}, V_{j2}	volume of jackets 1, 2
F_{r1}, F_{r2}	reactor flow rates
F_s	feed split to reactor 2
F_b	flow rate from reactor 1 to reactor 2
F_m	flow rate from reactor 2 to product
F_p	product flow rate
F_{jn1}	nominal jacket 1 flow rate
F_{jn2}	nominal jacket 2 flow rate
κ_{j1}, κ_{j2}	controller gain
τ_{j1}, τ_{j2}	integral time constant
y variable (binary)	**description**
y_{r1}, y_{r2}	existence of reactor 1 and 2

which has the initial condition $\mu(t_0) = 0$. Thus, the controllability objective is the minimization of μ at the final time.

Table 4: Parameters for the reactor network problem

Description	Parameter	Value
Heat of reaction	ΔH	$-3000 Btu/lbmol$
Heat transfer coefficient	U	$300 Btu/(hr ft^2 {}^\circ R)$
Energy of activation	E/R	$15075^\circ R$
Kinetic rate constant	k_0	$4.08 \times 10^1 0 hr^{-1}$
Liquid density	ρ	$50 lb/ft^3$
Liquid heat capacity	C_p	$0.75 Btu/(lb^\circ R)$
Coolant density	ρ_j	$62.3 Btu/(ft^{3\circ} R)$
Coolant heat capacity	C_j	$1.0 Btu/(lb^\circ R)$
Feed flow rate	F_f	$100 ft^3/hr$
Feed composition	C_f	$1 lbmol A/ft^3$
Feed temperature	T_f	$600^\circ R$
Coolant inlet temperature	T_{ji1}	$530^\circ R$
Coolant inlet temperature	T_{ji2}	$530^\circ R$
Coolant cost	$Cost_{cool}$	$3.74 \times 10^{-6} \$/ft^3$

The mathematical model for the superstructure is the following:

$$
\begin{aligned}
F_f &= F_{r1} + F_s \\
F_{r2} &= F_s + F_b \\
C_{ri2} F_{r2} &= C_f F_s + C_{ro1} F_b \\
T_{ri2} F_{r2} &= T_f F_s + T_{ro1} F_b \\
V_{r1} \frac{dC_{ro1}}{dt} &= C_{ri1} F_{r1} - C_{ro1} F_{ro1} - k_1 V_{r1} C_{ro1} \\
V_{r1} \frac{dT_{ro1}}{dt} &= T_{ri1} F_{r1} - T_{ro1} F_{ro1} - \frac{\Delta H}{\rho C_p} k_1 V_{r1} C_{ro1} - \frac{U}{\rho C_p} A_2 (T_{ro1} - T_{jo1}) \\
V_{r2} \frac{dC_{ro2}}{dt} &= C_{ri2} f_{r2} - C_{ro2} f_{ro2} - k_2 V_{r2} C_{ro2} \\
V_{r2} \frac{dT_{ro2}}{dt} &= T_{ri2} f_{r2} - T_{ro2} f_{ro2} - \frac{\Delta H}{\rho C_p} k_2 V_{r2} C_{ro2} - \frac{U}{\rho C_p} A_2 (T_{ro2} - T_{jo2}) \\
F_{r1} &= F_m + F_b \\
F_p &= F_m + F_{r2} \\
C_p F_p &= C_{ro1} F_m + C_{ro2} F_{r2} \\
T_p F_p &= T_{ro1} F_m + T_{ro2} F_{r2} \\
V_{j1} \frac{dT_{jo1}}{dt} &= T_{ji1} F_{j1} - T_{jo1} F_{jo1} + \frac{U}{\rho_j C_j} A_1 (T_{ro1} - T_{jo1}) \\
V_{j2} \frac{dT_{jo2}}{dt} &= T_{ji2} F_{j2} - T_{jo2} F_{jo2} + \frac{U}{\rho_j C_j} A_2 (T_{ro2} - T_{jo2}) \\
k_1 &= k_0 e^{\frac{-E}{RT_{ro1}}} \\
k_2 &= k_0 e^{\frac{-E}{RT_{ro2}}}
\end{aligned}
\tag{25}
$$

The volume of the reactor and the heat transfer area are determined by the dimensions of the reactor.

$$\begin{array}{l} V_{r1} = \frac{\pi}{4} D_{r1}^2 H_{r1} \\ V_{r2} = \frac{\pi}{4} D_{r2}^2 H_{r2} \\ A_1 = \pi D_{r1} H_{r1} \\ A_2 = \pi D_{r2} H_{r1} \end{array} \tag{26}$$

Assuming the jacket has a four inch clearance, the volume of the jacket is determined by the following:

$$\begin{array}{l} V_{j1} = A_1 \frac{1}{3} ft \\ V_{j2} = A_2 \frac{1}{3} ft \end{array} \tag{27}$$

The PI control equations are the following:

$$\begin{array}{rcl} \frac{dI_{tro1}}{dt} & = & T_{ro1} - T_{ro1}^{\star} = 0 \\ \frac{dI_{tro2}}{dt} & = & T_{ro2} - T_{ros}^{\star} = 0 \\ F_{j1} & = & F_{jn1} + \kappa_{j1}(T_{ro1} - T_{ro1}^{\star}) + \frac{\kappa_{j1}}{\tau_{j1}} I_{tro1} = 0 \\ F_{j2} & = & F_{jn2} + \kappa_{j2}(T_{ro2} - T_{ro2}^{\star}) + \frac{\kappa_{j2}}{\tau_{j2}} I_{tro2} = 0 \end{array} \tag{28}$$

The problem has a fixed time horizon of $t_0 = 0$ and $t_f = 5hr$ and a final time point constraint on the product composition:

$$C_p(t_f) \leq 0.025$$

The initial condition for the DAE system is the steady-state solution for the given values of the x variables. The dynamics are caused by a 10% increase step disturbance in the feed temperature modeled by

$$T_f = 600^\circ R + 60^\circ R/(1 + exp[-50hr(t - 0.5hr)])$$

The ϵ constraint method is applied by minimizing the total cost objective and incorporating the controllability objective as an end time constraint:

$$\mu(t_f) \leq \epsilon$$

The value of ϵ is varied from \$291,050 (the economic optimum) to \$401,712 (the controllability optimum) to generate the noninferior solution set shown in Figure 3.

The noninferior solution set has two regions which correspond to the single reactor and two reactor designs. The lower cost and higher ISE region

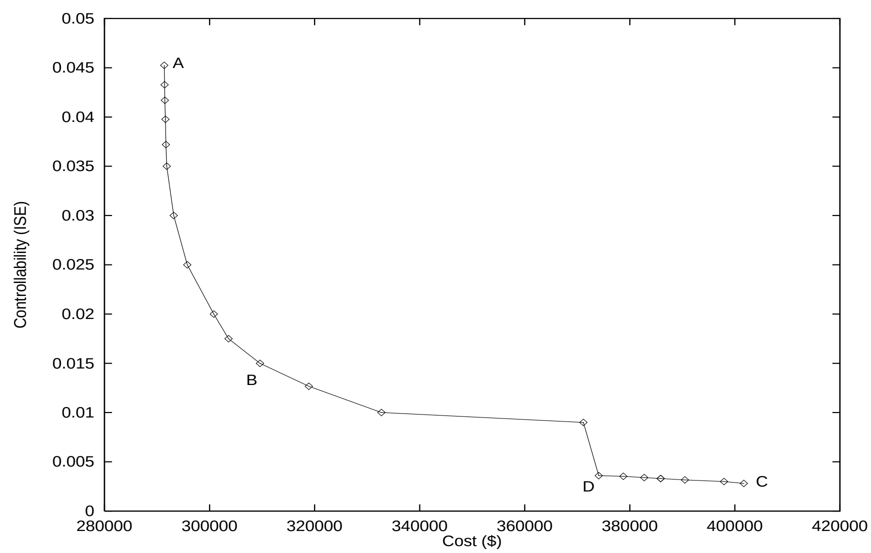

Figure 3: Noninferior solution set for the reactor network example.

corresponds to the two reactor design and the higher cost lower ISE region corresponds to the single reactor. The single reactor is more controllable because it incorporates a larger reactor and thus has more surface area available for heat transfer. The solutions for three of the designs are given in Table 5. The jump in the noninferior solution set is from the two reactor design to the single reactor design and design **D** corresponds to the minimum cost single reactor design.

Designs **A** and **B** correspond to designs with two reactors and design **C** has only a single reactor. All of the reactors in designs **A** and **B** operate at a temperature of $620^{\circ}R$ while the reactor in design **C** operates at $619.3^{\circ}R$. The dynamic responses of the reactor temperatures for reactors 1 and 2 in designs **A** and **B** are shown in Figures 4 and 5 respectively. The dynamic response of the reactor temperature for the reactor in design **C** is shown in Figure 6.

The dynamic responses of all the reactors are shown in Figure 7 in order to compare the responses. Since the controllability of the process was based on the all of the reactor temperatures in the process, design **C** has the best controllability measure. However, if the processes are compared based on

Table 5: Solution results for three reactor designs

Solution	**A**	**B**	**C**
Total Cost (\$)	291400	309610	401720
Capital Cost (\$)	186340	216820	320970
Utility Cost (\$)	105060	92790	80750
ISE	0.04524	0.015	0.0028
$D_{r1}(m)$	14.28	18.48	24.80
$D_{r2}(m)$	9.471	7.256	—
$H_{r1}(m)$	5.791	6.161	8.307
$H_{r2}(m)$	3.157	2.419	—
$V_{r1}(m)$	927.0	1653	4012
$V_{r2}(m)$	222.4	100.0	—
$T^{\star}_{r1}$	620	620	619.3
$T^{\star}_{r2}$	620	620	—
F_{jn1}	765.5	693.2	616.1
F_{jn2}	36.13	14.76	—
κ_{j1}	413.7	536.07	898.5
κ_{j2}	34.45	10.29	—
τ_{j1}	1.751	1.775	1.769
τ_{j2}	0.1681	0.0100	—

the responses of the product temperatures (outlet temperatures of reactor 2 in designs **A** and **B**), designs **A** and **B** exhibit better responses than design **C** and design **A** has the best response. Although the overall process may not be more controllable, the two reactors have a greater effect on damping the effect of the disturbance on the product.

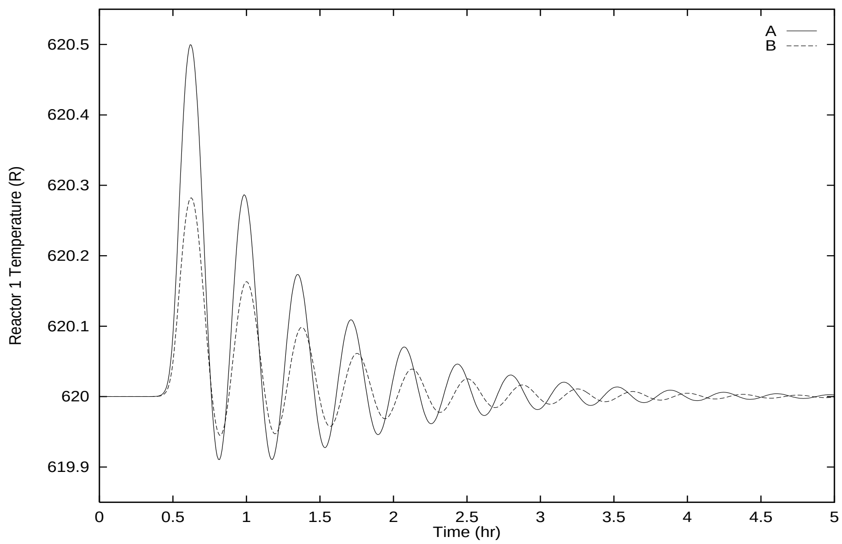

Figure 4: Dynamic responses of the temperatures in reactor 1

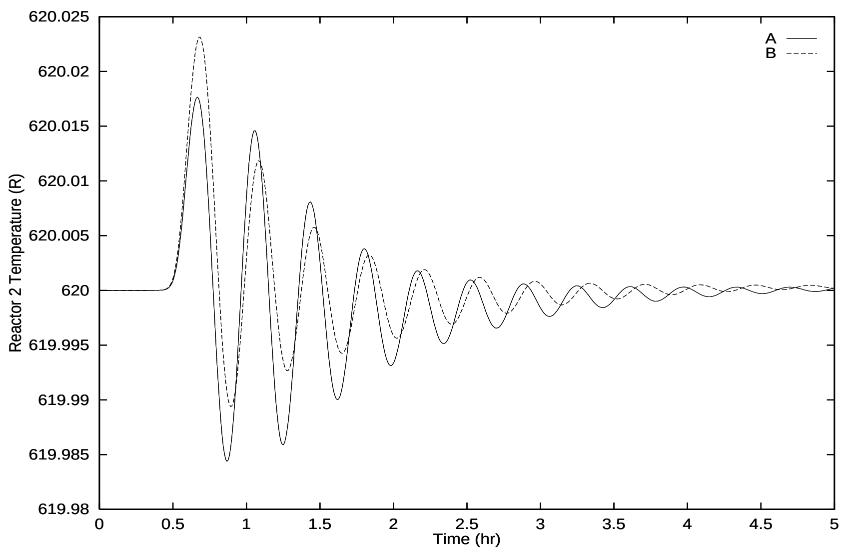

Figure 5: Dynamic responses of the temperatures in reactor 2

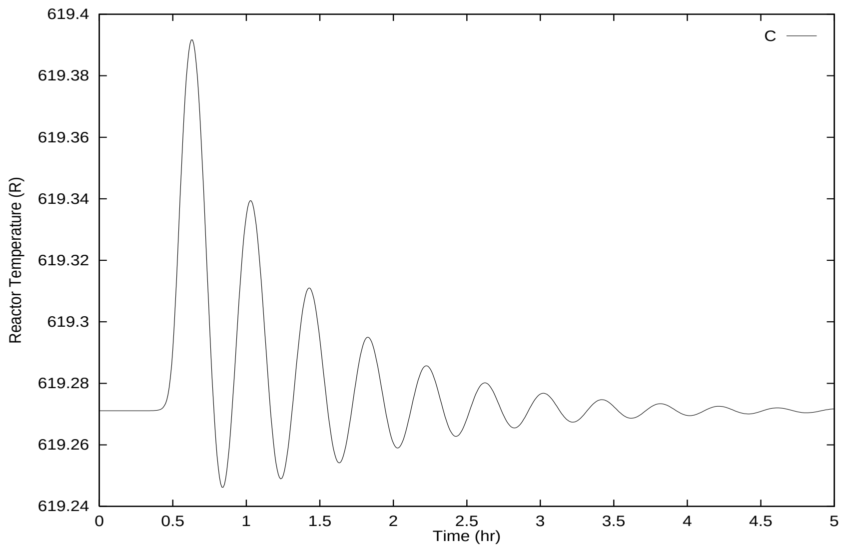

Figure 6: Dynamic response of the temperature in reactor for design **C**

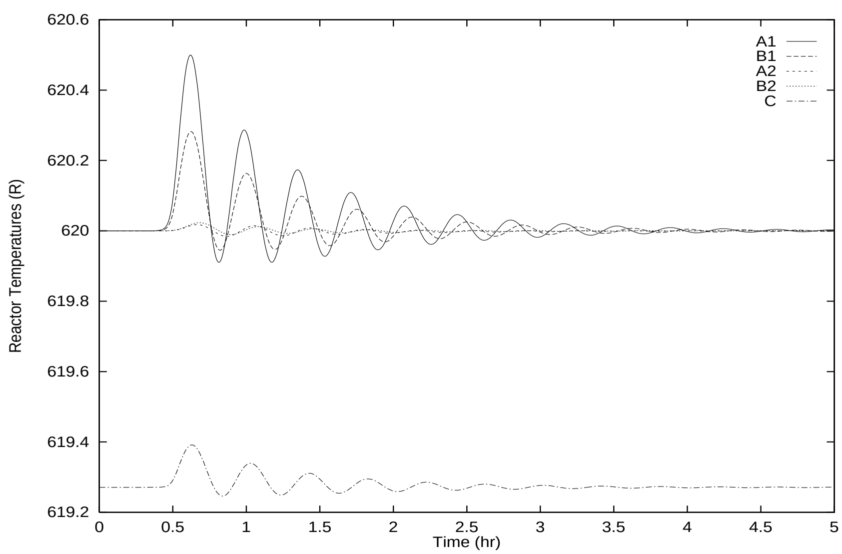

Figure 7: Dynamic response of all the reactor temperatures

6.2 Example 2—Binary Distillation

This example illustrates the proposed approach for the design of a binary distillation column. The goal is to design a process which separates a saturated liquid feed into bottoms and distillate products of specified purity. The number of trays, location of the feed, diameter of the column, flow rates and compositions must be determined. The superstructure considered for this problem is shown in Figure 8. The superstructure includes a PI control scheme for the control of the distillate and bottoms composition. The vapor boilup is used to control the bottoms composition and the reflux rate is used to control the distillate composition.

For the development of the mathematical model, the assumptions of equimolar overflow, constant relative volatility (α), partial reboiler, and total condenser are made. The structural alternatives are represented by the binary variables p_i and q_i which represent the existence of the feed and reflux respectively to tray i. The location of the reflux determines the number of trays for the column since there is no liquid flow in the trays above the reflux location.

The continuous time invariant variables in the model are the tray liquid holdup, M, tray hydraulic time constant, β, steady-state reflux ratio, R_{ss}, steady-state vapor boilup, V_{ss}, column diameter, D_c, and the controller gains and time constants K_V, K_R, τ_V, and τ_R.

The dynamic variables in the model are the liquid compositions, x_i, vapor compositions, y_i, liquid flow rate from each tray, L_i, bottoms and distillate flow rates, B and D, vapor boilup, V, and the reflux flow rate R. First order lags between the calculated control and the control level are included. For the composition measurements, a fifth order system is used to approximate a 5 minute deadtime between the actual value and the measured value. The parameters for the problem are listed in Table 6

Table 6: Parameters for the binary distillation problem

Parameter	symbol	value
Relative volatility	α	2.5
Height over the weir	h_w	$0.0254m$
Payback period	β_{pay}	$4yr$
Tax factor	β_{tax}	0.4

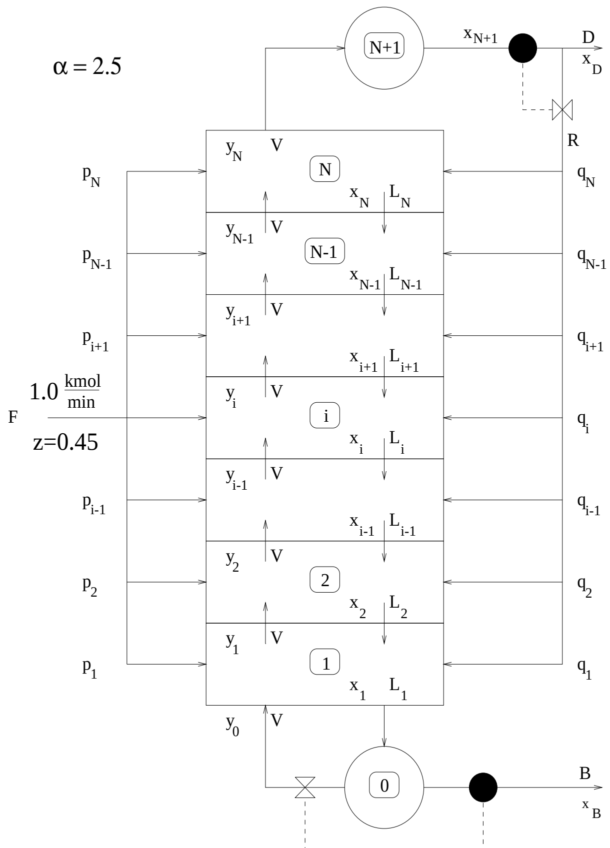

Figure 8: Superstructure for Binary Distillation Example

The full model for the binary distillation column is outlined below. The parameters for this problem are the same as those used in [14].

- Reboiler Component Balance

$$M_R \frac{dx_B}{dt} = L_1(x_1 - x_B) + V(x_B - y_B)$$

- Tray component balances

$$M \frac{dx_i}{dt} = L_{i+1}(x_{i+1} - x_i) + V(y_{i-1} - y_i) + p_i f(z - x_i) + q_i r(x_D - x_i)$$

- Condenser Component balance

$$M_C \frac{dx_D}{dt} = V(y_N - x_D)$$

- Reboiler Total Balance

$$\beta \frac{dB}{dt} = L_1 - V - B$$

- Tray total balances

$$\beta \frac{dL_i{}'}{dt} = L_{i+1} - L_i + p_i F + q_i R$$

- Condenser Total balance

$$\beta \frac{dD}{dt} = V - R - D$$

- Reboiler Equilibrium

$$y_B = \frac{\alpha x_B}{1 + x_B(\alpha - 1)}$$

- Tray equilibrium

$$y_i = \frac{\alpha x_i}{1 + x_i(\alpha - 1)}$$

- Measurement lags for the distillate and bottoms compositions (fifth order system and a five minute delay)

$$\frac{d^5 x_{B,m}}{dt^5} + 5\frac{d^4 x_{B,m}}{dt^4} + 10\frac{d^3 x_{B,m}}{dt^3} + 10\frac{d^2 x_{B,m}}{dt^2} + 5\frac{dx_{B,m}}{dt} + x_{B,m} = x_B$$

$$\frac{d^5 x_{D,m}}{dt^5} + 5\frac{d^4 x_{D,m}}{dt^4} + 10\frac{d^3 x_{D,m}}{dt^3} + 10\frac{d^2 x_{D,m}}{dt^2} + 5\frac{dx_{D,m}}{dt} + x_{D,m} = x_D$$

- PI controllers

$$\frac{dI_B}{dt} = x_{B,m} - x_B^\star$$

$$\frac{dI_D}{dt} = x_{D,m} - x_D^\star$$

$$V_c = V_{ss} + K_V(x_{B,m} - x_B^\star) - \frac{K_V}{\tau_V} I_B$$

$$R_c = R_{ss} + K_R(x_{D,m} - x_D^\star) - \frac{K_R}{\tau_R} I_D$$

- Final control lags

$$0.9\frac{dV}{dt} = V_c - V$$

$$0.5\frac{dR}{dt} = R_c - R$$

For the tray hydraulics, the Francis weir formula is used to obtain molar hold-ups, M, and tray time constants, β as functions of the column diameter. Both are assumed to time invariant and the same for all trays. The reboiler and condenser hold-ups are ten time the tray holdups and the reboiler and condenser time constants are 100 time the tray time constant.

$$M = 7.538115(((0.0014134/D_c)^{2/3}) + h_w)D_c^2$$

$$\beta = 0.05271 D_c^{1.3333}$$

The diameter of the column must be large enough to avoid flooding within the column. The flooding within the column is determined by the vapor flow rate in the column and the appropriate constraint to ensure that the column diameter is large enough is the following:

$$D_c \geq 0.6719\sqrt{V_{ss}}$$

The number of trays in the column is determined by the position of the reflux using the following constraint:

$$N_t = \sum_i (i)(q_i)$$

The following logical constraints are included to ensure the existence of one feed, the existence of one reflux, that the feed enters on tray 4 or above, that the reflux enters on tray ten or above, and that the reflux enters at least four trays above the feed.

$$\sum_{i=1}^{N} p_i = 1$$

$$\sum_{i=1}^{N} q_i = 1$$

$$\sum_{i=1}^{N} (i)(p_i) \geq 4$$

$$\sum_{i=1}^{N}(i)(q_i) \geq 10$$

$$\sum_{i=1}^{N}(i)(q_i) - (i)(p_i) \geq 4$$

The economic objective for the process is the annualized cost:

$$\text{cost} = \beta_{\text{tax}}\text{cost}_{\text{util}} + \text{cost}_{\text{cap}}/\beta_{\text{pay}}$$

$$\begin{aligned}\text{cost} \quad = \quad & 7756V_{ss} + 3.075(615 + 324D_c^2 \\ & +486(6 + 0.76N_t)D_c) + 61.25N_t(0.7 + 1.5D_c^2)\end{aligned}$$

The controllability objective is the sum of the time weighted ISE of the distillate and bottoms compositions:

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

The ISE for the two compositions could be included as separate controllability measures, but since both have the same magnitude, they are treated as having the same weight factor. Thus, they are included into a single controllability objective. In cases where the controllability objectives exhibit different characteristics or variations, different weight factors can be used to account for these different characteristics.

The initial condition for this problem is the steady-state solution along with the values of the controls set to their nominal values. The dynamics for the problem are caused by a step disturbance in the feed composition:

$$z = 0.45 + \frac{0.9}{1 + e^{-10(t-10)}}$$

The ϵ-constraint method is applied to the multiobjective problem by imposing the following end-point constraint:

$$\mu(t_f) \leq \epsilon$$

The MINLP/DAE problem is solved using GBD with the adjoint problem since the problem has $\boldsymbol{y}$ variables in the DAE system. The value of ϵ is varied from 0.01 to 0.5 to generate the noninferior solution set which is shown in Figure 9. Three points along the noninferior solution set are indicated: The minimum cost process, **A**, the minimum ISE process, **C**, and

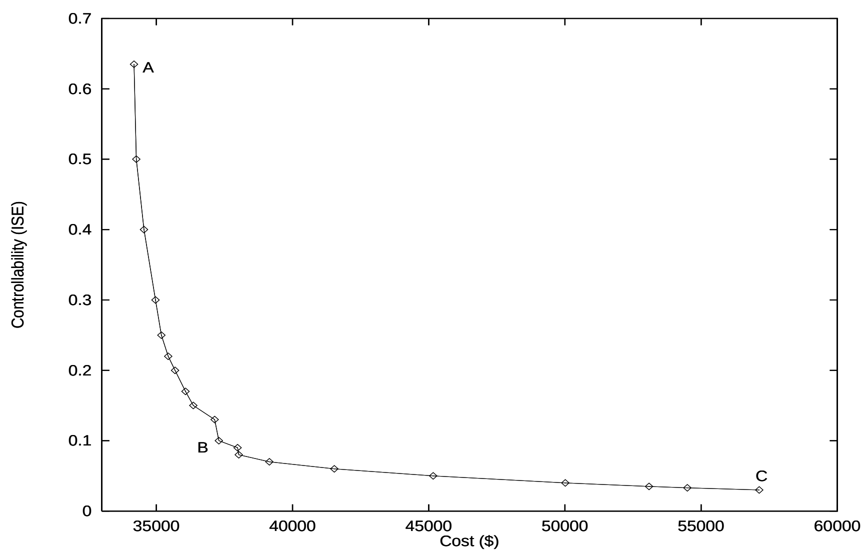

Figure 9: Noninferior solution set for the distillation column example

an intermediate process, **B**. The specific results for these three columns are shown in Table 7.

The noninferior solution set provides a way of quantitatively assessing the tradeoffs between the design and control of the process. The amount of cost incurred for obtaining a more controllable process can be obtained.

Since the dynamics are included in the solution of the problem, the dynamic responses are obtained as part of the solution. The dynamic responses of the bottoms and distillate compositions for the three columns are shown in Figures 10 and 11.

The controllability of the distillation process is observed to increase when the number of trays in the column is increased. The controllability is also increased by increasing the vapor boilup and diameter of the column. The larger column both in diameter and in height has a greater damping effect on the disturbance than the smaller columns. In comparing the dynamic responses of the three solutions, the improvement in the dynamic operation of the process can be seen.

Table 7: Solution results for three columns

Solution	**A**	**B**	**C**
Total Cost ($)	34182	37293	57131
Capital Cost ($)	24428	25602	45833
Utility Cost ($)	9754	11691	11298
ISE	0.635	0.100	0.03
Trays	16	15	25
Feed Tray	8	5	5
$D_c(m)$	0.7535	0.8250	1.050
$R(kmol/min)$	0.8097	1.059	1.009
$V(kmol/min)$	1.258	1.507	1.457
K_V	2.636	8.137	8.907
$\tau_V(min)$	20.55	18.23	10.39
K_R	-0.1078	-1.048	-5.677
$\tau_R(min)$	0.4827	4.696	20.65

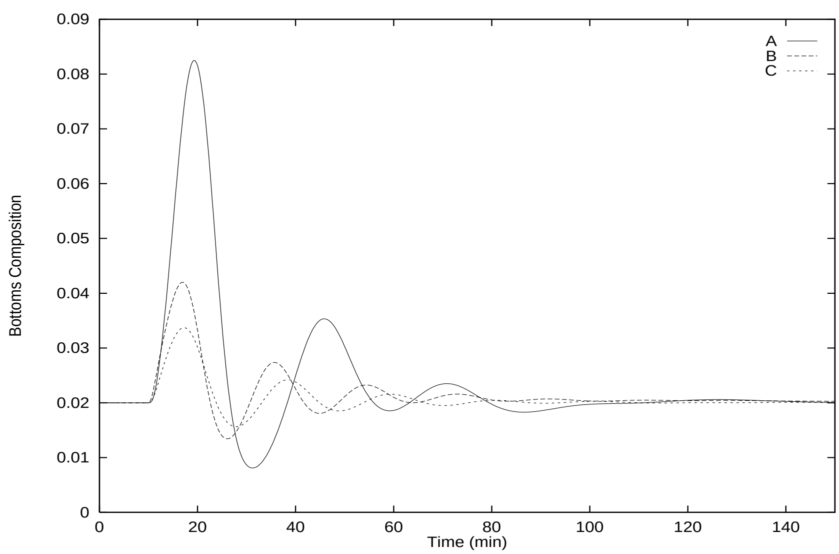

Figure 10: Dynamic responses of bottoms compositions for three solutions

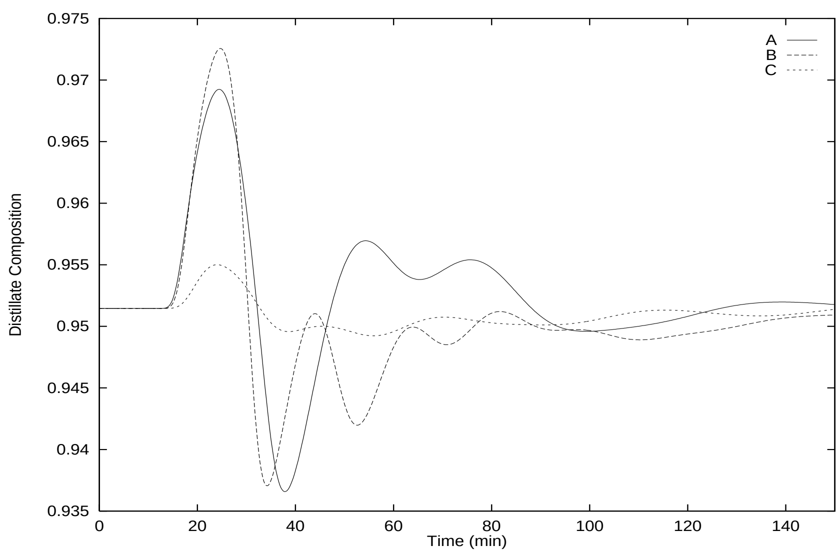

Figure 11: Dynamic responses of distillate compositions for three solutions

6.3 Example 3—Reactor-Separator-Recycle System

As a third example, the design of a process involving a reaction step, a separation step, and a recycle loop is considered. The parameters for the problem and the design follows the work in [15]. Fresh feed containing A and B flow into a an isothermal 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 shown in Figure 12 has the same distillation column as in the previous example with the addition of a reaction step. The solution requires the determination of the same parameters for the distillation column as in the previous example along with the size of the reactor.

The additional dynamic variables for the problem are the reactor outlet flow rate, F_c, and the reactor composition, z_c. The volume of the reactor, V_r is the additional time invariant variable. The reactor is mathematically modeled using the following equations:

- Total balance

$$F_c = F_r + D$$

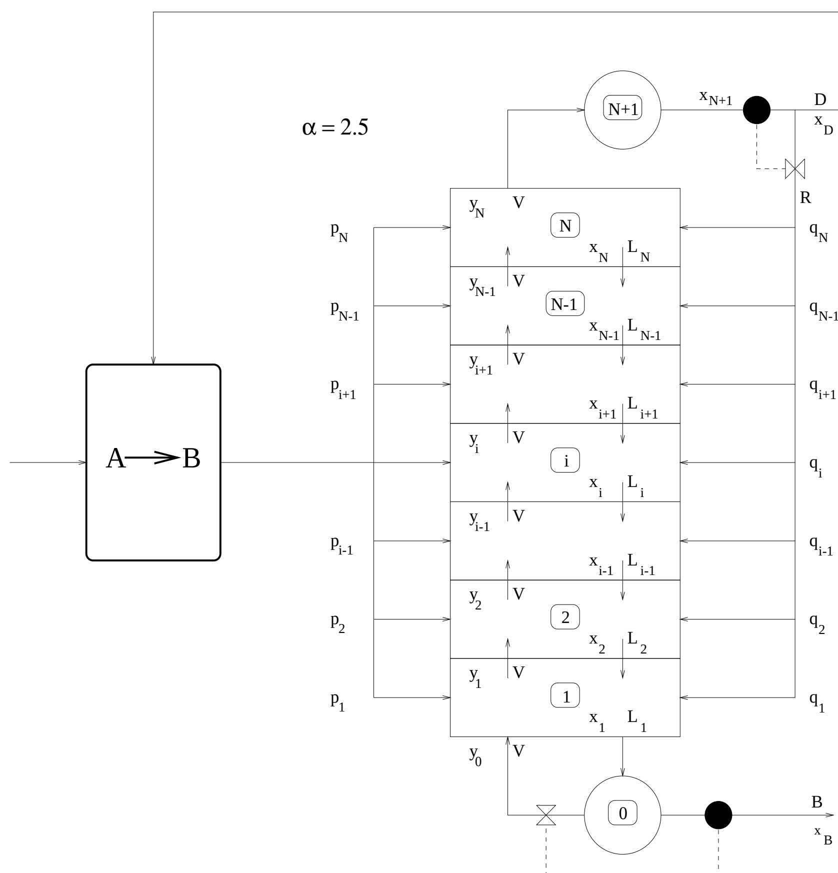

Figure 12: Superstructure for Reactor-Separator-Recycle system

- Component Balance

$$V_r \frac{dz_c}{dt} = F_r z_r + D x_D - F_c z_c - V_r k z_c$$

The same model equations are used for the distillation column.

For this problem, the single output is the product composition. However, the same two possible control loops are considered for the operation of the distillation column. The bottoms (product) composition is controlled by the vapor boil-up and the distillate composition is controlled by the reflux rate.

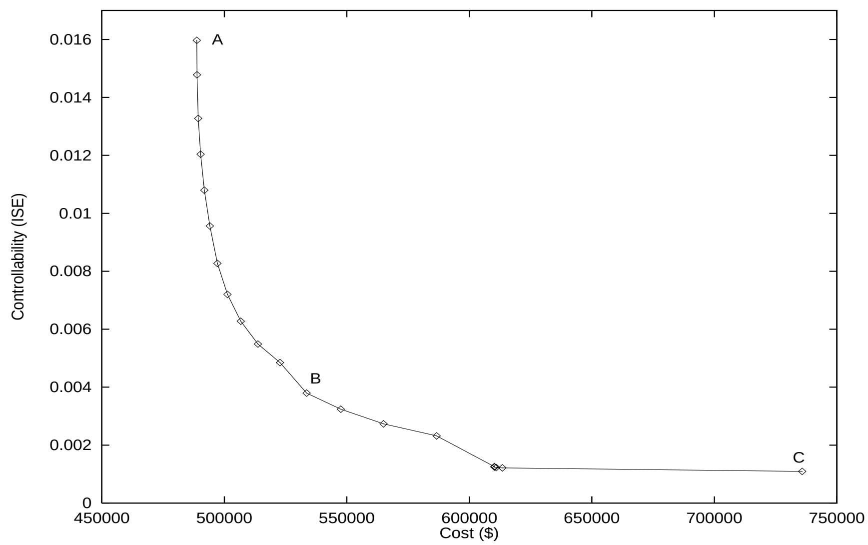

Figure 13: Noninferior solution set for the Reactor–Separator–Recycle System

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. The derivation and data for the cost function can be found in [15].

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

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

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

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

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

The controllability is the time weighted ISE for the product composition:

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

Table 8: Solution 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

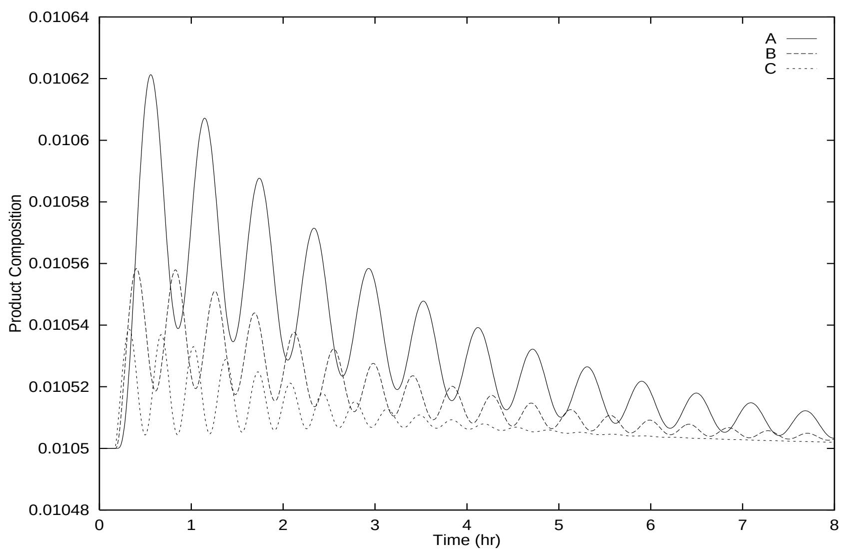

Figure 14: Dynamic responses of product compositions for three designs

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.

7 Conclusions

This work presented a method for systematically analyzing the interaction between the design economics and dynamic controllability. The mathematical programming framework of process synthesis has been applied to the problem by postulating a process superstructure and modeling with DAEs. The resulting problem formulation is a multiobjective MIOCP which is solved to establish the trade-offs between two objectives representing the economic and controllability aspects of the process. The multiobjective problem was solved using an ϵ-constraint method to reduce the problem to the solution of multiple MIOCP problems. A parameterization method has been applied to the optimal control problem reducing it to an MINLP/DAE problem. Several solution strategies for solving the MINLP/DAE problem have been presented. These strategies differ based on the structure of the MINLP/DAE problems and assumptions that can be made. The outlined solution procedure was effectively applied to three example problems including rector network synthesis, binary distillation, and a reactor-separator-recycle system.

One of the key issues in assessing the tradeoffs between the design a control of a process is the measurement of the controllability of the process. This work focused on using ISE as a controllability measure despite a number of drawbacks associated with it. Future work should address the development and usage of more suitable controllability measures for nonlinear processes.

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.

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