Simultaneous Design and Control Optimization under Uncertainty in Reaction/Separation Systems

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Abstract

In this paper, we overview recent advances towards the integration of process design, process control and process operability in separation and reaction/separation systems that were developed within our group at Imperial College. Based on novel mixed integer dynamic optimization algorithms, a simultaneous strategy is presented featuring high fidelity dynamic models, explicit consideration of structural process and control design aspects (such as number of trays, pairing of manipulated and controlled variables) through the introduction of 0-1 variables, and explicit consideration of time-varying disturbances and time-invariant uncertainties. The application of this strategy to two typical (a separation and a reactive separation) systems is discussed.

Keywords

Process design, Process control, Uncertainty, Operability, Mixed-integer dynamic optimization

Introduction

The need to consider operability issues at an early phase of process design is now becoming widely accepted in both academia and industry. As a result of this, in recent years, a number of methodologies and tools have been reported for taking account of the interactions between process design and process control, with well over fifty publications since 1982 plus several international workshops and dedicated conference sessions (see Van Schijndel and Pistikopoulos, 2000). Despite these developments, however, it is observable that a large proportion of the work in this field:

- has concentrated on the application of metrics (e.g., condition number) that provide some measure of a system's controllability, but may not relate directly and unambiguously to real performance requirements;
- relies on steady-state or simple, usually linear dynamic models for processes;
- does not account for the presence of both time-varying disturbances and time-invariant (or relatively slowly varying) uncertainties; and
- does not involve selection of the best process design and the best control scheme, taking into account both discrete and continuous decisions.

Van Schijndel and Pistikopoulos (2000) also put forward a number of key challenges that lie ahead in the area of Process Design for Operability. One such challenge is the need for a rigorous and efficient solution of the underlying optimization problem, which is at the heart of the mathematical representation of the simultaneous process and control design problem.

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The aim of this paper is to give a brief overview of some recent advances, towards this endeavor, and its application to typical separation and reactive separation problems, carried out whithin our group at Imperial College.

Simultaneous Design and Control Under Uncertainty Framework

As discussed in Van Schijndel and Pistikopoulos (2000), the problem of the integration of process design, process control and process operability can be conceptually posed as follows:

$$\text{minimize} \quad \text{Expected Total Annualized Cost} \qquad \text{(P)}$$

subject to

Differential-Algebraic Process Model
Inequality Path Constraints
Control Scheme Equations
Process Design Equations
Feasibility of Operation (over time)
Process Variability Constraints

To determine Process and Control Design

A general, algorithmic framework for solving (P) was proposed by Mohideen et al. (1996). Its steps, schematically shown in Figure 1, can be summarized as follows:

Step 1. Choose an initial set of scenarios for the uncertain parameters.

Step 2. For the current set of scenarios, determine the optimal process and control design by solving the (multi-period) mixed-integer dynamic optimization

(MIDO) problem:

$$\min_{\substack{\mathbf{d},\mathbf{y},\\ \mathbf{u_v^1},\mathbf{u_v^2},\ldots,\mathbf{u_v^{ns}}}} \sum_{i=1}^{ns} w_i.\phi\left(\dot{\mathbf{x}}^i(t_f),\mathbf{x}^i(t_f),\mathbf{z}^i(t_f),\mathbf{u_t}^i(t_f),\mathbf{u_v}^i,\boldsymbol{\nu}^i(t_f),\boldsymbol{\theta}^i,\mathbf{d},\mathbf{y},t_f\right) \tag{1}$$

subject to

$$\begin{aligned}
\mathbf{f}\left(\dot{\mathbf{x}}^i(t),\mathbf{x}^i(t),\mathbf{z}^i(t),\mathbf{u_t}^i(t),\mathbf{u_v}^i,\boldsymbol{\nu}^i(t),\boldsymbol{\theta}^i,\mathbf{d},\mathbf{y}\right) &= \mathbf{0}\\
\mathbf{c}\left(\mathbf{x}^i(t),\mathbf{z}^i(t),\mathbf{u_t}^i(t),\mathbf{u_v}^i,\boldsymbol{\nu}^i(t),\boldsymbol{\theta}^i,\mathbf{d},\mathbf{y}\right) &= \mathbf{0}\\
\mathbf{g}\left(\dot{\mathbf{x}}^i(t),\mathbf{x}^i(t),\mathbf{z}^i(t),\mathbf{u_t}^i(t),\mathbf{u_v}^i,\boldsymbol{\nu}^i(t),\boldsymbol{\theta}^i,\mathbf{d},\mathbf{y}\right) &\leq \mathbf{0}\\
i = 1,...,ns&
\end{aligned}$$

where $\mathbf{d}$ includes the continuous process design variables and controllers' tuning parameters; $\mathbf{y}$ comprises the binary variables for the process and the control structure (corresponding to whether a manipulated variable is paired with a particular controlled variable or not); $\mathbf{u_v}$ is the set of time-invariant operating variables; i is the index set for the scenarios of the uncertain parameters $\boldsymbol{\theta}$; ns is the number of scenarios; $w_i,\ i = 1,...,ns$, are discrete probabilities for the selected scenarios ($\sum_{i=1}^{ns} w_i = 1$); ϕ is a cost function; $\mathbf{x}(t)$ is the vector of differential states; $\mathbf{z}(t)$ is the vector of algebraic variables; $\mathbf{u_t}(t)$ denotes the set of time-varying manipulated (control) variables; $\nu(t)$ represents the time-varying disturbances; $\mathbf{f} = \mathbf{0}$ and $\mathbf{c} = \mathbf{0}$ represent the differential and algebraic equations (DAEs), respectively, for the process and control system, for which consistent initial conditions are given; and $\mathbf{g} \leq \mathbf{0}$ represents the set of constraints (end, point and path) that must be satisfied for feasible operation.

Step 3. Test the process and control design from Step 2 for feasibility over the whole ranges of the uncertain parameters by solving the dynamic feasibility test problem:

$$\chi(\mathbf{d},\mathbf{y}) = \max_{\boldsymbol{\theta}} \min_{\mathbf{u_v}} \max_{l\in L,\ t\in[0,t_f]} g_l(\cdot) \tag{2}$$

subject to

$$\begin{aligned}
\mathbf{f}\left(\dot{\mathbf{x}}(t),\mathbf{x}(t),\mathbf{z}(t),\mathbf{u_t}(t),\mathbf{u_v},\boldsymbol{\nu}(t),\boldsymbol{\theta},\mathbf{d},\mathbf{y}\right) &= \mathbf{0}\\
\mathbf{c}\left(\mathbf{x}(t),\mathbf{x_a}(t),\mathbf{u_t}(t),\mathbf{u_v},\boldsymbol{\nu}(t),\boldsymbol{\theta},\mathbf{d},\mathbf{y}\right) &= \mathbf{0}
\end{aligned}$$

If $\chi(\mathbf{d},\mathbf{y}) \leq 0$, feasible operation can be ensured dynamically for all values of $\boldsymbol{\theta}$ within the given ranges. In this case, the algorithm terminates; otherwise, the solution of Equation 2 identifies a critical scenario that is added to the current set of scenarios before returning to Step 2.

Remarks

1. If the active set formulation of Grossmann and Floudas (1987) is used to solve (2), as proposed by Dimitriadis and Pistikopoulos (1995) and Mohideen et al. (1996), then the problem, like (1), corresponds to a MIDO problem.
2. The formulation (P) is an exact closed-loop, dynamic analogue of the steady-state problem of optimal design with fixed degree of flexibility (Pistikopoulos and Grossmann, 1988).
3. The solution strategy shown in Figure 1 and described above, is a closed-loop dynamic analogue of the flexible design algorithm of Grossmann and coworkers (see Biegler et al., 1997, chapter 21).
4. Different control design criteria can be used for example, decentralized PI-control, as discussed in Mohideen *et al.*, multivariable PI-control as discussed in Kookos and Perkins (2000) or Q-parameterization methods, as discussed in Swartz et al. (2000).
5. To date, the framework has been applied to single- and double-effect (heat integrated) distillation systems (Mohideen et al., 1996), to rigorously modeled double-effect systems (Bansal et al., 2000c), and an industrial two column system (Ross et al., 1999), but with control model simplifications, fixed discrete decisions and simplification in the treatment of uncertainty.
6. The integrated design and control problem requires the solution of MIDO problem. Until recently, there were no reliable methods for dealing with such problems. Therefore, it is still imperative to develop rigorous theory and efficient methods to accomplish this.
7. The proposed decomposition scheme, as shown in Figure 1, requires the repetitive solution of two

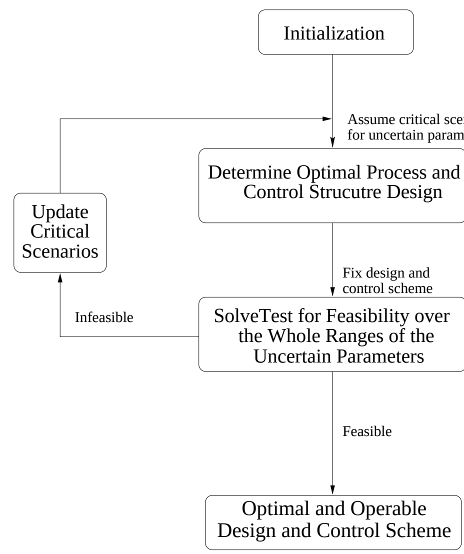

Figure 1: Decomposition algorithm of Mohideen et al. (1996).

MIDO problems in the design and the feasibility stage. It would be theoretically and computationally advantageous to avoid this iterative procedure, by solving in a single stage first, the feasibility problem and subsequently, the design problem, as it has been done for steady state systems by Bansal et al. (2000a). Currently, an endeavor is made towards adopting such a conceptual approach for the interactions of design and control under uncertainty and any progress in that area will be reported in the future.

In the next section an algorithm for solving mixed integer dynamic optimization problems is outlined. This algorithm is utilized in the simultaneous process and control design in the general case, where discrete decisions about the design and control structure are considered.

Mixed-Integer Dynamic Optimization (MIDO)

Optimal Control with the incorporation of binary variables, hence, Mixed Integer Dynamic Optimization (MIDO), plays a key role in methodologies that address the interactions of Design and Control (Mohideen et al., 1996; Schweiger and Floudas, 1997; Bahri et al., 1997; Kookos and Perkins, 2000). The simultaneous design and control framework described in the previous section involves the solution of MIDO problems in Steps 2 and 3. Moreover, MIDO is also encountered in several other modeling and optimization applications of chemical and process systems engineering. Avraam et al. (1999) used MIDO for addressing the issue of optimization on hybrid systems and recently, Barton et al. (2000) discuss the application of MIDO on the same area. Narraway and Perkins (1994) posed the Control Structure Selection problem in a Mixed Integer optimal control formulation. MIDO has also been employed for the design of batch / semi batch processes (Allgor and Barton, 1999; Barton et al., 1998; Sharif et al., 1998), dynamic optimization under uncertainty (Dimitriadis and Pistikopoulos, 1995; Samsatli et al., 1998) and for the reduction of kinetic mechanism models (Androulakis, 2000).

A number of algorithms have very recently started to appear in the open literature for solving MIDO problems. A common approach is to decompose directly the MIDO problem into a series of primal problems (upper bounds on the solution) and master problems (lower bounds on the solution). The primal problems correspond to continuous dynamic optimization problems where the values of the binary variables are fixed. These are commonly solved using control vector parameterization (CVP) techniques, where only the time-varying control variables are discretized. According to those techniques the differential system is initially integrated and then the gradients are calculated either via parameter perturbations or more accurately by integrating the sensitivity (Vassiliadis et al., 1994) or adjoint (Sargent and Sullivan, 1977) DAE system. The size of the sensitivity equations is proportional to the optimization parameters whereas the size of the adjoint system is approximately proportional to the number of constraints.

The MIDO algorithms that employ CVP for the primal problems mainly differ in how they construct the master problems, where the latter correspond to mixed-integer linear programs (MILPs) or non-linear programs (MINLPs) whose solutions give new sets of binary values for subsequent primal problems. Generalized Benders' Decomposition-based (GBD-based) approaches (Mohideen et al., 1997; Ross et al., 1998; Schweiger and Floudas, 1997), Outer Approximation-based (OA-based) approaches (Sharif et al., 1998), approaches based on "screening models" (Allgor and Barton, 1999) and "steady state models" (Kookos and Perkins, 2000) have been developed. These MIDO algorithms tend to depend on a particular type of method for integrating the DAE system in the primal problems and require the solution of a complex intermediate problem in order to construct the master problem. In the case of Allgor and Barton (1999) the method is case study-specific whereas the approach of Kookos and Perkins (2000) cannot in general be applied to intrinsic dynamic systems such as batch or semi-batch processes. In our approach, a variant of the Generalized Benders decomposition (Geoffrion, 1972; Floudas, 1995) method is employed for formulating the master problem. This is described next.

Generalized Benders Decomposition Approach for the Solution of MIDO Problems

Consider a general MIDO formulation:

$$\min_{u,d,y} \ \phi(\dot{x}(t_f), x(t_f), z(t_f), u(t_f), d, y, t_f) \tag{3}$$

subject to

$$\begin{aligned}
0 &= f(\dot{x}(t), x(t), z(t), u(t), d, y, t)\\
0 &= c(x(t), z(t), u(t), d, y, t)\\
0 &= r(x(t_0), \dot{x}(t_0), z(t_0), u(t_0), d, y, t_0)\\
0 &\geq g(\dot{x}(t), x(t), z(t), u(t), d, y, t)\\
0 &\geq q(\dot{x}(t_f), x(t_f), z(t_f), u(t_f), d, y, t_f)\\
&\quad t_o \leq t \leq t_f
\end{aligned}$$

Here, $x \in \Re^{n_x}, z \in \Re^{n_z}$ are the vectors of the differential states and the algebraic variables respectively. The vectors $u \in \Re^{n_u}, d \in \Re^{n_d}$ represent the control and the time-invariant design variables, whereas $y \in \{0,1\}^{n_y}$ is the vector of the discrete binary variables. The functions f, c and r represent the differential equations, the algebraic equations and their initial conditions respectively. The objective function is denoted by ϕ and the path and end point constraints by g and q respectively. The binary variables y participate only in a linear form in the objective function, the differential system and the constraints, since this is a necessary condition for applying GBD to a mixed integer optimization problem.

The *primal problem* is constructed by fixing the binaries to a specific value $y = y^k$. Then the problem given by Equation 3 becomes an optimal control problem that is solved with control vector parameterization. The control variables u are discretized to time-invariant parameters. From now on, the new total set of optimization variables will be denoted as v and includes the design and the parameterized controls $v = \{u_1, u_2, .., u_{N_u}, d\}$ $v \in \Re^{n_u \cdot N_u + n_d}$. The path constraints are converted to end-point constraints by introducing additional differential equations (e.g., Sargent and Sullivan, 1977) and state variables.

In GBD-based approaches the *master problem* is constructed using the dual information of the primal at the optimum solution. The *dual information* is embedded in the *Lagrange multipliers* μ of the constraints q and the *adjoint* time-dependent variables $\lambda(t), p(t)$ that are associated with the differential system of equations, i.e. f,c. Despite the fact that the Lagrange multipliers are calculated directly from the primal problem solution, the evaluation of the adjoint variables requires an extra integration of the so-called adjoint DAE system. This differential system has the form (Bryson and Ho, 1975; Vassiliadis, 1993):

$$
\begin{aligned}
-\frac{d\{[\frac{\partial f}{\partial \dot{x}}]^T \cdot \lambda(t)\}}{dt} &= -[\frac{\partial f}{\partial x}]^T \cdot \lambda(t) - [\frac{\partial c}{\partial x}]^T \cdot p(t) \\
0 &= -[\frac{\partial f}{\partial z}]^T \cdot \lambda(t) - [\frac{\partial c}{\partial z}]^T \cdot p(t) \\
(\frac{\partial f}{\partial \dot{x}})^T_{t_f} \cdot \lambda(t_f) &= -\{(\frac{\partial \phi}{\partial x})^T_f + (\mu)^T \cdot (\frac{\partial q}{\partial x})^T_f \\
&\quad + [(\frac{\partial f}{\partial x})^T \; (\frac{\partial c}{\partial x})^T]_f \cdot \omega_f\}
\end{aligned}
\tag{4}
$$

Equation 4 involves a backwards integration and can be computationally expensive. After the adjoint functions are calculated the master problem is constructed and has the following form:

$$
\min_{y,\eta} \; \eta \tag{5}
$$

subject to

$$
\begin{aligned}
\eta \geq \; & \phi + (\mu^k)^T \cdot q \\
& + (\omega_f^k)^T \cdot \begin{bmatrix} f \\ c \end{bmatrix}_f + (\omega_0^k)^T \begin{bmatrix} f \\ c \end{bmatrix}_o + (\rho^k)^T \cdot r \\
& + \int_{t_o}^{t_f} \begin{bmatrix} \lambda^k(t) \\ p^k(t) \end{bmatrix}^T \cdot \begin{bmatrix} f \\ c \end{bmatrix}_t dt \\
& \qquad k = 1, K \quad k \in K
\end{aligned}
$$

ρ, ω_f and ω_0 are multipliers that are evaluated from the first order optimality conditions of the optimal control primal problem (Vassiliadis, 1993). The master problem is a relaxation of the equivalent to the MIDO, dual problem (Bazaraa et al., 1993) since the dual multipliers (Lagrange μ and adjoints λ, p) and the non-complicating continuous variables (x,z,v) remain fixed. The consecutive solutions of the master problem generate a series of supporting functions to the overall problem under several convexity assumptions (Floudas, 1995). If those assumptions do not hold the relax master problem might rule out parts of the feasible region where several local optima could lie decreasing the probability of detecting the global minimum. Nevertheless, the method ensures local optimality in the sense that when the integers are fixed the primal problem converges to a local solution in the space of continuous variables (primal $\equiv$ valid upper bound).

The only variables that vary in the master problem are the binaries and the objective. The binaries participate in a linear form in the primal and master problems. As a result the master problem is an MILP and its solution apart from being lower bound to the MIDO problem also provides a new integer realization. If the lower bound evaluated at the master and the upper bound calculated in the primal cross then the solution is found and is equal to the upper bound, whereas if they do not cross the new integer set is augmented to the primal problem and the algorithm recommences.

The extra computationally demanding adjoint integration (Equation 4) limits the applicability of the method and renders the algorithm difficult to implement. Mohideen et al. (1997); Ross et al. (1998) employed a special numerical integration procedure for the primal dynamic optimization problem that brings some benefits in the adjoint calculation. However, these approaches restrict considerably the choice of primal solution techniques.

Recent developments in our group (Bansal et al., 2000b) show that the adjoint DAE system solution procedure can be eliminated by introducing an extra set of continuous optimization variables y_d, in the primal problem, that are fixed according to the equality constraint: $y_d - y^k = 0$. This gives rise to the following primal optimal control problem:

$$
\min_{v,y_d} \; \phi(\dot{x}(t_f), x(t_f), z(t_f), v, y_d, t_f) \tag{6}
$$

subject to

$$
\begin{aligned}
0 &= f(\dot{x}(t), x(t), z(t), v, y_d, t) \\
0 &= c(x(t), z(t), v, y_d, t) \\
0 &= r(x(t_0), \dot{x}(t_0), z(t_0), v, y_d, t_0) \\
0 &\geq q(\dot{x}(t_f), x(t_f), z(t_f), v, y_d, t_f) \\
0 &= y_d - y^k \\
& t_o \leq t \leq t_f
\end{aligned}
$$

The master problem is constructed in a similar mode:

$$\min_{y,\eta} \ \eta \tag{7}$$

subject to

$$\begin{aligned}\eta \geq\ & \phi(\dot{x}^k(t_f), x^k(t_f), z^k(t_f), v^k, y_d^k, t_f) \\ & + (\mu^k)^T \cdot q(\dot{x}^k(t_f), x^k(t_f), z^k(t_f), v^k, y_d^k, t_f) \\ & + (\omega_f^k)^T \cdot \begin{bmatrix} f \\ c \end{bmatrix}_f + (\omega_0^k)^T \begin{bmatrix} f \\ c \end{bmatrix}_o + (\rho^k)^T \cdot r \\ & + \int_{t_o}^{t_f} \begin{bmatrix} \lambda^k(t) \\ p^k(t) \end{bmatrix}^T \cdot \begin{bmatrix} f \\ c \end{bmatrix}_t dt \\ & + \Omega^k (y_d^k - y) \\ & \qquad\qquad k = 1, K \quad k \in K\end{aligned}$$

In the new primal formulation, Equation 6, the differential algebraic equations and the constraints do not include binaries any longer. Therefore at the master problem their associated terms are equal to zero due to the exact satisfaction of the DAE system and the complementarity conditions that apply to the constraints. By removing then those terms the master problem is simplified to the equation:

$$\min_{y,\eta} \ \eta \tag{8}$$

subject to

$$\begin{aligned}\eta \geq\ & \phi(\dot{x}^k(t_f), x^k(t_f), z^k(t_f), v^k, y_d^k, t_f) \\ & + \Omega^k (y_d^k - y) \\ & \qquad\qquad k = 1, K \quad k \in K\end{aligned}$$

In the modified equivalent master problem, Equation 8, all the terms are calculated at the solution of the primal problem and no adjoint calculations are required. Additionally, the formulation of the problem is considerably simplified compared to the original master problem structure of Equation 5.

However, the additional continuous optimization variables and the additional constraints may increase the computational effort for solving the primal problem while they may also introduce extra model complexity. Therefore, initially the primal is solved in its original form (Equation 3 with fixed binaries) and then a resolve session precedes the master problem where one additional optimization iteration is performed on the modified primal (Equation 6).

If the primal problem is infeasible the constraints are relaxed and a feasibility optimization problem is solved. The corresponding master problem is modified accordingly (Floudas, 1995; Mohideen, 1996). Integer cuts in the master problem formulation can also be included to exclude previous primal integer solutions.

The steps of the algorithm are briefly summarized below:

- Fix the values of the binary variables, $y = y^k$, and solve a standard dynamic optimization problem (Equation 3, kth primal problem). An upper bound, UB, on the solution to the MIDO problem is obtained from the minimum of all the primal solutions obtained so far.
- Re-solve the primal problem at the optimal solution (Equation 6) with additional constraints of the form $y_d - y^k = 0$, where y_d is a set of continuous search variables and y^k is the set of (complicating) binary variables. Convergence is achieved in one iteration. Obtain the Lagrange multipliers, Ω^k, corresponding to the new constraints.
- Construct the kth relaxed master problem from the kth primal solution, ϕ^k, and the Lagrange multipliers, Ω^k (Equation 8). This corresponds to the mixed-integer linear program (MILP) The solution of the master, η^k, gives a lower bound, LB, on the MIDO solution. If $UB - LB$ is less than a specified tolerance ϵ, or the master problem is infeasible, the algorithm terminates and the solution to the MIDO problem is given by UB. Otherwise, set $k = k + 1$, y^{k+1} equal to the integer solution of the master, and return to step 1.

The main advantage of the algorithm is that, even when the binary variables y participate within the DAE system (as they do for the distillation example presented later in this paper), the master problem does not require any direct dual information with respect to the DAE system and so no intermediate adjoint problem is required for its construction. The master problem, Equation 8, also has a very simple form compared to when adjoint variables are required (Mohideen et al., 1997; Schweiger and Floudas, 1997). Furthermore, the MIDO approach is independent of the type of method used for solving the dynamic optimization primal problems.

It should be noted, however, that since the algorithm is based GBD principles, shares the limitations of most decomposition methods. In particular, although a locally optimal solution is guaranteed when the integer variables are chosen as the complicating variables, the convexity conditions required for the algorithm to converge to the global optimum will not be satisfied by most process engineering problems. Investigation into the quality of solutions obtained from such MIDO algorithms is a current active research area.

Illustrative example

The application of the mentioned algorithm for solving Mixed Integer Dynamic Optimization problems is demonstrated through a process example that is taken from the MINOPT User's Guide (Schweiger et al., 1997). The case study examines a distillation column (Figure 2) that has a fixed number of trays and the objective is to determine the optimal feed location (discrete decision),

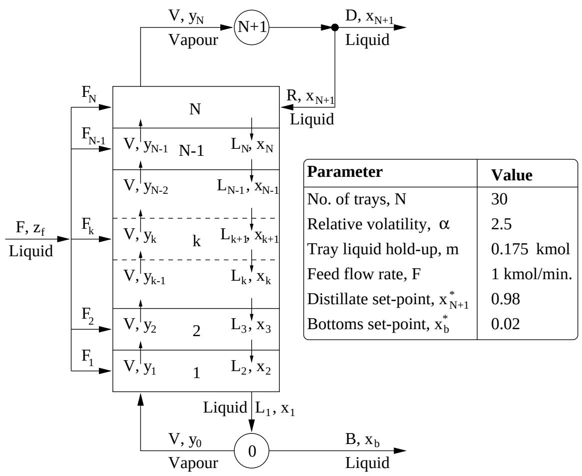

Figure 2: Illustrative example.

N° Iterations	1	2	3	4
Primal				
Feed Loc.	20	26	24	25
V (kmol/min)	1.223	1.783	1.411	1.543
R (kmol/min)	0.684	1.243	0.871	1.002
ISE	0.1991	0.1827	0.183	*0.1817*
UB	0.1991	0.1827	0.1827	*0.1817*
Master				
Feed Loc.	26	24	25	23
LB	0.158	0.1813	0.1815	0.185
Equivalent Number of Simulations		298		

Table 1: Results on illustrative MIDO example.

vapor boil-up, reflux flow rate (continuous decisions) in order to minimize the integral square error (ISE) between the bottoms and distillate compositions and their set-points. Several model assumptions are made in the model, such as: (i) constant liquid hold ups, (ii) constant relative volatility, (iii) no pressure drops, (iv) negligible vapor hold-ups. The system is initially at steady state and the dynamics are caused by a stepwise variation in the feed composition. Additionally, two constraints are necessary to be satisfied at the end of the time horizon, these being on the top and bottoms compositions ($x_d \geq 0.98, x_b \leq 0.02$). The proposed algorithm was applied in this example (Bansal, 2000) and produced the same results as Schweiger et al. (1997) that appear in Table 1.

Two more algorithms for solving MIDO problems are discribed in the Appendix. The first one also employs the GBD principles and aims at reducing even further the computational requirements of the MIDO approach whereas the other is based on Outer approximation for dealing with the binary variables and is expected to converge in less iterations between primal and master problems. However, it should be noted that those algorithms are still under development from an implementation point of view, therefore, they have not been applied to the simultaneous process and control design problem.

Process Examples

Next, two examples are presented that illustrate the characteristics of the framework for the integration for process and control design. The first one includes process and control discrete decisions and for that reason it utilizes extensively the developed MIDO approach. In the second example discrete degrees of freedom are not considered.

Distillation System—(Benzene Toluene)

Here, an example is presented for demonstrating the features of the simultaneous process and control design framework and the utilization of mixed integer dynamic optimization within this framework. This example has been solved by Bansal et al. (2000b). The system under consideration, adapted from one presented by Viswanathan and Grossmann (1999), is shown in Figure 3. A mixture of benzene and toluene is to be separated into a top product with at least 98 mol% benzene and a bottom product with no more than 5 mol% toluene. The system is subject to uncertainty in the feed flow rate and the cooling water inlet temperature (where the latter can be described dynamically by a slow sinusoid representing diurnal, ambient variations), as well as a high-frequency sinusoidal disturbance in the feed composition. The objective is to design the distillation column and its required control scheme at minimum total annualized cost (comprising capital costs of the column, internals and exchangers, and operating costs of the steam and cooling water utilities), capable of feasible operation over the whole of a given time horizon, where feasibility is defined through the satisfaction of constraints such as product quality specifications; minimum column diameter requirement due to flooding; fractional entrainment limit; temperature driving forces in the reboiler and condenser; limit on the heat flux in the reboiler; limit on the cooling water outlet temperature; above atmospheric pressure operation for the column; limits on the liquid levels in the reflux drum and reboiler; and limits on the flow rates of steam and cooling water. Solution of the problem thus requires the determination of (i) the optimal process design, in terms of the number of trays and feed location (discrete decisions), and the column diameter, condenser and reboiler surface areas (continuous decisions); and (ii) the optimal control design, in terms of the pairings of manipulated and controlled variables (discrete decisions), and the tuning parameters for the given control structure (continuous decisions).

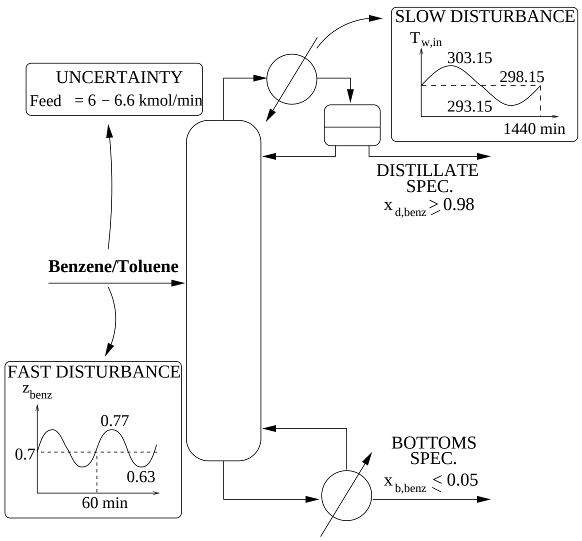

Figure 3: Distillation example.

Modeling Aspects. Due to the complexity and highly constrained nature of the problem described above, it is likely that a simplified dynamic model using "traditional" assumptions (such as constant molal overflow, relative volatility, liquid and vapor hold-ups) will be inadequate for realistically portraying the operability characteristics of the distillation system over time. A rigorous model is thus developed along similar lines to that used by Bansal et al. (2000c); however here, binary variables yf_k and yr_k are incorporated in order to account for the locations of the feed and reflux trays, respectively, where $yf_k = 1$ if all the feed enters tray k, and is zero otherwise, and $yr_k = 1$ if the reflux enters tray k, and is zero otherwise. This leads to a mixed-integer dynamic distillation model that is considerably more detailed than those that have already been reported (Mohideen et al., 1996; Schweiger and Floudas, 1997). The principal differential-algebraic equations (DAEs) for the trays are given below. A full list of nomenclature, values of the parameters, details of the DAEs for the reboiler, condenser and reflux drum, cost correlations for the objective function and inequality path constraints, can be found in Bansal (2000).

For $k = 1, ..., N$, where N is an upper bound on the number of trays required, and $i = 1, ..., NC$, where NC is the number of components:

Component molar balances:

$$\left(\sum_{k'=k}^{N} yr_{k'}\right) \cdot \frac{dM_{i,k}}{dt} = L_{k+1} \cdot x_{i,k+1} + V_{k-1} \cdot y_{i,k-1} + F_k \cdot z_{i,f} + R_k \cdot x_{i,d} - L_k \cdot x_{i,k} - V_k \cdot y_{i,k}.$$

Molar energy balances:

$$\left(\sum_{k'=k}^{N} yr_{k'}\right) \cdot \frac{dU_k}{dt} = L_{k+1} \cdot h_{k+1}^l + V_{k-1} \cdot h_{k-1}^v + F_k \cdot h_f + R_k \cdot h_d^l - L_k \cdot h_k^l - V_k \cdot h_k^v.$$

Component molar hold-ups:

$$M_{i,k} = M_k^l \cdot x_{i,k} + M_k^v \cdot y_{i,k}.$$

Molar energy hold-ups:

$$U_k = M_k^l \cdot h_k^l + M_k^v \cdot h_k^v - 0.1 \cdot P_k \cdot Vol_{tray}.$$

Volume constraints:

$$\frac{M_k^l}{\rho_k^l} + \frac{M_k^v}{\rho_k^v} = Vol_{tray}.$$

Definition of Murphree tray efficiencies:

$$y_{i,k} = y_{i,k-1} + Eff_{i,k} \cdot \left(y_{i,k}^* - y_{i,k-1}\right).$$

$$Eff_{i,k} = a_{i,k} + (1 - a_{i,k}) \cdot \sum_{k'=1}^{k} yr_{k'}.$$

Equilibrium vapor phase composition:

$$\Phi_{i,k}^v \cdot y_{i,k}^* = \Phi_{i,k}^l \cdot x_{i,k}.$$

Mole fractions normalization:

$$\sum_{i=1}^{NC} x_{i,k} = \sum_{i=1}^{NC} y_{i,k} = 1.$$

Liquid levels:

$$Level_k = \frac{M_k^l}{\rho_k^l \cdot A_{tray}}.$$

Liquid outlet flow rates:

$$L_k = 110.4 \cdot \rho_k^l \cdot Length_{weir} \cdot \left(Level_k - Height_{weir}\right)^{1.5}.$$

Pressure driving force for vapor inlet:

$$P_{k-1} - P_k = 1e - 5 \cdot \left(\sum_{k'=k}^{N} yr_{k'}\right) \cdot \left(\alpha \cdot vel_{k-1}^2 \cdot \tilde{\rho}_{k-1}^v + \beta \cdot \tilde{\rho}_k^l \cdot g \cdot Level_k\right).$$

Vapor velocities:

$$vel_{k-1} = \frac{1}{60} \cdot \left(\frac{V_{k-1}}{\rho_{k-1}^v \cdot A_{holes}}\right).$$

Fractional entrainment for 80% flooding factor:

$$ent_k = 0.224e - 02 + 2.377 \cdot exp\left(-9.394 \cdot FLV_k^{0.314}\right).$$

Sherwood flow parameter:

$$FLV_k = \frac{\tilde{L}_k}{\tilde{L}_k} \cdot \left(\frac{\tilde{\rho}_k^v}{\tilde{\rho}_k^l}\right)^{0.5}.$$

Flooding velocity:

$$vel_k^{flood} = 60 \cdot \left(\frac{\sigma_k^l}{20}\right)^{0.2} \cdot K1_k \cdot \left(\frac{\tilde{\rho}_k^l - \tilde{\rho}_k^v}{\tilde{\rho}_k^v}\right)^{0.5}.$$

Empirical coefficient:

$$K1_k = 0.0105 + 0.1496 \cdot Space^{0.755} \cdot exp\left(-1.463 FLV_k^{0.842}\right).$$

Minimum allowable column diameter and area:

$$D_{col,k}^{min} = \left(\frac{4 \cdot A_{col,k}^{min}}{\pi}\right)^{0.5}.$$
$$A_{net,k}^{min} = 0.9 \cdot A_{col,k}^{min}.$$
$$A_{net,k}^{min} = \frac{V_k}{\rho_k^v \cdot Floodfrac \cdot vel_k^{flood}}.$$

Feed and reflux flow rates to each tray:

$$F_k = F \cdot yf_k.$$
$$R_k = R \cdot yr_k.$$

Only one tray each receives feed and reflux; feed must enter below reflux:

$$\sum_{k=1}^{N} yf_k = \sum_{k=1}^{N} yr_k = 1.$$
$$yf_k - \sum_{k'=k}^{N} yr_{k'} \leq 0.$$

The complete distillation model constitutes a system of $[N(7NC+27)+15NC+56]$ DAEs in $[N(7NC+27)+15NC+64]$ variables (after specification of the feed and utilities' inlet conditions), of which $[N(NC+1)+3NC+5]$ are differential state variables. For the case study in this paper with $N=30$ and $NC=2$, there are 1316 DAEs in 1324 variables (101 states). The remaining eight variables consist of the three continuous design variables for optimization (column diameter, surface areas of the reboiler and the condenser), and the five manipulated variables (reflux, distillate, cooling water, steam and bottoms flow rates), whose values are determined by the tuning parameters of the control scheme used.

Application of the Framework.

Step 1. An initial set of two scenarios, $[6, 6.6]$, is chosen with weights $[0.75, 0.25]$. These correspond to the nominal and upper values, respectively, of the feed flow rate.

Step 2. Since the distillation column does not operate at very high purity, advanced control techniques are not required, and so multi-loop proportional-integral (PI) controllers are considered. For the purposes of this study, the control structure is considered to be a square system of measured and manipulated variables. The possible manipulated variables are: the reflux flow, R, the distillate flow, D, the cooling water flow, F_w, the steam flow, F_s and the bottoms flow, B. The set of the measured variables consists of: the distillate composition, x_d, the liquid level in the reflux drum, $Level_{drum}$, the pressure of the condenser, P_{cond} and the bottoms composition, x_b. The pairing between those variables, however, which is not known a priori, is treated as a discrete decision about the control design and is left to be determined through the optimization. One integer variable, y_k, is assigned to each possible control pairing and the modeling of the control structure selection is carrying out similarly to Narraway and Perkins (1994).

The MIDO problem (1) for this example consists of approximately 2700 DAEs and 216 inequality path constraints, with 85 binary search variables (thirty for the feed, thirty for the reflux location and twenty five for the control structure selection) and 18 continuous search variables (column diameter, surface areas of the reboiler and condenser, and gains, reset times and set-points for each of the five control loops). The problem was solved using the algorithm outlined in the section *Mixed Integer Dynamic Optimization*, with *gPROMS/gOPT* (PSE, 1999) used for solving the dynamic optimization primal problems and GAMS/CPLEX (Brooke et al., 1992) for the MILP master problems.

Step 3. In this example there are no time-invariant operating variables, and so the dynamic feasibility test, Equation 2, reduces to a conventional dynamic optimization problem with a single maximisation operator in the objective. Testing the design and control system resulting from Step 2 gives $\chi = 0$, indicating that there are no more critical scenarios, so the algorithm terminates.

Table 2 shows the iterations carried out between the Primal & the Master Problems. The economically optimal process and control design that gives feasible operation for all feed flow rates in the range 6-6.6 $kmol\ min^{-1}$ is summarized in Tables 3 and 4. Table 3 also compares the process design with the optimal steady-state, but dynamically inoperable, nominal and flexible designs. The latter was obtained through application of the analogous, steady-state algorithm to that described in §2 (Biegler et al., 1997). It can be seen that in order to accommodate feed flow rates above the nominal value of 6 $kmol\ min^{-1}$ requires more over-design when the dynamic behavior of the system is accounted for than when only steady-state effects are considered. This illustrates a weakness of considering design and control in a sequential manner.

Figures 4 and 5 show the dynamic simulations of the

Iteration Number	1	2	3	4	5
Primal Problem Solution					
Discrete decisions					
No. of Trays	25	24	23	22	24
Feed Tray	15	14	13	13	13
Control Scheme*	2	1	1	1	1
Process design					
D_{col} (m)	2.03	1.99	1.99	2.00	2.00
S_{reb} (m^2)	127.6	134.2	140.0	138.9	138.0
S_{cond} (m^2)	91.45	85.03	84.13	84.02	85.78
Controllers' gains					
$K_{\sqcup,1}$ $(x_{1,d})$	6.70	33.74	48.85	70.00	32.10
$K_{\sqcup,2}$ (L_d)	-105.0	-41.29	-18.64	-24.55	-25.39
$K_{3,3}$ $(P_c)^\dagger$	-28.00	-31.44	-29.24	-26.57	-36.16
$K_{\sqcup,4}$ $(x_{1,b})$	9.71	-2.22	-2.38	-3.37	-0.93
$K_{\sqcup,5}$ (L_0)	-1042	-600.0	-560.1	-580.5	-550.0
Reset times					
$\tau_{\sqcup,1}$	160.0	87.3	100.0	143.2	77.2
$\tau_{\sqcup,2}$	530.0	568.2	568.9	568.9	684.5
$\tau_{\sqcup,3}$	9935	3483	3615	5032	2809
$\tau_{\sqcup,4}$	2325	59.8	66.3	61.7	150.6
$\tau_{\sqcup,5}$	663.6	693.7	662.1	664.2	695.2
Set-points					
$set_{1,1}$	0.9883	0.9849	0.9843	0.9835	0.9853
$set_{1,2}$	0.5368	0.0668	0.0773	0.0746	0.0703
$set_{1,3}$	1.1944	1.2800	1.3022	1.3164	1.2694
$set_{1,4}$	0.0182	0.0223	0.0250	0.0293	0.0179
$set_{1,5}$	0.6002	0.8995	0.8994	0.8980	0.8995
Costs					
(100k\ yr^{-1}$)					
Capital	1.941	1.883	1.858	1.823	1.894
Operating(1)‡	6.367	6.268	6.287	6.334	6.269
Operating(2)§	7.220	7.122	7.136	7.194	7.097
Expected	8.521	8.364	8.357	8.372	8.370
UB	**8.521**	**8.364**	**8.357**	**8.357**	**8.357**
Master Problem Solution					
No. of Trays	24	23	22	24	22
Feed Tray	14	13	13	13	11
Control Scheme	1	1	1	1	1
LB	**8.242**	**8.282**	**8.341**	**8.355**	**8.357**
$UB - LB \leq 1e-4$	**No**	**No**	**No**	**No**	**Yes STOP**

*Control scheme 1: $R - x_{1,d}$, $D - Level_d$, $F_w - P_c$, $F_s - x_{1,b}$, $B - Level_0$.
*Control scheme 2: $R - x_{1,d}$, $D - Level_d$, $F_w - P_c$, $B - x_{1,b}$, $F_s - Level_0$.
†For $K_{3,3}$, the cooling water flow rate is scaled (0.01 F_w).
‡Nominal feed flow $F = 6 kmolmin^{-1}$.
§Feed flow upper bound $F = 6.6 kmolmin^{-1}$.

Table 2: Progress of iterations for the multi-period MIDO design and control problem.

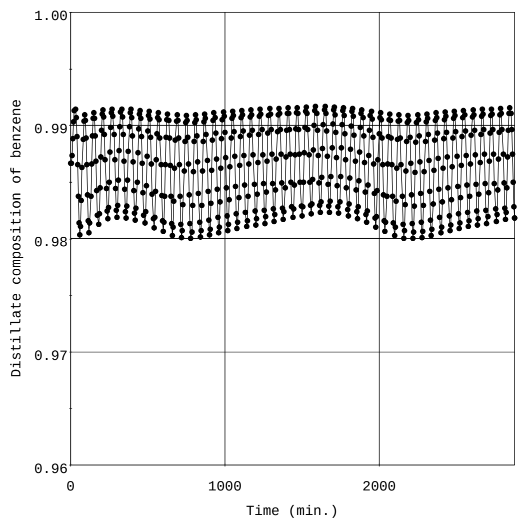

Figure 4: Controlled distillate composition at feed flow rate of 6.6 $kmol\ min^{-1}$.

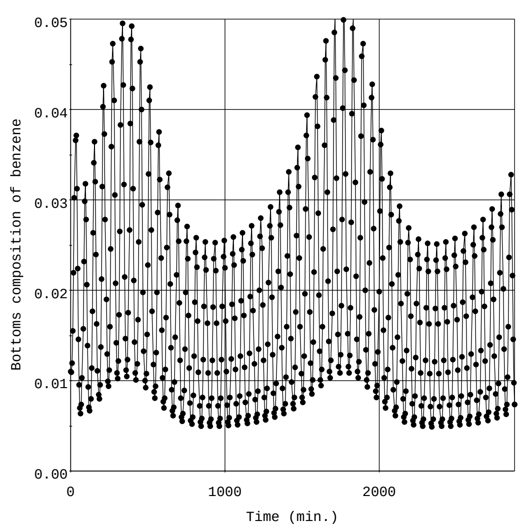

Figure 5: Controlled bottoms composition at feed flow rate of 6.6 $kmol\ min^{-1}$.

controlled compositions, that are given as part of the solution of the MIDO problem. Notice how one of the compositions, in this case the distillate, is tightly controlled relative to the other (in fact, the bottoms composition loop is open—see Table 4). This effect of controlling both compositions with one tight loop and one loose loop is due to the negative interaction of the two control loops, and is a common feature of distillation control reported in the literature (Kister, 1990).

Variable	SS nominal	SS flexible	Dynamic
No. of trays	23	23	26
Feed location	12	12	14
D_{col} (m)	1.82	1.91	1.99
S_{reb} (m^2)	113	116	134
S_{cond} (m^2)	83	83	88
Capital cost	169	175	195
Operating cost	591	607	641
Total (\$ $k\ yr^{-1}$)	760	782	836

Table 3: Steady-state *vs.* dynamically operable design.

Loop	K	τ (min)	Set-point
$R - x_d$	5.10	25.69	0.9867
$D - Level_{drum}$	-39.29	566.41	0.5187
$F_w - P_{cond}$	-44.81	7766.61	1.2183
$F_s - x_b$	0	250	0.0110
$B - Level_{reb}$	-501.93	663.96	0.8997

Table 4: Control design from simultaneous framework.

Reactive Distillation System—(Production of ethyl-acetate)

Here the problem that is considered is the production of ethyl acetate from the esterification of acetic acid and ethanol, as shown in Figure 6 (Georgiadis et al., 2000, 2001). The saturated liquid mixture is fed at a rate of 4885 mol/h in order to produce a top product with at least 0.52% ethyl acetate composition and a bottom product of no more than 0.26% ethyl acetate. Reaction takes place in all 13 trays of the column. The objective is then to design the column and the control scheme at minimum total cost, able to maintain feasible operation over a finite time horizon of interest (24 hours); subject to (i) high-frequency sinusoidal disturbances in the acetic acid inlet composition; (ii) "slow-moving" disturbance in the cooling water inlet temperature; (iii) product quality specifications; (iv) flooding, entrainment and minimum column diameter requirements; (v) thermodynamic feasibility constraints for the heat exchangers and (vi) operating pressure limits for the column.

The basis of the detailed model has been presented in our previous work (Schenk et al., 1999). The model includes details that are normally neglected, such as:

- Detailed flooding and entrainment calculations for each tray and 'subsequent' calculation of 'critical' points in the column and the minimum allowable column diameter.
- Equation for the pressure drop for each tray

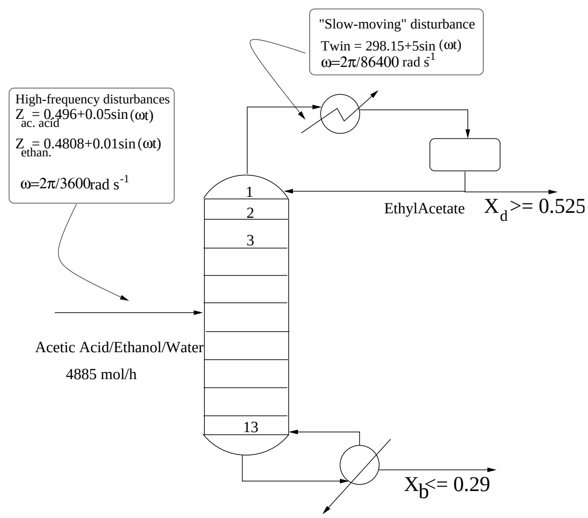

Figure 6: Schematic illustration of the reactive distillation system.

- Liquid hydraulics and liquid level on each tray and in the auxiliary units by using modified Francis weir formulae.
- The liquid-vapour equilibrium has been represented accurately using non-ideal models.

The model and its steady-state analogue have been implemented within gPROMS (PSE, 1999).

Sequential Design. A systematic sequential design and control approach is first carried out. The nominal and flexible steady-state designs are initially obtained via an optimization based approach. The nominal column design obtained is not feasible for the whole range of uncertain cooling water temperatures. The flexible design is obtained by applying a steady-state multiperiod approach that corresponds to equation (1). Three degrees of freedom (reflux ratio, steam flow rate and cooling water flow rate) can, in principle, be adjusted to offset the effects of the uncertainty. The following cases were considered (i) all three degrees of freedom allowed to vary ("best-case" design) and (ii) no degrees of freedom allowed to vary ("worst-case" design). The different optimal designs and resulting annual costs for the nominal and the two cases considered are shown in Table 5. Note that D refers to column diameter and S refers to the surface area of the heat exchange coil in the reboiler, Reb, or the condenser, Cond.

Both, the "best-case" and the "worst-case" flexible designs were dynamically tested in the presence of the sinusoidal feed composition disturbance and the "slow-moving" profile for the cooling water inlet temperature which ranges between suitable lower and upper bounds. As expected, there were a large number of constraints violations for both designs, and so they both require a

Design Variable	Nominal	Case 1	Case2
D (m)	6.09	6.09	6.12
$S_{Reb}(m^2)$	280	286	325
$S_{Cond}(m^2)$	417	458	498
Capital Cost (\$ myr^{-1})	0.45	0.46	0.47
Operating Cost (\$ myr^{-1})	3.95	3.99	4.35
Total Cost (\$ myr^{-1})	4.40	4.45	4.82

Table 5: Comparison of different designs for the reactive distillation example.

control scheme in order for feasibility to be maintained. The control structure considered here has been proven to be stable and exhibit satisfactory performance. The control loops are $(R - X_d)$, $(F_{stream} - X_b)$ and $(F_{water} - P_c)$ where R is the reflux ratio, F_{stream} is the steam flowrate and F_{water} the cooling water flowrate. Finally, x_d and x_b are the distillate and bottom compositions and the pressure in the condenser. The dynamic equations of the PI controllers are properly incorporated into the model. No set of controller's tuning parameters (gains, reset times, set-points and biases) could be found for either design that would enable all the system constraints to be satisfied over the entire time horizon. In particular the "best-case" design produced large constraint violations whereas the "worst-case" design exhibit the major operability bottleneck in the minimum column diameter requirements that are related to flooding. Then only the minimum column diameter was modified accordingly and a new steady-state flexible design was obtained.

The next step in the sequential design approach is to identify the optimal tuning of the controller's gains, reset times, set-points and biases keeping the modified "worse case" design fixed and optimizing the total annualized cost of the system over a fixed time-horizon. The operating variables obtained with that procedure along with the process design variables calculated in the previous step, i.e. column diameter, heat exchange areas comprise the results of the sequential design depicted in Table 6.

Simultaneous Process and Control Design. The sequential strategy outlined above has illustrated that interactions do exist between process design and process control. However, a more systematic approach for exploiting these interactions is to also include the process design variables as optimization variables whilst optimizing the controller settings. The framework presented in §2 is adopted. However, all the features of the general approach were not exploited fully, i.e. the design and control structural decisions remained fixed. The optimization variables are the design variables (column diameter and heat exchanger areas) and the gains, reset time, set points and biases of the controllers. The prob-

Quantity	Sequential	Simultaneous
D (m)	6.3	6.37
$S_{Reboiler}$ (m^2)	325	315
$S_{Condenser}$ (m^2)	498	425
PI1 Controller (top compositions control)		
Gain	747	181
Reset Time	1	0.59
Set-Point	0.54	0.527
PI2 Controller (bottom compositions control)		
Gain	1959	4573
Reset Time	12000	7294
Set Point	0.1	0.22
PI3 Controller (Condenser pressure control)		
Gain	-9500	-10400
Reset Time	0.603	1.32
Set-Point	1.023	1.023
Capital Cost ($ Million)	0.48	0.48
Operating Cost ($ Million)	4.37	4.17
Total Cost ($ Million)	4.85	4.63

Table 6: Results on the reactive distillation example.

lem is again solved as a large scale dynamic optimization problem with 12 optimization variables and a number of path and end-point inequality constraints describing the feasible operation of the process.

The optimal design, controller tuning parameters and associated costs are shown in Table 6 and compared with the results obtained using the sequential strategy with optimally tuned controllers. The simultaneous strategy has the same capital costs and lower operating costs leading to a 5% total annual cost savings ($220,000 per year). It is interesting to note that the simultaneous approach is able to give a fully operational system with an annual cost in between the costs of the "best-case" and "worst case" while the sequential approach gives a system which is more expensive than the "worst-case" optimal flexible design. This clearly demonstrates how a simultaneous approach can exploit the interactions between design and control to give process designs that are cheaper and more easily controlled than those found by even state-of the-art sequential approaches. It is also interesting to observe the different control settings adopted by the two approaches. As can be seen from Table 6 the simultaneous approach gives tighter bottom product composition that is closer to the constraint boundary; also tighter top product control and almost identical pressure control. The economic impact of this control action is the reduction in the operating costs.

Conclusions

This paper demonstrates the progress that has been made in simultaneous process and control design under uncertainty. A well-established decomposition framework for that purpose is reviewed. This framework in its general form requires the repetitive solution of mixed integer dynamic optimization problems. An algorithm for MIDO that has been recently developed by our group for that purpose is outlined.

Two process examples are considered that demonstrate the applicability and the benefits of the developed methods in the context of the integration of process design, process control and process operability. The first example considers the separation of a binary mixture and utilizes the novel MIDO algorithm for treating control, design and discrete structural decisions. The second example studies the process and control design of a reactive distillation system and does not take into account discrete decisions.

Future work will mainly focus on improving the convergence properties of the current MIDO methodologies and developing a more efficient single-stage approach for dealing with the inevitable presence of the uncertainty as opposed to the current decomposition (two-stage) approach. Also other control technology will be considered, such as multivariable PI controllers (Kookos and Perkins, 2000), as opposed to decentralized PI controllers that are almost exclusively used so far and in addition, an effort will be made to address synthesis issues that have not been fully considered within a mixed integer dynamic optimization framework.

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References

Allgor, R. J. and P. I. Barton, "Mixed—integer dynamic optimization I: problem formulation," *Comput. Chem. Eng.*, **23**, 567–584 (1999).

Androulakis, I. P., "Kinetic Mechanism Reduction Based on an Integer Programming Approach.," *AIChE J.*, **46**(2), 361–371 (2000).

Avraam, M. P., N. Shah, and C. C. Pantelides, "A Decomposition Algorithm for the Optimisation of Hybrid Dynamic Processes," *Comput. Chem. Eng.*, pages Suppl. S451–S454 (1999).

Bahri, P. A., J. A. Bandoni, and J. A. Romagnoli, "Integrated Flexibility and Controllability Analysis in Design of Chemical

Processes," *AIChE J.*, **43**(4), 997–1015 (1997).

Bansal, V., R. Ross, J. D. Perkins, and E. N. Pistikopoulos, "The interactions of design and control: double-effect distillation systems," *J. Proc. Cont.*, **10**, 219–227 (2000c).

Bansal, V., J. D. Perkins, and E. N. Pistikopoulos, "Parametric Programming Algorithms for the Flexibility Analysis and Design of Linear Process Systems," *AIChE J.*, **46**(2), 335–354 (2000a).

Bansal, V., J. D. Perkins, E. N. Pistikopoulos, R. Ross, and J. M. G. van Schijndel, "Simultaneous Design and Control Optimization under uncertainty," *Comput. Chem. Eng.*, **24**(2-7), 261–266 (2000b).

Bansal, V., *Analysis, Design and Control Optimization of Process Systems under Uncertainty*, PhD thesis, Imperial College, University of London (2000).

Barton, P. I., R. J. Allgor, W. F. Feehery, and S. Galan, "Dynamic Optimization in a Discontinuous World," *Ind. Eng. Chem. Res.*, **37**(3), 966–981 (1998).

Barton, P. I., J. R. Banga, and S. Galan, "Optimization of hybrid discrete/continuous systems," *Comput. Chem. Eng.*, **24**(9-10), 2171–2182 (2000).

Bazaraa, M. S., H. D. Sherali, and C. M. Shetty, *Nonlinear Programming. Theory and Applications*. Wiley, New York (1993).

Biegler, L. T., I. E. Grossmann, and A. W. Westerberg, *Systematic Methods of Chemical Process Design*. Prentice Hall (1997).

Brooke, A., D. Kendrick, and A. Meeraus, *GAMS Release 2.25: A User's Guide*. San Francisco: The Scientific Press (1992).

Bryson, A. E. and Y. Ho, *Applied Optimal Control*. Taylor & Francis, New York (1975).

Dimitriadis, V. D. and E. N. Pistikopoulos, "Flexibility analysis of dynamic systems," *Ind. Eng. Chem. Res.*, **34**, 4451–4462 (1995).

Duran, M. A. and I. E. Grossmann, "An outer approximation algorithm for a class of mixed integer nonlinear programs," *Math. Prog.*, **36**(3), 307–339 (1986).

Floudas, C. A., *Nonlinear and Mixed-Integer Optimization*. New York: Oxford University Press (1995).

Geoffrion, A. M., "Generalized Benders decomposition," *J. Optim. Theo. Appl.*, **10**, 237–260 (1972).

Georgiadis, M. C., R. Gani, and E. N. Pistikopoulos, A Synthesis Method for Hybrid Separation, Technical report, European Commission, Research Contract No: JOE3-CT97-0085 (2000).

Georgiadis, M. C., M. Schenk, R. Gani, and E. N. Pistikopoulos, "The Interactions of Design, Control and Operability in Reactive Distillation Systems," *Proc. of ESCAPE-11*, pages 997–1002 (2001). Denmark May 2001.

Grossmann, I. E. and C. A. Floudas, "Active constraint strategy for flexibility analysis in chemical processes," *Comput. Chem. Eng.*, **11**, 675–693 (1987).

Kister, H. Z., *Distillation Operation*. New York: McGraw-Hill (1990).

Kookos, I. K. and J. D. Perkins, An algorithm for simultaneous process design and control (2000). Submitted for publication to the Ind. Eng. Chem. Res.

Mohideen, M. J., J. D. Perkins, and E. N. Pistikopoulos, "Optimal design of dynamic systems under uncertainty," *AIChE J.*, **42**, 2251–2272 (1996).

Mohideen, M. J., J. D. Perkins, and E. N. Pistikopoulos, "Towards an efficient numerical procedure for mixed integer optimal control," *Comput. Chem. Eng.*, **21**, S457–S462 (1997).

Mohideen, J. M., *Optimal design of Dynamic Systems under Uncertainty*, PhD Dissertation, Imperial College of Science, Technology and Medicine, London (1996).

Narraway, L. and J. D. Perkins, "Selection of Process control Structure based on economics," *Comput. Chem. Eng.*, **18**, Suppl. S511–S515 (1994).

Pistikopoulos, E. N. and I. E. Grossmann, "Optimal Retrofit Design for Improving Process Flexibility in Linear Systems," *Comput. Chem. Eng.*, **12**(7), 719–731 (1988).

PSE, *gPROMS Advanced User's Guide*. Process Systems Enterprise Ltd., London (1999).

Ross, R., V. Bansal, J. D. Perkins, and E. N. Pistikopoulos, A Mixed-Integer Dynamic Optimization Approach to Simultaneous Design and Control, In *AIChE Annual Meeting*, Paper 220e, Miami Beach Florida, US. American Institute of Chemical Engineering (1998).

Ross, R., V. Bansal, J. D. Perkins, E. N. Pistikopoulos, G. L. M. Koot, and J. M. G. Schijndel, "Optimal design and control of an industrial distillation system," *Comput. Chem. Eng.*, **23**, S875–S878 (1999).

Sakizlis, V., V. Bansal, R. Ross, J. D. Perkins, and E. N. Pistikopoulos, "New Algorithms for Mixed-Integer Dynamic Optimization," *Proc. of ESCAPE-11*, pages 273–278 (2001). Denmark May 2001.

Samsatli, N. J., L. G. Papageorgiou, and N. Shah, "Robustness Metrics for Dynamic Optimization Models under Parameter Uncertainty," *AIChE J.*, **44**(9), 1993–2006 (1998).

Sargent, R. W. H. and G. R. Sullivan, Development of an Efficient Optimal Control Package, In *Proc. 8th IFIP conf. optimization techniques*, Wurzuburg. IFIP (1977).

Schenk, M., R. Gani, D. Bogle, and E. N. Pistikopoulos, "A hybrid modelling approach for separation systems involving distillation," *Chem. Eng. Res. Des.*, **77**(A6), 519–534 (1999).

Schweiger, C. A. and C. A. Floudas, Interaction of design and control: optimization with dynamic models, In Hager, W. W. and P. M. Pardalos, editors, *Optimal Control: Theory, Algorithms and Applications*, pages 388–435. Kluwer (1997).

Schweiger, C. A., A. Rojnuckarin, and C. A. Floudas, *MINOPT: User's Guide*. Princeton University, software version 2.0 edition (1997).

Sharif, M., N. Shah, and C. C. Pantelides, "On the Design of Multicomponent Batch Distillation Columns," *Comput. Chem. Eng.*, **22**, Suppl. S69–S76 (1998).

Swartz, C. L. E., J. D. Perkins, and E. N. Pistikopoulos, Incorporation of Controllability in Process Design Through Controller Parameterization, In *Process Control and Instrumentation 2000*, pages 49–54. University of Strathclyde (2000).

Van Schijndel, J. M. G. and E. N. Pistikopoulos, Towards the Integration of Process Design, Process Control & Process Operability—Current Status & Future Trends, In Malone, M. F., J. A. Trainham, and B. Carnahan, editors, *Foundations of Computer-Aided Process Design*, volume 96, pages 99–112, Breckenridge, Colorado. American Institute of Chemical Engineers (2000).

Vassiliadis, V. S., R. W. H. Sargent, and C. C. Pantelides, "Solution of a class of multistage dynamic optimization problems. 1. Problems without path constraints.," *Ind. Eng. Chem. Res.*, **33**(9), 2111–2122 (1994).

Vassiliadis, V., *Computational Solution of Dynamic Optimization Problems with General Differential—Algebraic Constraints*, PhD Dissertation, Imperial College of Science, Technology and Medicine, London (1993).

Viswanathan, J. and I. E. Grossmann, "A Compined penalty function and Outer Approximation method for MINLP Optimization," *Computers and Chemical Engineering*, **14**(7), 769–780 (1999).

Appendix

Adjoint Based Algorithm on Mixed Integer Dynamic Optimization

From the discussion on mixed integer dynamic optimization the conclusion drawn is that an efficient adaptation of Generalized Benders Decomposition in MIDO requires the simplification of the master problem construction and the reduction or possible elimination of the dual information calculations. An algorithm for achieving that is presented in the main document and here an alternative approach is outlined aiming at reducing the computational requirements of the linked subproblems. The details of this approach can be found in Sakizlis et al. (2001).

According to the original GBD-approach in MIDO (Schweiger and Floudas, 1997; Mohideen et al., 1997) after the solution of the primal optimal control problem an additional subproblem has to be solved that involves the backwards integration of the so-called adjoint DAE system, Equation 4. Since this can be computationally expensive, a method is developed for eliminating the extra calculations by adapting an adjoint-based approach for evaluating the gradients of the constraints and the objective function of the primal optimal control problem. This provides at the optimal solution of the primal a set of vectors of adjoint variables that are associated with the constraints and the objective function, denoted as $[\lambda_\phi(t)\ p_\phi(t)]$, $[\lambda_q(t)\ p_q(t)]$ respectively. Those adjoint functions are given by the same linear DAE system as the adjoint functions that are necessary for the master problem construction. However, $[\lambda_\phi(t)\ p_\phi(t)]$, $[\lambda_q(t)\ p_q(t)]$ are given by different final conditions as opposed to $[\lambda(t), p(t)]$. Their final conditions are:

$$[\frac{\partial f}{\partial \dot{x}}]^T_{t_f} \cdot \lambda_\phi(t_f) = -[(\frac{\partial \phi}{\partial x})^T_f + [(\frac{\partial f}{\partial x})^T\ (\frac{\partial c}{\partial x})^T]_f \cdot (\omega_f)_\phi]$$
$$[\frac{\partial f}{\partial \dot{x}}]^T_{t_f} \cdot \lambda_q(t_f) = -[(\frac{\partial q}{\partial x})^T_f + [(\frac{\partial f}{\partial x})^T\ (\frac{\partial c}{\partial x})^T]_f \cdot (\omega_f)_q]$$

The linear properties of the adjoint differential system and its boundary conditions, enable the evaluation of the adjoint variables required for the master problem $[\lambda, p]$ as a function of $[\lambda_\phi\ p_\phi]$, $[\lambda_q\ p_q]$ from the equation:

$$\begin{bmatrix} \lambda(t) \\ p(t) \end{bmatrix} = \begin{bmatrix} \lambda_\phi(t) \\ p_\phi(t) \end{bmatrix} + \mu^T \cdot \begin{bmatrix} \lambda_q(t) \\ p_q(t) \end{bmatrix} \tag{9}$$

Equation 9 can be proved using the transition matrix theory. Using that approach, the rigorous adjoint integration for the master problem derivation is not required any more after the primal has terminated and the derivation of the dual information is reduced exclusively to Equation 9.

Even if the easily obtained time-dependent functions $\lambda(t), p(t)$ are supplied to the master problem many calculations are still required due to the presence of the time integral in Equation 5 and the usually complicated non-linear functions involved in the DAE system. In order to simplify further the master problem equations f,c are decomposed in terms of the binary and continuous variables:

$$\begin{aligned} f &= f'(\dot{x}, x, z, v, t) + f^y(\dot{x}, x, z, v, t) \cdot y \\ c &= c'(x, z, v, t) + c^y(x, z, v, t) \cdot y \\ r &= r'(\dot{x}_o, x_o, z_o, v, t_o) + r^y(\dot{x}_o, x_o, z_o, v, t_o) \cdot y \end{aligned} \tag{10}$$

f^y, c^y, r^y are a matrices of dimensions $n_x \times n_y$, $n_z \times n_y$, $n_x \times n_y$ respectively. This separation is allowed, since the binaries participate in the DAE in a linear form (variant-2 of GBD). At the primal solution though:

$$f = 0 \;\; c = 0 \;\; r = 0 \tag{11}$$

So, $(f')^k$ can be written as:

$$(f')^k = -(f^y)^k \cdot y^k \tag{12}$$

Similarly for c', c^y, r', r^y. Finally we have:

$$\begin{aligned} f &= (f^y)^k \cdot (y - y^k) \\ c &= (c^y)^k \cdot (y - y^k) \\ r &= (r^y)^k \cdot (y - y^k) \end{aligned} \tag{13}$$

Once Equation 13 is substituted in Equation 5 the modified master problem becomes:

$$\min_{y,\eta} \ \eta \tag{14}$$

subject to

$$\begin{aligned} \eta \geq \phi + (\mu^k)^T \cdot q + \{(\omega_f^k)^T \cdot \begin{bmatrix} (f^y)^k \\ (c^y)^k \end{bmatrix}_f \\ + (\omega_0^k)^T \begin{bmatrix} (f^y)^k \\ (c^y)^k \end{bmatrix}_o + (\rho^k)^T \cdot (r^y)^k \\ + \int_{t_o}^{t_f} [(\lambda^k)^T\ (p^k)^T] \cdot \begin{bmatrix} (f^y)^k \\ (c^y)^k \end{bmatrix}_t dt\} \cdot (y - y^k) \end{aligned}$$

In this manner, the size of the master problem formulation is significantly reduced. The multiplier of the binary terms $y - y^k$ corresponds to a time dependent vector of size equal to the dimensions of the binaries n_y. This vector does not contain any integer terms and hence, it remains fixed throughout the master problem solution. In order to evaluate the components of that vector it suffices to transform the contained integrals to an ODE system of size n_y introducing differential states of zero initial conditions. Then by solving numerically the ODE system the construction of the master problem is completed. Alternatively, if the formulation of Equation 5 was retained, every equation that contains a binary term would have to be integrated. So the size of that corresponding ODE system would be of order of magnitude $O(n_x + n_z) >> n_y$.

From an implementation point of view, Equation 14 is easier to construct than Equation 5 because the matrices f^y, c^y, r^y are the Jacobians of the DAE with respect to the binaries and are simply generated (numerically or analytically) using well-established commercial codes or algorithms.

The master optimization problem consists of the binary variables and the continuous objective. The other variables are fixed. Since the optimization variables participate in a linear form, the problem is an MILP and it is solved with the current well-established methodologies (e.g. branch and bound algorithm).

The steps of the algorithm are summarized as follows:

1. Fix the values of the binary variables, $y = y^k$, and solve a standard dynamic optimization problem (k^{th} primal problem). An upper bound, UB, on the solution to the MIDO problem is obtained from the minimum of all the primal solutions obtained so far.
2. At the solution of the primal problem, using Equation 9, obtain the adjoint functions $\lambda(t), p(t)$.
3. Use the problem variables $x(t), z(t), v$, the adjoint functions $\lambda(t), p(t)$ and the Lagrange multipliers of the constraints μ to construct the k^{th} relaxed master problem, Equation 14, from the k^{th} primal solution. The Master problem corresponds to a Mixed -integer linear program (MILP), that its solution provides the lower bound, LB, on the MIDO solution. If UB-LB is less than a specified tolerance ϵ, or the master problem is infeasible, the algorithm terminates and the solution to the MIDO problem is given by UB. Otherwise, set $k = k + 1$ and y^{k+1} equal to the integer solution of the master problem and return to step 1.

This alternative algorithm eliminates completely the adjoint evaluation and does not require any resolve session after the primal problem is solved. It also manages to simplify considerably the master problem construction. Moreover, descpite the fact that it is restricted to using only an adjoint based gradient evaluation procedure for the primal optimal control problem it is not confined to a particular type of DAE integrator as in Mohideen et al. (1997); Ross et al. (1998).

An Outer Approximation Based Method for Mixed Integer Dynamic Optimization

The algorithms presented on Mixed Integer dynamic optimization are based on Generalized Benders decomposition for obtaining the lower bound to the problem. Therefore, the results that they will produce will be equivalent. Despite the benefits of GBD, that among others are the simple modeling of the discrete decisions and the straight forward formulation of the master problem, the lower bounds that are generated are relatively relaxed since in every master problem, only a single constraint is added to the iterative procedure. This can increase the number of the subsequent problem solutions deteriorating the convergence properties. A desired reduction in the primal-master iterations can be achieved by adapting another decomposition approach for constructing the master problem based on Outer Approximation (Duran and Grossmann, 1986). An outline of the concepts that enable the application of OA to MIDO is presented here.

The application of OA to an MINLP problem requires the participation of the integer variables in the equalities, inequalities and objective in a linear and separable form. The translation of this condition to MIDO makes imperative the removal of the binary variables from the DAE system. The reason being that even if the binaries participate linearly in the DAE their implicit contribution to the objective and the constraints is non-linear due to the non-linearities introduced by the dynamics. The removal of the binaries from the dynamic system is done in a way similar to the one presented in the main document. Namely, an extra set of continuous search variables y_d is introduced in the primal problem, that are fixed according to the double inequality constraint: $y_d - y^k \geq 0, y_d - y^k \leq 0$. This gives rise to the following primal optimal control problem:

$$\min_{v, y_d} \ \phi(\dot{x}(t_f), x(t_f), z(t_f), v, y_d, t_f) \tag{15}$$

subject to

$$\begin{aligned}
0 &= f(\dot{x}(t), x(t), z(t), v, y_d, t) \\
0 &= c(x(t), z(t), v, y_d, t) \\
0 &= r(x(t_0), \dot{x}(t_0), z(t_0), v, y_d, t_0) \\
0 &\geq q(\dot{x}(t_f), x(t_f), z(t_f), v, y_d, t_f) \\
0 &\leq y_d - y^k \\
0 &\geq y_d - y^k \\
& t_o \leq t \leq t_f
\end{aligned}$$

The master problem that aims to generate a lower bound, is constructed by linearizing the constraints and the objective around the primal optimal point only in the space of the search variables (v, y_d). The resultant master problem is:

$$\min_{y, y_d, v, \eta} \ \eta \tag{16}$$

subject to

$$\begin{aligned}
\eta &\geq \phi(\dot{x}^k(t_f), x^k(t_f), z^k(t_f), v^k, y_d^k, t_f) \\
&\qquad + \frac{d\phi}{dv} \cdot (v - v^k) + \frac{d\phi}{dy_d} \cdot (y_d - y_d^k) \\
0 &\geq q(\dot{x}^k(t_f), x^k(t_f), z^k(t_f), v^k, y_d^k, t_f) \\
&\qquad + \frac{dq}{dv} \cdot (v - v^k) + \frac{dq}{dy_d} \cdot (y_d - y_d^k) \\
0 &\leq y_d - y \\
0 &\geq y_d - y
\end{aligned}$$

In this master formulation in every k^{th} iteration a set of inequality constraints equal to the number of the original constraints plus one is added. Therefore, if the number of constraints is relatively high the lower bounds generated by OA will be tighter than the ones produced from GBD, hence the algorithm convergence will be achieved in less iterations.

A summary of the steps of the OA algorithm are presented below:

1. Fix the values of the binary variables, $y = y^k$, and solve a standard dynamic optimization problem (k^{th} primal problem). An upper bound, UB, on the solution to the MIDO problem is obtained from the minimum of all the primal solutions obtained so far.
2. At the solution of the primal problem add the extra set of continuous search variables y_d and the inequality constraints: $y_d - y^k \geq 0$,$y_d - y^k \leq 0$. Resolve the primal problem at the optimal solution. Convergence is achieved in one iteration and the gradients: $\frac{d\phi}{dy_d}$,$\frac{d\phi}{dy_d}$,$\frac{dq}{dv}$ and $\frac{dq}{dy_d}$ are evaluated via numerical integration of the sensitivity (Vassiliadis et al., 1994) or the adjoint DAE system (Sargent and Sullivan, 1977).
3. Use the problem continuous optimization variables and the corresponding gradients for formulating the master problem, Equation 16. The Master problem corresponds to a Mixed -integer linear program (MILP), that its solution provides the lower bound, LB, on the MIDO solution. If UB-LB is less than a specified tolerance ϵ, or the master problem is infeasible, the algorithm terminates and the solution to the MIDO problem is given by UB. Otherwise, set $k = k + 1$ and y^{k+1} equal to the integer solution of the master problem and return to step 1.

This presented algorithm for MIDO has the potential of providing tighter (higher) lower bounds to the overall problem thus accelerating the MIDO solution convergence.