# Simultaneous Process Design and Process Control: Application to Complex Separation Systems

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**Abstract**

The design and control of a literature-based double-effect and an industrial azeotropic distillation system are considered. Rigorous dynamic modelling is used to capture the key operability characteristics of each process. The economic and operational benefits of considering the process design and process control tasks simultaneously are explored with the aid of advanced dynamic optimization techniques. The inclusion of structural decisions into the optimization is a very challenging area of research. In this regard, algorithmic developments are presented which show potential for the efficient solution of the resulting large-scale mixed-integer dynamic optimization problems.

*Keywords*: Dynamic modelling, Design, Process control, Dynamic Optimization

## 1 Introduction

During the past two decades, there has been a growing awareness amongst academia and industrial practitioners that operability issues need to be considered explicitly at an early phase of process design. Mathematical frameworks have been developed for incorporating steady-state flexibility requirements into process design (see Grossmann and Straub, 1991, for a review), as well as for the identification and treatment of factors limiting dynamic operability (Morari and Perkins, 1994).

In recent years, new algorithms have been developed which utilise state-of-the-art dynamic optimization methods to enable the solution of realistic process engineering problems (see, for example, Walsh and Perkins, 1996 and Mohideen *et al.*, 1996a). The objective of this paper is to demonstrate the economic and operability benefits that can be obtained by using such advanced techniques. Two design and control studies are presented, namely:

- a double-effect distillation system
- a high-purity industrial distillation system

Both studies involve the solution of very large-scale dynamic optimization problems due to the rigorous modelling required to capture the operability characteristics of these complex systems.

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In each study only the continuous variables relating to the process and control design are optimized. The inclusion of structural (integer) decisions leads to very challenging mixed-integer dynamic optimization (MIDO) problems. The final part of the paper describes theoretical and algorithmic developments which show potential for the efficient solution of such large-scale MIDO problems.

# 2 Study 1: Double-Effect Distillation

## 2.1 Background and process description

Double-effect distillation systems, where the overhead vapour from one column is used to supply the reboiler heat for another column operating at a lower pressure, have the potential to greatly reduce utility costs. However, they are not extensively used in industry since it is perceived that the operation of a double-effect system will always be more difficult and will pose higher requirements on the quality of the design and control system than for a single column.

We consider the separation of an equimolar mixture of methanol and water into purer components (see Fig. 1). The saturated liquid mixture, at 330 $K$, is fed at a rate of 750 $mol/s$ in order to produce a top product with at least 96% methanol and a bottom product with no more than 4% methanol. The objective is to design the columns and control scheme at minimum total annualised cost (capital costs plus operating costs), able to maintain feasible operation over a finite time horizon of interest, subject to: (i) parametric uncertainty in the inlet temperature of the cooling water to the low-pressure column (LPC) condenser; (ii) a sinusoidal disturbance in the feed composition; (iii) the product quality specifications; (iv) flooding and minimum column diameter requirements; (v) entrainment limits; (vi) thermodynamic feasibility constraints for the heat exchangers; and (vii) operating pressure limits for the columns.

In this study a split-feed double-effect configuration is used (Fig. 1) with a fixed process structure based on that from Chiang and Luyben (1988). The control structure is also fixed using the optimal structure found by Mohideen *et al.* (1996b) with an additional pressure control loop. Two state-of-the-art optimization strategies are employed. In the first, the design and control tasks are considered sequentially, while in the second, design and control are optimized simultaneously and the potential synergistic benefits of such an approach investigated. In both cases, multi-loop proportional-integral (PI) controllers are used in order to challenge the perception that advanced control strategies are necessary for the successful operation of double-effect distillation systems (Seborg *et al.*, 1989; Han and Park, 1996).

## 2.2 Dynamic Model

A rigorous, multi-component dynamic model has been developed within the *g*eneral *PRO*cess *M*odelling *S*ystem or *gPROMS* (Process Systems Enterprise, 1998a) to describe the design and operation of distillation systems. This model is independent of the process and control structure, and different alternatives can be readily constructed by changing the inter-connections between

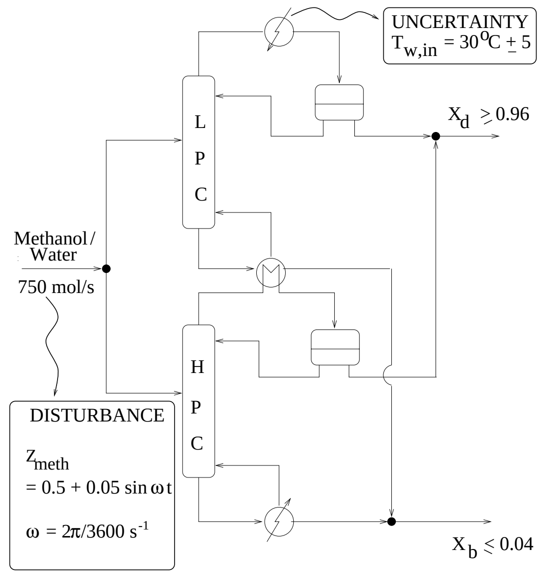


Figure 1: Double-effect distillation example

relevant units.

The model relaxes many of the assumptions used in double-effect distillation studies in the literature and has the following key features (Bansal *et al.*, 1999):

- dynamic material and energy balances for every tray, reboiler, condenser and all auxillary units;
- the consideration of both liquid and vapour, mass and energy hold-ups within the balances;
- the accurate representation of the vapour-liquid equilibria using non-ideal physical properties models (*e.g.* Wilson models for activity coefficients);
- the use of Murphree tray efficiencies;
- the consideration of liquid hydraulics and level on each tray;
- equations for determining the pressure drop from tray to tray; and
- detailed flooding and entrainment calculations for each tray and subsequent evaluation of "critical" points in the columns and the minimum allowable column diameters.

## 2.3 Sequential Design and Control

A sophisticated sequential approach for design and control is outlined schematically in Fig. 2. The step-by-step results obtained using this strategy are reported in Bansal *et al.* (1999).

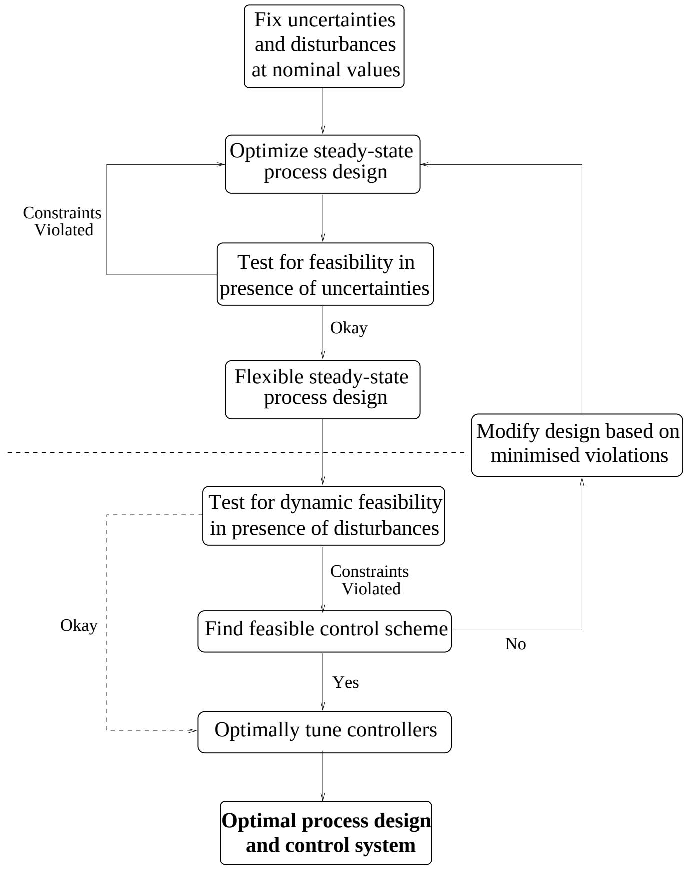


Figure 2: Outline of sequential design and control strategy

Note that the final stage of the sequential approach involves the optimal tuning of the controllers' gains, reset times, set-points and biases. This may be done, for example, using either an economic objective or one which provides a measure of control quality (e.g. a normalised ISE). Note also that a pareto-optimal curve of cost *vs.* ISE could be drawn up by solving the economic problem with an extra inequality constraint to bound the value of the ISE.

In either case, the resulting dynamic optimization problems are large-scale and involve approximately 4000 differential-algebraic model equations (180 differentiable states) and 20 inequality path constraints to enforce process feasibility. The problems were solved using the *gOPT* dynamic optimization interface (Process Systems Enterprise Ltd., 1998b) for *gPROMS*.

The ISEs and total annualised costs for the two extreme points of the pareto-optimal curve are shown in Table 1. Given the very high price one has to pay in order to minimise the ISE ($150,000 per year in utility costs), and the fact that all the process feasibility constraints are enforced in both cases, it is logical to use the economically tuned control scheme.

| Quantity | min ISE | min Cost |
|---|---|---|
| ISE | 21 | 100 |
| Total Cost ($m/yr) | 3.66 | 3.51 |

Table 1: Comparison of results obtained by tuning controllers on a quality of control basis and an economic basis.

### 2.4 Simultaneous Design and Control Strategy

Fig. 3 illustrates the steps of a general mathematical framework for simultaneous design and control proposed by Mohideen *et al.* (1996a). For the example in this paper, with a fixed uncertainty profile (see Fig. 4), the approach reduces to a single step after initialisation.

Here, the expected total annual cost of the system is minimised subject to the differential-algebraic process model; the PI-control scheme equations; the disturbance profile; the uncertainty profile; and the inequality feasibility constraints. The optimization variables are all the design variables (column diameters and heat exchanger areas), and the gains, reset times, set points and biases of the controllers. The problem is solved as a large-scale, dynamic optimization problem involving approximately 4000 variables (180 differentiable state variables), 20 optimization variables and 20 inequality path constraints describing feasible operation of the process.

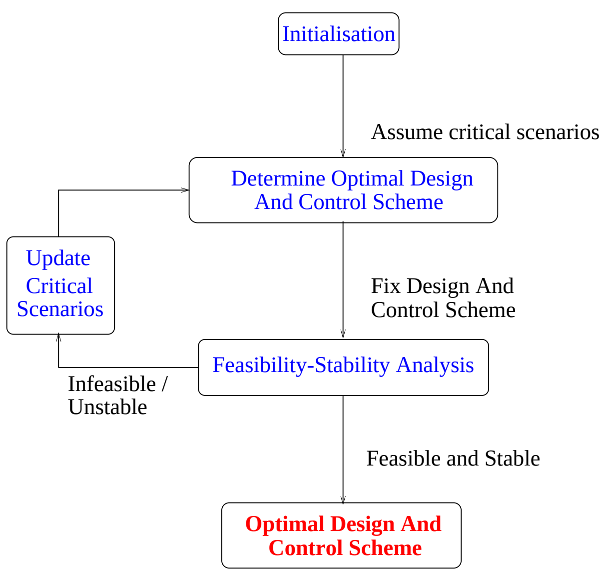


Figure 3: Outline of simultaneous design and control strategy

The optimal design, controller tuning parameters and associated costs are shown in Table 2 and are compared with the results obtained using the sequential strategy with economically tuned controllers. The double-effect system resulting from the simultaneous strategy has lower capital costs and lower operating costs, leading to a total annual cost saving of about $100,000 per year.

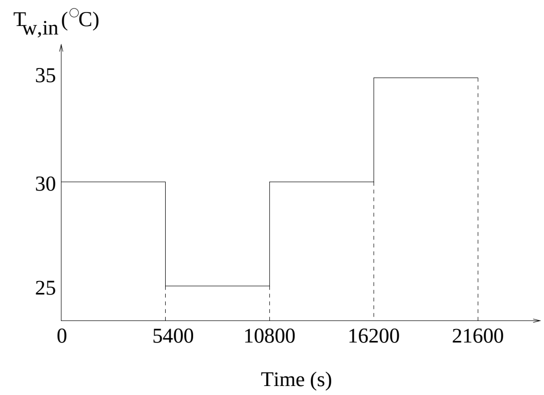


Figure 4: Profile of the uncertain cooling water temperature

| Quantity | Sequential | Simultaneous |
|---|---|---|
| $D_{HPC}$ $(m)$ | 2.27 | 2.27 |
| $D_{LPC}$ $(m)$ | 3.00 | 3.00 |
| $S_{HPCReb}$ $(m^2)$ | 470 | 410 |
| $S_{LPCCond}$ $(m^2)$ | 279 | 291 |
| $S_{Exch}$ $(m^2)$ | 956 | 942 |
| Gain, PI1 | -204 | -400 |
| Reset Time, PI1 | 6357 | 6369 |
| Set-Point, PI1 | 0.037 | 0.038 |
| Gain, PI2 | -2250 | -1103 |
| Reset Time, PI2 | 3577 | 5000 |
| Set-Point, PI2 | 1.11 | 1.09 |
| Gain, PI3 | 406 | 408 |
| Reset Time, PI3 | 649 | 738 |
| Set-Point, PI3 | 0.960 | 0.960 |
| **ISE** | **100** | **85** |
| **Capital Cost** | **0.74** | **0.72** |
| **Operating Cost** | **2.77** | **2.70** |
| **Total Cost** | **3.51** | **3.42** |

Table 2: Comparison of process designs and controller tuning parameters resulting from sequential and simultaneous strategies.

It is interesting to observe that the ISE for the simultaneously obtained system is 15% less than that of the sequentially obtained system. This demonstrates how in this case a simultaneous approach exploits the interactions between design and control to give a process design which is cheaper *and* more satisfactorily controlled than that found by a state-of-the-art sequential approach.

The economic benefits from using a simultaneous approach are likely to increase when more dramatic uncertainty and disturbance scenarios are considered and when the process and control structural issues are taken into consideration within the optimization framework.

# 3 Study 2: Industrial Distillation System

## 3.1 Background and project objectives

The system under consideration is shown in Fig. 5. A ternary feed of iso-propanol (IPA), water and normal propanol (NPA) is to be separated, with the desired product being the IPA/water azeotrope which is drawn off near the top of column I.

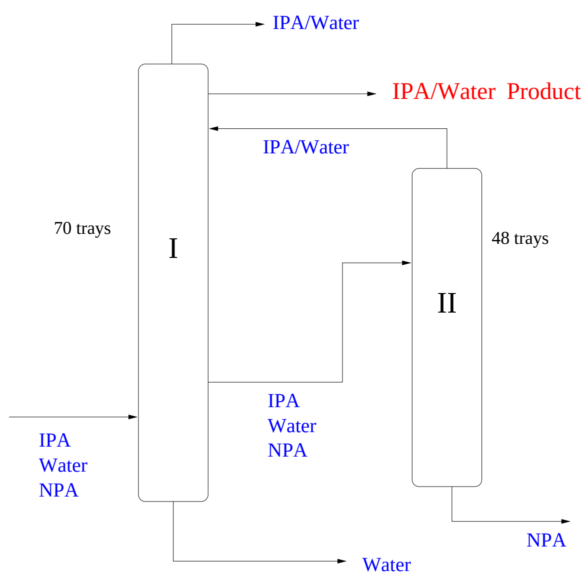


Figure 5: Schematic of the industrial distillation system

Most of the separation of the IPA/water azeotrope occurs in the lower part of column I, accompanied by large temperature gradients. In the same region there is a buildup of NPA due highly non-ideal, liquid phase interactions between the non-polar NPA and polar water molecules. Disturbances in the feed flow and composition may dramatically affect the temperature and composition profiles, thus changing the location of the peak NPA concentration, and the resulting feed composition to column II. In the absence of good control, two scenarios are possible and have been observed:

1. If the peak NPA concentration moves too high in column I, column II becomes overloaded with water and valuable IPA is lost from its bottoms stream;
2. If the peak NPA concentration moves too low in column I, there is a sharp build-up of liquid flows and the lower section of column I becomes flooded.

Detrimental effects on process economics include the production of off-specification material, a reduction in throughput to avoid flooding, and, should flooding occur, the shut-down and re-starting of the plant.

The objectives of this study are two-fold:

1. To address the operability difficulties experienced with the current process design;
2. To propose a new process design and control system with improved economics and operability.

In order to meet the first objective, rigorous modelling and simulation, sensitivity analyses, and control system design are carried out. For the second objective, process and control design decisions are optimized simultaneously within a mathematical programming framework and the potential benefits of such an integrated design approach are investigated.

## 3.2 Addressing the Operability Problems of the Existing Design

### 3.2.1 Development of Dynamic Model

The key features of the *gPROMS* dynamic model for the industrial system are similar to those described earlier for the double-effect case study, with the difference being in the modelling of the non-ideality of the liquid and vapour phase thermo-physical properties.

The complexity of the large-scale distillation system leads to around 27,000 differential and algebraic equations that must be solved during simulation. However, by utilising the *gPROMS* Foreign Object Interface to Multiflash (Process Systems Enterprise, 1998b) for carrying out the physical property calculations, the number of equations that *gPROMS* must handle directly is reduced to approximately 10,000. This leads to dramatic reductions in computational times.

### 3.2.2 Sensitivity Analyses and Controller Design

Steady-state analyses showed that, due to the high-purity azeotropic separation in column I, the temperature, composition and liquid load profiles are highly sensitive to changes in material flows. For example, a 2% (2.8 tonnes per hour) increase in the feed flow rate leads to a dramatic 19% (27 tonnes per hour) increase in the peak internal liquid flow rate in the bottom section of column I, thus demonstrating why flooding is often a problem in practice.

Based on the insights gained from the sensitivity analyses a mass balance-based control scheme was developed, which involved temperature control in column I through manipulation of the product flow rate (Ross *et al.*, 1999). Additional inventory control in the reboilers and reflux drums is provided by manipulating the associated outlet flow rates, with controller tuning based on the Internal Model Control rules (Morari and Zafiriou, 1989).

With the inventory controllers in place, the temperature controller was optimally tuned using *gOPT*. A normalised integral square error (ISE) performance measure was used for this purpose. Fig. 6 compares the open and closed-loop dynamic behavior of the controlled temperature and the liquid flow rate leaving the feed tray for a 2.4% step increase in the feed flow rate. The optimally tuned control scheme gives rapid disturbance rejection and prevents the dramatic decrease in tray temperature and increase in liquid load experienced in the open-loop system.

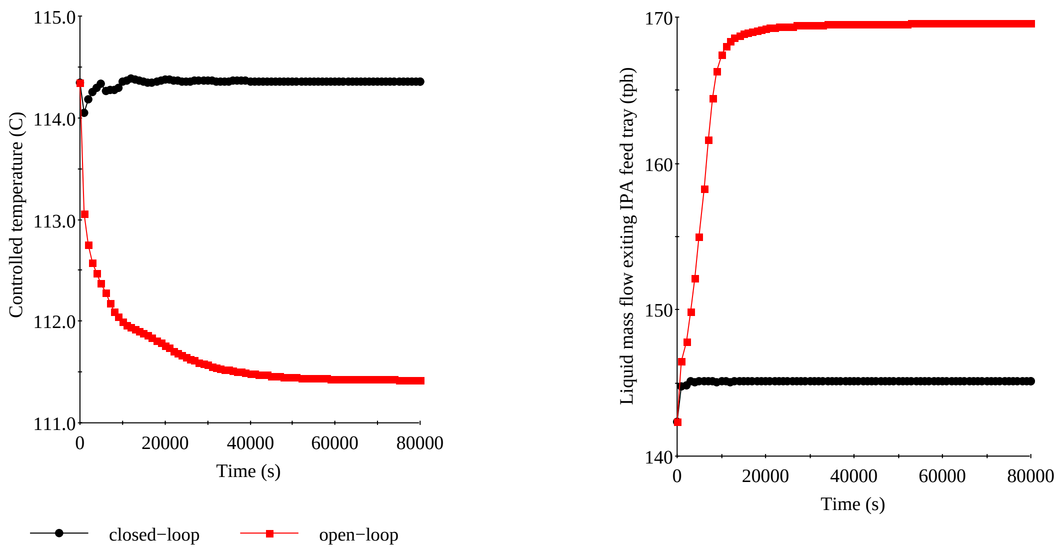


Figure 6: Open- *vs.* closed-loop performance: controlled temperature and peak liquid flow

## 3.3 Simultaneous Optimization of Process Design and Control

Having successfully addressed the operability problems of the existing design, the objective here is to determine the optimal system that would have resulted if a state-of-the-art, simultaneous optimization approach to design and control had been used at the outset, and to investigate its potential economic and operability benefits.

The formulation of the simultaneous design and control optimization problem is:

$$\begin{array}{ll} \textit{min} & \text{Expected Total Annualised Cost} \\ \\ \textit{s.t.} & \text{Differential-Algebraic process model} \\ & \text{PI control scheme equations} \\ & \text{Uncertainty in feed flow rate } (\pm\ 8\%) \\ & \text{Sinusoidal IPA feed composition } (\pm\ 5\%) \\ & \text{Inequality path constraints} \end{array}$$

This corresponds to a very large-scale dynamic optimization problem involving approximately 10,000 model equations (not including 17,000 physical property equations), with about 600 differentiable states. The objective function consists of annualised capital costs (calculated from Guthrie correlations: Douglas, 1988) and annual operating costs (Shell data). There are 7 path inequality constraints describing feasible operation of the process, namely a minimum column diameter/flooding constraint and a fractional entrainment limit for each column; composition constraints on the NPA and the water in the azeotrope product near the top of column I; and a composition constraint on the IPA in the bottom product of column II. The variables being optimized include 6 design variables (two column diameters, both reboiler duties and the two flow rates between columns I and II); and the gain and reset time of the PI-controller in the temperature-product flow rate loop. Note that the process structure (numbers of trays, feed and draw-off locations) and control structure are fixed at this stage, but future work will involve the inclusion of these integer decisions into the optimization.

The simultaneous design and control problem was solved in *gPROMS/gOPT* and leads to a design and control system which is 6% ($300,000 per year) cheaper than the existing design and optimally tuned control scheme reported earlier in this paper. The new distillation system design has a reduced capacity in column I (7% smaller diameter; 9% lower reboiler duty) and an increased capacity in column II (1% larger diameter; 24% higher reboiler duty). By increasing the draw-off rate from column I to column II, more NPA can be removed from column I, allowing for its reboiler duty to be reduced while still maintaining the product quality specifications. The overall savings then result because column I dominates the economics of the process.

# 4 Mixed-Integer Dynamic Optimization

## 4.1 Mathematical formulation

The iterative decomposition algorithm for simultaneous design and control (outlined in Fig. 3) alternates between a multi-period design sub-problem (which determines an optimal process design and control system able to tolerate a given set of critical uncertainty/disturbance scenarios) and a time-varying feasibility analysis step (which identifies a new set of critical scenarios for the fixed structure and design).

Both sub-problems involve the solution of mixed-integer dynamic optimization problems, a general form of which is given below:

$$
\left.
\begin{array}{c}
\min\limits_{u(t),d,t_f,y} \quad \phi\left(y,d,x\left(t_f\right)\right) + \int_{t_0}^{t_f} f^0(y,d,x\left(t\right),u\left(t\right),t)dt = F^0\left(y,d,x,u\right) \\
\\
\text{subject to} \\
\\
\begin{array}{ll}
F\left(y,d,\dot{x}\left(t\right),x(t),u\left(t\right),t\right) = 0 & \forall\, t \in [t_0,t_f] \\
q\left(y,d,x\left(t\right),t\right) \le 0 & \forall\, t \in [t_0,t_f] \\
h_e\left(y,d,x\left(t_f\right)\right) = 0 & e \in E \\
h_g\left(y,d,x\left(t_f\right)\right) \le 0 & g \in G
\end{array} \\
\\
u \in U = \{u : u(t) \in \Omega \quad \forall\, t \in [t_0,t_f]\} \subseteq \Re^{n_u} \\
d \in D \\
y \in Y = \{0,1\}^{n_y} \\
x \in X \subseteq \Re^{n_x}
\end{array}
\right\} \quad (1)
$$

where $y$ is the vector of 0-1 variables and $d$ denotes time-invariant continuous variables in the convex compact set $D$. Here, $x(t) \in \Re^{n_x}$ are continuous variables describing the state of the dynamic system, $u(t) \in \Re^{n_u}$ are controls whose optimal time variations on the interval $[t_0,t_f]$ are required and $\Omega$ is a convex compact set. Note that the integer variables appear not only in the path ($q$) and endpoint constraints ($h_e$ and $h_g$), but also in the DAE system.

Returning to Fig 3, we see that in the multi-period sub-problem, integer variables correspond to discrete design decisions (such as the interconnection of units and the control structure), whereas in the feasibility analysis sub-problem integer variables arise from the active set strategy used to determine new critical scenarios.

### 4.2 Existing solution approaches

Currently, a common approach to solving MIDO problems is through orthogonal collocation on finite elements, where the overall problem is transformed into a large-scale mixed-integer nonlinear programming (MINLP) problem and solved by existing decomposition algorithms (such as Generalized Benders Decomposition (GBD) or Outer Approximation/Equality Relaxation (OA/ER)). In transforming the problem to a MINLP, both the states and the control variables are discretised. As a result, the efficient use of this approach is limited to relatively small-scale problems, since for problems with many differential-algebraic equations (DAEs) the number of parameters to be optimized grows rapidly and the problem becomes unwieldy, if not impossible to solve at present.

Another approach to solving MIDO problems is to use control parameterisation and sensitivity-based arguments for solving the primal (dynamic optimization) problem (Schweiger and Floudas, 1997). Thereafter an intermediate adjoint problem is solved to provide the dual information needed to formulate the relaxed master problem. The benefit of this approach is that the primal problem is solved in the reduced-space. However, the intermediate adjoint problem may often be expensive.

### 4.3 Proposed solution procedure for large-scale systems

In light of the difficulties mentioned above, an alternative approach for solving MIDO problems has been proposed by Mohideen *et al.* (1997). The method aims to combine the benefits of the above two approaches and is briefly discussed below, with further details in Ross *et al.* (1998).

A schematic of the prototype software implementation of the approach is shown in Fig. 7. In the primal (dynamic optimization) problem, the differential-algebraic model equations are substituted by discrete-time implicit equations resulting from the integration of the system by an implicit Runge-Kutta method. Efficient adjoint-based arguments are used to calculate the reduced gradients and the (dynamic) optimization is only carried out over the reduced space of the control variables (Pytlak, 1999).

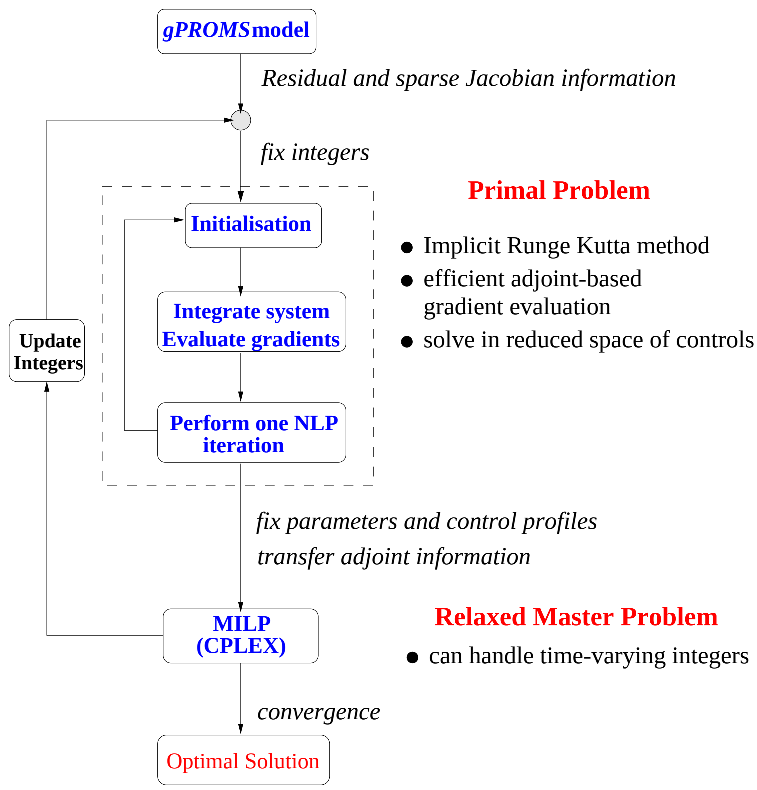


Figure 7: Prototype software implementation for large-scale MIDO problems

The dual information required for the construction of the master problem is directly available from the adjoint variables of the primal problem (thus avoiding an intermediate adjoint problem).

With the algorithmic benefits mentioned above, together with the convenience of using *gPROMS* as a front-end to define the dynamic system, it is envisaged that the solution of large-scale integrated design and control problems should become a manageable task. The implementation is currently being tested on a number of problems and results will be reported shortly.

# 5 Conclusions

The effective design and operation of complex separation systems requires a systematic treatment of design and control issues. The use of rigorous, high-fidelity models is a necessity for accurately capturing the key dynamic features and for identifying process bottlenecks in such systems. The application of advanced dynamic optimization techniques enables improved economic and control performance to be achieved, especially when process design and control issues are tackled simultaneously. These benefits have been demonstrated on both a theoretical and an industrial system. However, to fully exploit the synergy between design and control, the optimization of structural decisions needs to be included. Techniques for the efficient solution of large-scale mixed-integer dynamic optimization thus remain a key area of research.

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