

A Robust and Efficient Mixed-Integer Non-Linear Dynamic Optimization Approach for Simultaneous Design and Control

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Abstract

In this work, we propose a new algorithm for addressing the simultaneous design and control problem through the robust and efficient solution of a Mixed-Integer Dynamic Optimization (MIDO) problem. The algorithm is based on the transformation of the MIDO problem into a Mixed-Integer Nonlinear Programming (MINLP) program through the discretization of the MIDO problem. In this approach both the manipulated and controlled variables are discretized along the expected solution trajectory. This leads to a MINLP problem whose solution provides the full manipulated and controlled time variable profiles and the process design structure aiming to reduce operability problems. The new algorithm for addressing the solution of the MIDO problem has been applied to a system of two series connected continuous stirred tank reactors where a first order reaction takes place. Our results demonstrate that the new approach is able to efficiently address the solution of the simultaneous design and control problem in a systematic way.

1. Introduction

In the last 20 years there have been important efforts aiming at providing methodologies for tackling process design and control in a simultaneous and integrated framework (Bansal et al., 2002; Sakizlis et al., 2004). Some initial efforts were directed toward steady-state indicators that addressed potential control problems. However, as the operability problem features strong dynamic variations, its assessment requires that the problem be approached using a dynamic framework. The simultaneous design and control problem (SDCP) can be cast as an optimization problem. As both integer and continuous variables are embedded into this problem, the SDCP must be naturally formulated as a Mixed-Integer Dynamic Optimization (MIDO) problem. The integer variables take care of variables that can only take integer values (i.e. number of control loops, number of distillation columns, number of trays, etc), while the continuous variables are normally related to design variables (i.e. flows, temperatures, composition, etc). As many real chemical processes feature strong nonlinear behavior around optimal

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design regions, it is likely that the MIDO problem gives rise to a highly nonlinear optimization formulation.

From an optimization point of view, two major approaches have been proposed for tackling the solution of the MIDO problem. Some approaches (Bansal et al., 2002; Sakizlis et al., 2004) have suggested to solve the MIDO problem as a sequence of primal and master problems resembling optimization decomposition strategies as Benders decomposition and the Outer-Approximation algorithm. The primal problem corresponds to a dynamic optimization problem, while the master problem is formulated as a MILP. On the other hand, the full discretization (FD) of the dynamic model has been suggested to address the solution of the MIDO problem (Biegler et al., 2002). In the FD approach, the MIDO problem is cast as a MINLP for which efficient solution strategies have been reported. Recently Grossmann (2002) has reviewed the numerical algorithms for solving MINLPs; these include Outer Approximation (OA) and Branch and Bound (BB).

In this work we propose an FD approach to tackle the simultaneous design and control problem cast as a MIDO problem. The FD approach leads to an MINLP whose solution is addressed using the branch and bound (BB) method as proposed by Fletcher and Leyfer (1994). One advantage of this BB method, compared against the OA approach, is that nonlinearities in the discrete variables can be directly handled by the MINLP solver.

2. Simultaneous Approach for Design and Control

By using the FD approach a dynamic optimization problem can be cast as an NLP. From an algorithmic point of view, the solution of the MIDO problem involves solving a dynamic optimization problem that involves both integer and continuous variables. Therefore, by applying the FD approach, the MIDO problem is finally transformed into a MINLP.

In the FD approach the states and the manipulated variables are discretized along the expected solution trajectory. When binary variables are not part of the continuous model to be discretized, the procedure gives rise to an NLP. Moreover, if binary variables are part of the model, the FD approach will give rise to an MINLP. It is worth mentioning that, when discretizing a continuous model in which binary decision variables are embedded, the binary variables are not subject to discretization. Therefore, in order to explain the FD approach as applied to a model involving continuous and binary variables, it is only necessary to explain how the discretization of the continuous variables is addressed. Some of the discretization techniques proposed for the FD of dynamic optimization problems have been discussed elsewhere (Flores-Tlacuahuac et al., 2004) and only a short summary will be discussed here.

In the FD approach both the manipulated and controlled variables are discretized along the expected solution trajectory. This leads to a nonlinear programming problem whose solution provides the full manipulated and controlled time variable profiles. Due to the fact that fast variations in the controlled variables might arise, the whole solution space is commonly divided into time intervals called finite elements. Inside each finite element the differential-algebraic equations are satisfied at Radau collocation points. This approach corresponds to a fully implicit Runge-Kutta method with high order accuracy and stability properties.

2.1 Formulation

A common requirement in the closed-loop control of chemical processes refers to disturbance rejection. In order to get minimum time closed-loop disturbance rejection capabilities, the following optimization problem can be formulated:

$$\text{Min} \int_0^{t_f} \|z(t) - \hat{z}(t)\|^2 dt \quad (1)$$

$$\text{s.t. Semi-explicit DAE model: } \frac{dz}{dt} = F(z(t), x(t), u(t), t, p, y) \quad (2)$$

$$0 = G(z(t), x(t), u(t), t, p, y) \quad (3)$$

$$\text{Initial conditions: } z(0) = z^0 \quad (4)$$

Bounds:

$$\begin{aligned} z^L &\leq z(t) \leq z^U \\ x^L &\leq x(t) \leq x^U \\ u^L &\leq u(t) \leq u^U \\ p^L &\leq p \leq p^U \end{aligned} \quad (5)$$

where F is the vector of right hand sides of differential equations in the DAE model, G is the vector of algebraic equations, assumed to be index one, z is the differential state vector, z^0 are the initial values of z , $\hat{z}$ is the set-point vector, x is the algebraic state vector, u is the control profile vector, p is a time-independent parameter vector and y is the vector of binary variables. Additional details of the optimization formulation can be consulted elsewhere (Flores-Tlacuahuac et al., 2004).

3. Example of MIDO

3.1 Problem Formulation

When using MINLP methods to address the SDCP problem, the first step consists of proposing a superstructure of processing alternatives. Such a superstructure contains all the potential solutions the designer would like to consider. The optimal solution is embedded in such representation. It is clear that this step is a crucial one since, if a poor superstructure is proposed, then we would not be able to get the best potential solution. Therefore, the solution will be optimal only with respect to the embedded processing superstructure.

The objective of the simultaneous design and control problem is to design the 2 series-connected CSTR system, and its associated control system, so that the conversion at the second reactor outlet is maximized. Since, normally conversion is not measured on-line, maximum conversion will be achieved through the closed-loop control of the second reactor temperature T_2 . The cooling system of the reaction train may be operated either in a co-current or counter-current form. The manipulated variables candidates are the cooling water flow rate Q_c and the feed stream temperature T_f . The binary variables y_1 ; y_2 ; y_3 ; y_4 ; y_5 ; y_6 , when set to one, stand for Co-current flow rate, Counter-current flow rate, $T_f \rightarrow T_1$ control pairing, $T_f \rightarrow T_2$ control pairing, $Q_c \rightarrow T_1$ control pairing, and $Q_c \rightarrow T_2$ control pairing, respectively. The superstructure of processing alternatives is shown in Figure 1.

$$\text{Min}_{x,u,y,p} \int_0^{t_f} (T_2^{sp} - T_2)^2 dt \quad (6)$$

Step Disturbances:

$$C_f = C_f^{nominal} + \alpha_d (e^{-\lambda t} - 1) \quad (7)$$

Mathematical Model:

$$\begin{aligned}
\frac{dC_1}{dt} &= \frac{(C_f - C_1)}{\theta} + r_{A1} \\
\frac{dT_1}{dt} &= \frac{(T_f - T_1)}{\theta} + \beta r_{A1} - \alpha(T_1 - T_{c1}) \\
\frac{dT_{c1}}{dt} &= \frac{y_1(T_{cf} - T_{c1}) + y_2(T_{c2} - T_{c1})}{\theta_c} + \alpha_c(T_1 - T_{c1}) \\
\frac{dC_2}{dt} &= \frac{(C_1 - C_2)}{\theta} + r_{A2} \\
\frac{dT_2}{dt} &= \frac{(T_1 - T_2)}{\theta} + \beta r_{A2} - \alpha(T_2 - T_{c2}) \\
\frac{dT_{c2}}{dt} &= \frac{y_1(T_{c1} - T_{c2}) + y_2(T_{cf} - T_{c2})}{\theta_c} + \alpha_c(T_2 - T_{c2})
\end{aligned} \tag{8}$$

Control System:

$$\begin{aligned}
T_f &= T_f^{bias} + K_p[y_3(T_1^{sp} - T_1) + y_4(T_2^{sp} - T_2)] + K_i I_f \\
Q_c &= Q_c^{bias} - K_p[y_5(T_1^{sp} - T_1) + y_6(T_2^{sp} - T_2)] - K_i I_c \\
\frac{dI_f}{dt} &= y_3(T_1^{sp} - T_1) + y_4(T_2^{sp} - T_2) \\
\frac{dI_c}{dt} &= y_5(T_1^{sp} - T_1) + y_6(T_2^{sp} - T_2)
\end{aligned} \tag{9}$$

Binary Constraints

$$\begin{aligned}
y_1 + y_2 &= 1 \\
y_3 + y_4 + y_5 + y_6 &= 1
\end{aligned} \tag{10}$$

In the objective function expression, given by Eqn (6), the decision variables are defined as follows: $x = [C_1; T_1; T_{c1}; C_2; T_2; T_{c2}]$, $u = [T_f; Q_c]$, $y = [y_1; y_2; y_3; y_4; y_5; y_6]$ and $p = [\theta; \theta_c; T_{cf}; K; \tau_i]$. It is worth noting that only the variables embedded in the x and u vectors are time variant. Notice that in equation (7), $\alpha_d = C_f^{nominal} - C_f^{final}$ where C_f^{final} stands for the final value of the feed stream composition (i.e. after the disturbance upsets the system), while λ is related to the disturbance time constant (θ_d) through $\lambda \approx (1/\theta_d)$.

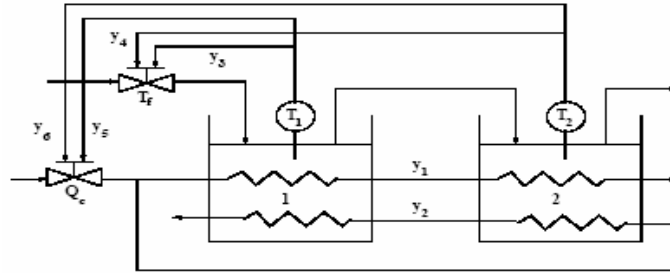


Figure 1: Superstructure of processing alternatives.

4. Results and Discussion

In order to evaluate the robustness of the FD approach for tackling SDC problems, several cases were analyzed. In all scenarios, it was assumed that the coupled reaction system always operates around the high sensitivity multiplicity region. Both increasing and decreasing step feedstream composition disturbances were applied to the system. It was also assumed that the controllers are just plain PI controllers. Therefore, the aims of the MIDO problem solution are: (a) to find the best cooling water configuration, (b) to compute reactor and cooling water residence times, (c) to select the control structure and (d) to select the PI controller tuning parameters so that the disturbance is rejected in minimum time, while keeping the second reactor temperature at its set-point. Two cases of these cases are presented here. Both cases assume that the reactor is operating around the high temperature and conversion region. The intermediate temperature region was not addressed as it requires a control system in each of the two reactors.

Case 1

In this case the feedstream composition decreases from 0.6 down to 0.55 mol/l. Under this situation the second reactor temperature T_2 decreases as well, as the heat released by the reaction diminishes. Therefore, the effect of the closed-loop control action will be to increase the second reactor temperature until it reaches its set-point temperature. The solution of the MIDO problem dictates that T_2 must be controlled by the first reactor feedstream temperature T_f , and that the cooling system must be countercurrent. The optimal values of the decision variables are: $\theta = 360$ s, $\theta_c = 100$ s, $K_p = 259\,791$ and $K_i = 5\,177\,800$. The reason why the $T_f \rightarrow T_2$ control pairing was selected is because the $T_2(s)/T_f(s)$ gain is higher than the $T_2(s)/Q_c(s)$ gain. Therefore, better disturbance rejection characteristics are obtained by employing the $T_f \rightarrow T_2$ control pairing. The selection of the type of cooling is influenced by the direction of the disturbance. As T_2 diminishes when the disturbance hits the system, the countercurrent cooling has a weaker influence on T_2 therefore allowing T_2 to recover more quickly. Figure 2 displays the feedstream temperature profile employed to reject the disturbance. Generally speaking, the solution of the MIDO problem shows good disturbance rejection capabilities. Here, the reactor residence time is about 6 min. and, from Figure 2, it can be noticed that the disturbance rejection is achieved in around one residence time, without excessive control energy.

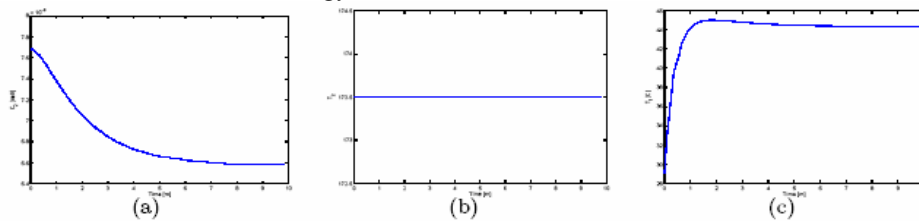


Figure 2: Case 1: Input/Output behaviour showing C_2 (a), T_2 (b) and T_f (c) vs. time.

Case 2

In this case the feedstream composition disturbance increases from 0.6 up to 0.65 as a step input. When the disturbance hits the system, the second reactor temperature T_2 starts rising. The solution of the MIDO problem once again selects the $T_f \rightarrow T_2$ control pairing. However, this time the cocurrent cooling is chosen. The optimal values of the decision variables are $\theta = 360$ s, $\theta_c = 100$ s, $K_p = 1\,610\,190$ and $K_i = 3\,673\,870$. In order to reject the disturbance, the feedstream temperature must be reduced until T_2 reaches its

set-point value. Once again, the reason why the $T_f \rightarrow T_2$ control pairing was selected is due to the fact that the $T_2(s)/T_f(s)$ gain is larger than the $T_2(s)/Q_c(s)$ gain. As T_2 rises, the selection of the cocurrent cooling affords better cooling capabilities, hence, leading to better disturbance rejection characteristics. Figure 3 displays the time profile of the reaction system states as well as the dynamic variation of the feedstream temperature. As can be noted, the closed-loop system exhibits good disturbance rejection characteristics. In fact, the disturbance is rejected in less than one reactor residence time. The larger values of the controller tuning parameters of this case, compared to the first case, demonstrate that the reaction system exhibits stronger nonlinearities depending on whether the feedstream composition is either decreased or increased.

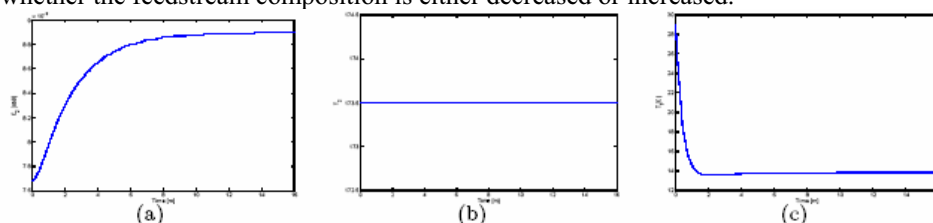


Figure 3: Case 2: Input/Output behaviour showing C_2 (a), T_2 (b) and T_f (c) vs. time.

5. Conclusions

From the analyzed cases, we note that good disturbance rejection was always achieved around the high temperature region independently of the size, shape and direction of the feedstream disturbance. It should be noted that in all the analyzed cases, the solution of the MIDO problem always selected the $T_f \rightarrow T_2$ control pairing. The selection of T_2 as the controlled variable is clear as it appears directly in the objective function. Regarding the manipulated variable, T_f has a greater influence on T_2 as compared to Q_c . However, because modifying Q_c is easier than changing T_f , one might wonder if the selected control pairing would remain the same if dynamic behaviour for T_f and Q_c would be modelled. It is interesting to note that, although the values of the reactor and cooling water residence times for both cases are almost the same, very different values of the controller tuning parameters were required to reflect the size, shape and direction of the feedstream composition disturbances.

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