Plantwide Control Structure Selection Methodology based on Economics: a Quadratic Approximation

Christos S. Patilas a,b, Ioannis K. Kookos a,b*

a University of Patras, Department of Chemical Engineering, Patras, Greece
b Research Infrastructure for Waste Valorisation and Sustainable Management of Resources, Patras, Greece

i.kookos@chemeng.upatras.gr

Abstract

The back-off methodology has been developed and refined in the last decades and offers a systematic tool for solving the simultaneous design and control problem. The first formulation of the methodology was based on linear process and control models. In previous work an improved formulation was proposed where use is made of a nonlinear process model that ensures improved accuracy but increases the complexity and the computational cost of the final problem. In this work, another formulation is presented which is based on the quadratic approximation of the objective function, resulting in a Mixed Integer Quadratic Programming (MIQP) formulation. This approximation can offer greater accuracy than the linear counterpart with a reasonable increase in the computational complexity. The three formulations are evaluated in a reactor-separator-recycle process.

Keywords: process control, control structure selection, mathematical programming

1. Introduction

In industry, processes are designed to operate at specific conditions dictated by economics, equipment capacity constraints and environmental and safety considerations. However, a wide range of disturbances may cause process operation to deviate from the optimal operating point which can not only cause performance deterioration but also operation infeasibility. These phenomena are treated with corrective actions in the form of control mechanisms. In designing those systems, the objective is to develop control structures that satisfy the constrains under the effect of disturbances with minimum performance loss. This is known as the Control Structure Selection Problem (CSSP) and refers to the synthesis of optimal regulatory control structures by considering both structural and parametric optimization issues.

A systematic method, that is known as the back-off methodology for simultaneous design and control, has been proposed and latter refined by Heath et al. (2000). More recently Psaltis et al. (2013) proposed some implementation improvements that made the application of the methodology possible to plantwide control problems.

The initial formulation of the method was based on linearized economics that ensure quick determination of the optimal solution at the expense of a possible loss in the accuracy due to the nonlinearities. In (Kookos and Perking, 2016) a new formulation is proposed which uses the nonlinear model of the process assuming that all design (structural) decisions have been made. This new formulation ensures improved accuracy.
and also offers the opportunity for the simultaneous consideration of process design and control. The nonlinear formulation increases the complexity and the computational cost of the final problem. Therefore, a new formulation based on the quadratic approximation of the objective function (economic penalty) is introduced resulting in a Mixed Integer Quadratic Programming (MIQP). This approximation can be more accurate when compared with the linear counterpart at reasonable increase in computational effort. A short review of the back-off methodology is first presented followed by the formulation of the quadratic approximation. Finally, all three formulations are evaluated in a case study involving a reactor-separator-recycle process (Luyben and Floudas, 1993).

2. Mathematical Framework and Formulation

Operation of chemical process systems may be modeled by a set of nonlinear differential and algebraic equations and inequality constraints that involve an \( n_x \) vector of state variables \( \mathbf{x}(t) \), an \( n_z \) vector of algebraic variables \( \mathbf{z}(t) \), an \( n_u \) vector of control variables \( \mathbf{u}(t) \), a vector of design variables that consist of continuous (\( \mathbf{d} \)) as well as integer (\( \mathbf{\Delta} \)) variables and an \( n_p \) vector of disturbances \( \mathbf{p}(t) \) (variables that are determined exogenously). Finally, \( J \) is the objective function usually used to evaluate the economic performance of the process. The control structure selection problem can be modeled as a Mixed Integer Non-Linear Programming (MINLP) and described by the following set of equations:

\[
\min_{\mathbf{x}(t), \mathbf{z}(t), \mathbf{u}(t), \mathbf{p}(t); \mathbf{d}, \mathbf{\Delta}} J(\mathbf{x}(t), \mathbf{z}(t), \mathbf{u}(t), \mathbf{p}(t); \mathbf{d}, \mathbf{\Delta})
\]

\[
st. \quad \mathbf{h}(\mathbf{x}(t), \mathbf{z}(t), \mathbf{u}(t), \mathbf{p}(t); \mathbf{d}, \mathbf{\Delta}) = 0
\]

\[
\mathbf{g}(\mathbf{x}(t), \mathbf{z}(t), \mathbf{u}(t), \mathbf{p}(t); \mathbf{d}, \mathbf{\Delta}) \leq 0
\]

For the ideal case, in which the uncertain parameters are set to their nominal values the above formulation is restricted to steady state. The solution of the steady state problem yields the optimum steady-state operating point which usually lies at the intersection of active constraints. In general, the uncertain parameters deviate from their nominal values and therefore the process operation may shift to the infeasible region.

In order to ensure the feasibility of the operation under the effect of disturbances, the back-off vector \( \mathbf{\mu} \) is introduced:

\[
\mu_k = \max_i |g_i^N - g_i^k|, \quad k = 1, 2, \ldots, n_g
\]

where, \( g_i^k \) is the value of the \( k \)-th constraint at the nominal optimal operating point. Each element of the back-off vector is defined as the maximum violation of the corresponding constraint over the time horizon. The magnitude of the back-off vector depends not only on the disturbance characteristics but also on the structure and the parameters of the regulatory control system.

The dynamic behavior of a process under the effect of disturbances, in a region close to a steady state point can be described with adequate accuracy by the linearization of Eq. (1) at the optimal operating point. Furthermore, to avoid the complexity of solving a dynamic problem, the system of differential and algebraic equations can be transformed into the frequency domain. The latter is performed by taking the Laplace transformation of the system and decompose the transformed variables into real (superscript R) and
imaginary (superscript I) parts. The final system of equations is described below in Eq. (3):

\[
\begin{align*}
0 &= AX^s + BU^s + EP^s + \omega X' \\
0 &= AX' + BU' + EP' - \omega X^s \\
Y^s &= CX^s + DU^s + FP^s \\
Y' &= CX' + DU' + FP' \\
\Sigma^s &= HX^s + PU^s + SP^s \\
\Sigma' &= HX' + PU' + SP'
\end{align*}
\]

If we set \( P^R = 1 \) and \( P^I = 0 \), we can obtain the frequency response of the system (i.e. the asymptotic response to sinusoidal variation of the disturbances with frequency \( \omega \)). However, the system of linear equations is underdetermined as 2\( n \) equations are missing. These are the equations that are needed to describe the controller in the frequency domain. To resolve this issue and simultaneously avoid the introduction of the controller design problem, the implementation of perfect control was proposed. Integer variables \( \Psi_j \) are introduced to denote the selection (\( \Psi_j = 0 \)) or not (\( \Psi_j = 1 \)) of potential controlled variable (CV) \( y_j \). In a similar way the integer variables \( \Theta_j \) are introduced to select (\( \Theta_j = 1 \)) or not (\( \Theta_j = 0 \)) a potential manipulated variable (MV) \( u_j \) in the regulatory control structure and perfect control is implemented through the following linear inequalities. Finally, consideration is also restricted to square control structures. The equations of the controller are presented in Eq. (4).

\[
\begin{align*}
-y_j^u \Psi_j &\leq y_j^s \Psi_j \quad j = 1, 2, ..., n_y \\
-y_j^u \Psi_j &\leq y_j' \Psi_j \\
-u_j^u \Theta_j &\leq U_j^R \leq u_j^u \Theta_j \\
-u_j^u \Theta_j &\leq U_j' \leq u_j^u \Theta_j \\
\sum_{j=1}^{n_y} \Psi_j + \sum_{j=1}^{n_u} \Theta_j &= n_y
\end{align*}
\]

Psaltis et al. (2013) have shown that the back-off vector can be determined accurately through a set of linear inequalities that avoid the need for the iterative application of the algorithm used earlier by Heath et al (2000).

\[
\Pi^R \Sigma^R + \Pi' \Sigma' \leq \mu
\]

For the linear formulation equations Eq. (3) - Eq. (5) can be combined with the state space model of the process and can be written in Eq. (6), where \( J_c \) and \( J_u \) are the gradients of the objective function with respect to the state and control vectors accordingly and EP_t_p is the economic penalty resulting from the occurrence of the disturbances. Additionally, the non-linear formulation is also presented in Eq. (6) and makes use of the linear approximation for the back-off estimation and the initial formulation Eq. (1) for the estimation of the economic penalty.
The proposed formulation has the same set of equations as the linear and a quadratic approximation of the economic penalty. The objective function of this formulation is stated below in Eq. (7), where $Q$ is the hessian matrix.

$$EP_{OP} = J'_x \delta x + J'_u \delta u + \frac{1}{2} \left[ \begin{array}{c} \delta x' \\ \delta u' \end{array} \right] Q \left[ \begin{array}{c} \delta x' \\ \delta u' \end{array} \right]$$

3. Case Study

The reactor-separator-recycle process examined in this case study is presented in Figure 1. Fresh feed of 90% A is fed into the reactor, where the first order irreversible reaction $A \rightarrow B$ takes place. The reactor product is then fed to the distillation column. The main product B is obtained as the bottom product, while unreacted A is recycled back to the reactor.

The design strategy of the process was based on a structural optimization problem for finding the optimal steady state regarding the topology and the operating point (Luyben and Floudas, 1993) and (Viswanathan and Grossmann, 1992).
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Table 1. Results of the CSSP- Nonlinear, Linear and Quadratic for 5% variation in Disturbances

<table>
<thead>
<tr>
<th>N₀</th>
<th>(EP_{nlp})</th>
<th>N₀</th>
<th>(EP_{lp})</th>
<th>N₀</th>
<th>(EP_{qp})</th>
<th>Manipulated</th>
<th>Controlled</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.01 %</td>
<td>1</td>
<td>0.00 %</td>
<td>1</td>
<td>0.00 %</td>
<td>F, L₁, V₁, R, D</td>
<td>N₀, x₀, x₁₂, N₁, NNT</td>
</tr>
<tr>
<td>2</td>
<td>0.14 %</td>
<td>2</td>
<td>0.08 %</td>
<td>2</td>
<td>0.21 %</td>
<td>F, L₁, V₁, R, D</td>
<td>N₀, x₂, x₁₂, N₁, NNT</td>
</tr>
<tr>
<td>3</td>
<td>0.32 %</td>
<td>3</td>
<td>0.21 %</td>
<td>3</td>
<td>0.21 %</td>
<td>F, L₁, V₁, R, D</td>
<td>N₀, x₃, x₂₁, N₁, NNT</td>
</tr>
<tr>
<td>4</td>
<td>0.56%</td>
<td>5</td>
<td>0.36 %</td>
<td>4</td>
<td>0.37 %</td>
<td>F, L₁, V₁, R, D</td>
<td>N₀, x₄, x₂₂, N₁, NNT</td>
</tr>
<tr>
<td>5</td>
<td>0.58 %</td>
<td>4</td>
<td>0.34 %</td>
<td>9</td>
<td>0.56 %</td>
<td>F, L₁, V₁, R, D</td>
<td>N₀, x₂, x₂₀, N₁, NNT</td>
</tr>
<tr>
<td>6</td>
<td>0.85 %</td>
<td>9</td>
<td>0.77 %</td>
<td>6</td>
<td>0.77 %</td>
<td>F, L₁, V₁, R, D</td>
<td>N₀, x₅, x₁₉, N₁, NNT</td>
</tr>
<tr>
<td>7</td>
<td>0.85 %</td>
<td>8</td>
<td>0.61 %</td>
<td>7</td>
<td>0.77 %</td>
<td>F, L₁, V₁, R, D</td>
<td>N₀, x₆, x₂₀, N₁, NNT</td>
</tr>
<tr>
<td>8</td>
<td>0.85 %</td>
<td>7</td>
<td>0.55 %</td>
<td>5</td>
<td>0.56 %</td>
<td>F, L₁, V₁, R, D</td>
<td>N₀, x₅, x₂₁, N₁, NNT</td>
</tr>
<tr>
<td>9</td>
<td>1.22 %</td>
<td>-</td>
<td>-</td>
<td>8</td>
<td>0.79 %</td>
<td>F, L₁, V₁, R, D</td>
<td>N₀, x₆, x₂₂, N₁, NNT</td>
</tr>
<tr>
<td>10</td>
<td>1.22 %</td>
<td>6</td>
<td>0.46 %</td>
<td>10</td>
<td>1.08 %</td>
<td>F, L₁, V₁, R, D</td>
<td>N₀, x₃, x₂₀, N₁, NNT</td>
</tr>
</tbody>
</table>

The mathematical problem for the optimal design of the process is a MINLP problem which was solved using the SBB solver available in GAMS. The optimal solution is presented in Figure 1. The state vector consists of the mole fractions of component A and the molar holdups in the reactor and the column. The potential MV are the reactor product flowrate \(F\), the vapor boilup \(V₁\), the bottom’s product flowrate \(L₁\), the reflux rate \(R\) and the recycle stream flow \(D\). The potential CV are the reactor’s holdup \(N₁\) and composition \(x₀\), the holdup of the reboiler \(N₁\) and condenser \(NNT\) and finally the composition of component A in all trays. It should be noted that for this case study the choice of compositions as CV rather than temperatures will not make any difference because it is well known that both of them are equivalent for binary mixtures. As a result, there are 5 potential MV and 26 CV giving rise to an exploding size of potential control structures. The CSSP was then solved applying the three formulations to determine the 10 most promising structures and to examine if the quadratic performs better when compared to the linear. Table 1 summarizes the results.

All structures make use of all MV resulting in 5x5 control structures. An RGA analysis was performed to design the interconnection between the variables. In all cases, the reactor holdup is controlled by the reactor’s outflow, the reboiler’s holdup by the bottom’s product flow and the condenser’s holdup by the reflux rate. Finally, the boilup is connected with a composition in the stripping section and the recycle stream flow (distillate) with a composition in the rectifying section. The best structure was identified by all formulations and makes use of the compositions of the bottom and distillate product streams. Direct control of variables that appear in design specifications is often unrealistic therefore, these were eliminated as CV to examine structures based on the compositions of the internal trays.

Based on the results, the quadratic formulation managed to identify all of the structures produced by the non-linear and rank them more accurately than the linear. Some selected structures were evaluated in closed loop simulations in a rather aggressive disturbance scenario, where the inlet flow \(F₀\) to the reactor was increased by 10 %, then decreased by 20 % and finally returned to the nominal point. The same procedure was followed for the composition \(x₀\). In the closed loop system, PI controllers were implemented and tuned via the ATV method. In Figure 2, the deviation of the composition in the bottom’s product is
presented. As expected, the most promising structure is CS1 in which the purity specifications are directly controlled. Apart from that, the performance of the other three structures is also smooth with small deviations of order \(10^{-3}\).

![Figure 2. Deviation of bottom’s product composition.](image)

Finally, in order to evaluate the economic performance of the structures, the cost of utilities regarding the examined time domain was calculated. More specifically, the examined structures resulted in 2001.4$, 2001.5$, 2001.6$, and 2001.7 $ accordingly. Considering the order of the resulted economic penalties, it can be said that all structures feature in the same cost. The difference between the cost although insignificant, manages to ascertain the ranking of the structures presented in Table 1. These findings prove that the proposed formulation is successful in identifying promising control structures in a systematic way based on economic performance and not on rules of thumb and heuristics.

**Conclusions**

This paper presents the main concepts of the back-off methodology for the CSSP problem. A new formulation is presented and evaluated for the reactor-separator-recycle process. The results are very promising and the new formulation may offer advantages in the study of even more aggressive non-linear processes. The back-off methodology in general, handles efficiently the CSSP and based on the size of the current case the proposed methodology is not size-limited.

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