PLANTWIDE CONTROL STRUCTURE SELECTION

C. Patilas[1,2], I. Kookos[1,2, *]
[1]Department of Chemical Engineering, University of Patras, Karatheodory 1, Rio, 26504, Patras, Greece
[2]INVALOR: Research Infrastructure for Waste Valorization and Sustainable Management of Resources, Patras, Greece
(*ikookos@chemeng.upatras.gr)

ABSTRACT

An important and challenging problem is the determination of appropriate control structures that minimize the loss of process performance under the effect of disturbances. This can be achieved by selecting subsets of controlled and manipulated variables and designing their interconnection. The methods of solving the control structure selection problem can be divided in two main categories: a) qualitative b)quantitative. The qualitative methodologies are based on heuristic and logical rules while quantitative consist of mathematical or optimization based techniques.

The proposed ('back-off') methodology is part of the quantitative methodologies and is able to rank potential control structures based on the operational cost. In this paper, the main ideas of the methodology are presented in short and the method is evaluated in a challenging system of a quaternary reactive distillation column.

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, based on these ideas has been proposed by Narraway and Perkins [3] and was latter refined by Perkins and his co-workers [1]. More recently Psaltis et al. [4] proposed some implementation improvements that made the application of the methodology possible to plantwide control problems. The back-off methodology is based on the assumption that the optimal steady state operating point is defined by the intersection of active constraints. This is a well-established fact that is critical to the design of successful control systems. However, perfect control of the active constraints cannot be achieved and, to make things even worse, the set of active constraints can vary under dynamic conditions and/or active constraints may not be measurable. In addition, a large number of potential manipulated variables and secondary measurements is usually available, consideration of which results in an exploding number of possible combinations that need to be considered before an optimal structure is established. In the back-off methodology mathematical programming techniques are utilized for the systematic representation of alternatives (superstructure representation) and the solution of the problem (quick ranking of alternatives and identification of optimal solution).

A short review of the back-off methodology is first presented and then in order to evaluate the usefulness of the systematic methodology one case study is considered and studied in detail. More specifically, a quaternary reactive distillation system is investigated. The results obtained, demonstrate the potential of the proposed methodology for solving efficiently challenging control structure selection problems in an efficient and effective way.

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 $\boldsymbol{x}(t)$, an n_z vector of algebraic variables $\boldsymbol{z}(t)$, an n_u vector of control variables $\boldsymbol{u}(t)$, a vector of design variables that consist of continuous ($\boldsymbol{d}$) as well as integer ($\boldsymbol{\Delta}$) variables and an n_p vector of disturbances $\boldsymbol{p}(t)$ (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:

$$\begin{gathered}\min_{\boldsymbol{x}(t),\boldsymbol{z}(t),\boldsymbol{u}(t),\boldsymbol{p}(t),\boldsymbol{\Delta}} J(\boldsymbol{x}(t),\boldsymbol{z}(t),\boldsymbol{u}(t),\boldsymbol{p}(t);\boldsymbol{d},\boldsymbol{\Delta})\\ s.t.\\ \boldsymbol{h}(\dot{\boldsymbol{x}}(t),\boldsymbol{x}(t),\boldsymbol{z}(t),\boldsymbol{u}(t),\boldsymbol{p}(t);\boldsymbol{d},\boldsymbol{\Delta})=0\\ \boldsymbol{g}(\boldsymbol{x}(t),\boldsymbol{z}(t),\boldsymbol{u}(t),\boldsymbol{p}(t);\boldsymbol{d},\boldsymbol{\Delta})\le 0\end{gathered} \tag{1}$$

For the ideal case, in which the uncertain parameters are set to their nominal values ($\boldsymbol{p}=\boldsymbol{p}_N$) 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 μ is introduced:

$$\mu_k = \max_t \left|g_k - g_k^N\right|,\ \ k = 1,2,\dots,n_g \tag{2}$$

where, g_k^N 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 the formulation (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 in the following formulation:

$$\begin{aligned} 0 &= \boldsymbol{A}\boldsymbol{X}^R + \boldsymbol{B}\boldsymbol{U}^R + \boldsymbol{E}\boldsymbol{P}^R + \omega\boldsymbol{X}^I\\ 0 &= \boldsymbol{A}\boldsymbol{X}^I + \boldsymbol{B}\boldsymbol{U}^I + \boldsymbol{E}\boldsymbol{P}^I - \omega\boldsymbol{X}^R\\ \boldsymbol{Y}^R &= \boldsymbol{C}\boldsymbol{X}^R + \boldsymbol{D}\boldsymbol{U}^R + \boldsymbol{F}\boldsymbol{P}^R\\ \boldsymbol{Y}^I &= \boldsymbol{C}\boldsymbol{X}^R + \boldsymbol{D}\boldsymbol{U}^R + \boldsymbol{F}\boldsymbol{P}^I\\ \boldsymbol{\Sigma}^R &= \boldsymbol{H}\boldsymbol{X}^R + \boldsymbol{P}\boldsymbol{U}^I + \boldsymbol{S}\boldsymbol{P}^R\\ \boldsymbol{\Sigma}^I &= \boldsymbol{H}\boldsymbol{X}^R + \boldsymbol{P}\boldsymbol{U}^I + \boldsymbol{S}\boldsymbol{P}^I \end{aligned} \tag{3}$$

If we set $\boldsymbol{P}^R = 1$ and $\boldsymbol{P}^I = 0$, we can obtain the frequency response of he system (i.e. the asymptotic response to sinusoidal variation of the disturbances with frequency ω). By taking several values of ω , the complete frequency response can be constructed. However, the system of linear equations (3) is undetermined as $2n_u$ 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 Narraway and Perkins [3] propose the implementation of perfect control. Integer variables Ψ_j are introduced to denote the selection ($\Psi_j = 0$) or not ($\Psi_j = 1$) of potential controlled variable y_j in the regulatory control structure and perfect control is implemented through the following linear inequalities.

$$\left.\begin{array}{r} -y_j^U\Psi_j \leq Y_j^R \leq y_j^U\Psi_j \\ -y_j^U\Psi_j \leq Y_j^I \leq y_j^U\Psi_j \end{array}\right| \; j = 1,2,\dots,n_y \tag{4}$$

In a similar way the integer variables Θ_j are introduced to select ($\Theta_j = 1$) or not ($\Theta_j = 0$) a potential manipulated variable u_j in the control structure.

$$\left.\begin{array}{r} -u_j^U\Theta_j \leq U_j^R \leq u_j^U\Theta_j \\ -u_j^U\Theta_j \leq U_j^I \leq u_j^U\Theta_j \end{array}\right| \; j = 1,2,\dots,n_u \tag{5}$$

Consideration is also restricted to square control structures.

$$\sum_{j=1}^{n_y}\Psi_j + \sum_{j=1}^{n_u}\Theta_j = n_y \tag{6}$$

Psaltis et al. [4] have shown that the back-of vector can be determined accurately through the following set of linear inequalities that avoid the need for the iterative application of the algorithm used by Narraway and Perkins [3] and Heath et al.[1]

$$\boldsymbol{\Pi}^R\boldsymbol{\Sigma}^R + \boldsymbol{\Pi}^I\boldsymbol{\Sigma}^I \leq \boldsymbol{\mu} \tag{7}$$

The overall formulation is coupled with the linearized system at steady state and can be written in formulation (8) ,where J_x and J_u are the gradient of the objective function with respect to the state and control vectors accordingly and EP is the economic penalty resulting from the occurrence of the disturbances calculated using a linearized model for the process economics.

$$\begin{gathered} \min_{\delta \boldsymbol{x},\delta\boldsymbol{u},\boldsymbol{\Theta},\boldsymbol{\Psi},\boldsymbol{\mu}} EP = J_x^T\delta\boldsymbol{x} + J_u^T\delta\boldsymbol{u} \\ s.t. \\ \boldsymbol{A}\delta\boldsymbol{x} + \boldsymbol{B}\delta\boldsymbol{u} = 0 \\ \boldsymbol{C}\delta\boldsymbol{x} + \boldsymbol{D}\delta\boldsymbol{u} = \delta\boldsymbol{y} \\ \boldsymbol{g}_N + \boldsymbol{H}\delta\boldsymbol{x} + \boldsymbol{P}\delta\boldsymbol{u} \leq -\boldsymbol{\mu} \\ -\delta\boldsymbol{x}^{\boldsymbol{U}} \leq \delta\boldsymbol{x} \leq \delta\boldsymbol{x}^{\boldsymbol{U}} \\ -\delta\boldsymbol{u}^{\boldsymbol{U}} \leq \delta\boldsymbol{u} \leq \delta\boldsymbol{u}^{\boldsymbol{U}} \\ \boldsymbol{\Theta_j},\boldsymbol{\Psi_j} \in \{\boldsymbol{0},\boldsymbol{1}\} \\ Eqs\; 3-7 \end{gathered} \tag{8}$$

QUATERNARY REACTIVE DISTILLATION CASE STUDY

The aim of this case study is to utilize the proposed methodology on a relatively large scale and challenging system. The reaction taking place in the column is the hydrolysis of methyl-lactate to lactic acid and methanol.

$$ML + W \leftrightarrow LA + MeOH \tag{9}$$

This reaction was thoroughly studied by Sanz et al. [5] and is expressed by the following kinetics.

$$R_i = k_{F,i}\left(a_{i,ML}a_{i,W} - \frac{a_{i,LA}a_{i,MeOH}}{K_{eq,i}}\right) \quad (10)$$

where, $a_{i,j}$ is the activity of component j in tray i and the units of the reaction rate are $kmol{\cdot}h^{-1}kg_{cat}^{-1}$. Furthermore, for the vapor-liquid equilibrium the NRTL activity model is considered, while the pressure is kept constant in the column at 1.013 bar. This system is a part of the downstream process of the bio-based production of polymer grade lactic acid. The column's specifications and topology were designed independently as a structural optimization problem, including the inequality constraints (11) presented below. The resulting nominal operating point combined with the topology of the column are presented in Figure 1.

$$\begin{aligned} g_1 &= 0.90 - z_{B,LA} \le 0 \\ g_2 &= z_{D,LA} - 0.001 \le 0 \\ g_3 &= 142 - Pr \le 0 \end{aligned} \quad (11)$$

where, $z_{B,LA}$, $z_{D,LA}$ are the lactic acid's mass fraction in the bottom's and distillate's product stream and Pr is the productivity of the process.
The potential controlled variables are the tray temperatures ($T_2 - T_{17}$). The manipulated variables are the heat duty of the reboiler (Q_{reb}) and the reflux rate (RR). The criterion used for the control structure ranking is the operational cost and more specifically the cost of utilities. The utilities of the process are the usage of high-pressure steam and cooling water for the reboiler and condenser respectively.
The results obtained by applying the proposed methodology are summarized in Table 1. where the five best structures are presented. In the best structure, only one manipulated variable is selected. More specifically, the temperature of the first internal tray (T_2) is controlled by the heat duty of the reboiler (Q_{reb}). Additionally, the best 2 by 2 structure consists of both manipulated variables controlling the temperatures T_2 and T_8.

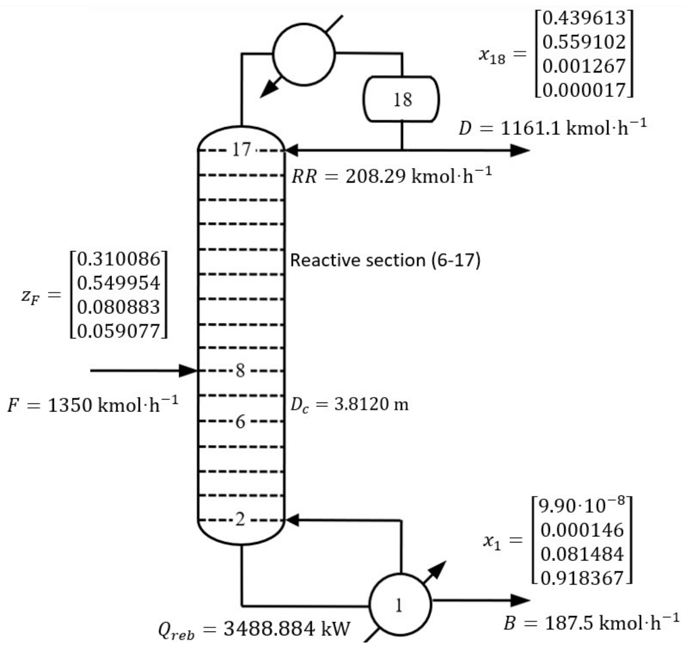

Figure 1. *Schematic representation of the reactive distillation column*

Table 1. Reactive distillation column control structure ranking

Rank	Structure			Economic Penalty (M$/y)
1	$\{T_2\}$	→	$\{u_1\}$	0.14742
2	$\{T_3\}$	→	$\{u_2\}$	0.15329
3	$\{T_2, T_8\}$	→	$\{u_1, u_2\}$	0.15578
4	$\{T_8, T_9\}$	→	$\{u_1, u_2\}$	0.15580
5	$\{T_9, T_{11}\}$	→	$\{u_1, u_2\}$	0.15580

The evaluation of the control structures consists of the comparison of the best 1 by 1 and 2 by 2 structures with a structure derived from the SVD methodology. In the latter, a singular value decomposition is performed on the gain matrices of the system and based on the maximum of every manipulated variable, the control structure is selected. On this case, the manipulated variables are controlling the temperatures T_3 and T_{11}. For all structures realistic PI controllers are implemented and the controllers' parameters were tuned using a parametric optimization technique. More specifically, the system is forced to a step sequence involving a ± 10 % step change in the feed flow followed by a ±2 °C step change in the set points of the measured temperatures. The objective function that must be minimized is described by Equation 12.

$$J = \int_0^\infty \sum \left|T_i - T_{sp}\right| dt + \int_0^\infty \sum \left|\frac{du_i}{dt}\right| dt \qquad (12)$$

The closed loop system was simulated for 100 h of operation and the responses of the manipulated variables, controlled variables and products' (distillate and bottom's) composition are shown in Figure 2. As can be observed, the performance of the closed loop system for all structures is smooth and the deviations of the controlled variables from their set points is small. A quantitative comparison of the deviations of the controlled variables concludes that the best structure (1 by 1) based on the proposed methodology exhibits the minimum error. In addition, the deviations of the two compositions (Figure 2 c, d) from the desired values are kept very small. Despite the fact that the composition of lactic acid in both product streams is not directly controlled, the deviations are kept in the order of 10^{-3} and 10^{-5} respectively.

Finally, in order to evaluate the economic performance of the structures, the cost of utilities regarding the examined time domain was calculated. More specifically, in the 1 by 1 structure the disturbance scenario cost 7798.2 $ while the two 2 by 2 structures resulted in 7831.2 $ and 7812.5 $ respectively. 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 of the structures derived from the proposed methodology, although insignificant, manage 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 in short, the main concepts of the back-off methodology for the control structure selection problem that was first proposed by Narraway and Perkins [3] and refined in the last decade from Heath et al. [1], Kookos et al. [2] and Psaltis et al. [4]. A challenging process that involves a quaternary reactive distillation system was investigated and the results are very promising. Based on the resulted economic penalties for the disturbance scenario, the ranking derived from the proposed methodology is verified. As a result, the proposed method handles

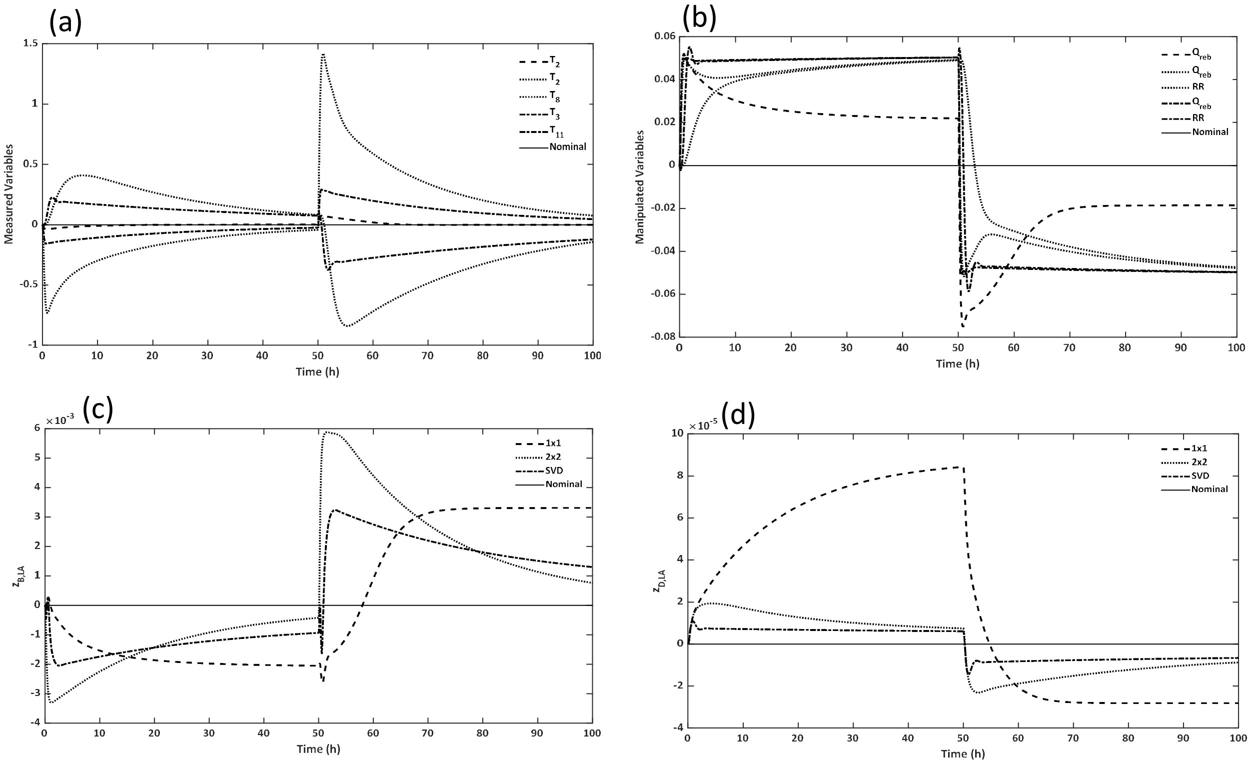

Figure 2. *(a) Response of measured variables, (b) Response of manipulated variables (c) Response of lactic acid's purity in the bottom's, (d) Response of lactic acid's purity in the distillate's*

efficiently processes with an aggressive non-linear nature and based on the size of the current case the back-off methodology is not size-limited.

ACKNOWLEDGEMENT

This work was supported by the project "INVALOR: Research Infrastructure for Waste Valorization and Sustainable Management" (MIS 5002495) which is implemented under the Action "Reinforcement of the Research and Innovation Infrastructure", funded by the Operational Programme "Competitiveness, Entrepreneurship and Innovation" (NSRF 2014-2020) and co-financed by Greece and the European Union (European Regional Development Fund).

European Union
European Regional Development Fund

HELLENIC REPUBLIC
MINISTRY OF ECONOMY & DEVELOPMENT
SPECIAL SECRETARY FOR ERDF & CF

EPAnEK 2014-2020
OPERATIONAL PROGRAMME
COMPETITIVENESS ENTREPRENEURSHIP INNOVATION

ΕΣΠΑ 2014-2020
ανάπτυξη - εργασία - αλληλεγγύη

Co-financed by Greece and the European Union

LITERATURE

[1] Heath JA, Kookos IK, Perkins JD. (2000). AIChE, 46(10): 1998-2016

[2] Kookos IK, Perkins JD. (2016). AIChE, 62: 3056-3064

[3] Narraway LT, Perkins JD. (1993). Ind. Eng. Chem. Res. 32: 2681-2692

[4] Psaltis A, Kookos IK, Kravaris C. (2013). Comp. Chem. Eng. 52:240-248

[5] Sanz M.t, Murga R, Beltran S, Cabezas J.L. (2004), Ind. Eng. Chem. 43:2049-2053