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Modifier-Adaptation methodology for RTO applied to Distillation Columns

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Abstract: Optimal process operation is not always guaranteed due to the presence of significant uncertainty about the plant models that are used to make decisions, for example in Real time optimization, and also due to the differences between control architecture layers which operate on different time-scales and use different kind of models. Modifier adaptation is a methodology that achieves optimality despite the presence of uncertainty by using plant measurements. This paper presents the Nested modifier-adaptation methodology applied to the operation of distillation columns and the results obtained are compared with the previous modifier adaptation methodology using dual control optimization.

Keywords: Real Time Optimization, modifier-adaptation, uncertainty, distillation columns, optimization problems

1. INTRODUCTION

The management of large scale systems, such as petrochemical industry, consists of making decisions that have to satisfy process specifications and constraints on many variables. In addition, these decisions should be optimal with respect to efficiency, economy, environment, etc. This problem requires the use of large models and optimization methods.

In modern refineries, optimal operation is typically addressed by a hierarchical structure as shown in Fig.1. The upper layer is Real-Time Optimization (RTO), at this level, medium-term decisions are made on a time scale of hours to a few days by considering economical objectives explicitly. The optimum operating point obtained by RTO layer is passed to lower-level controllers that include basic control and multivariable predictive control (MPC).

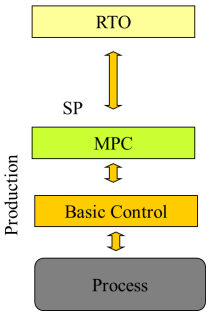

Fig. 1. Hierarchical control structure.

This structure is required for the management of large and complex plants, but optimal operation is not guaranteed since process models are inaccurate, so the optimum of the process could not be the same as the optimum of the model. In addition, layers of control structure use different models for making decisions, RTO typically involves nonlinear first-principles models that describe the steady-state behaviour of the plant whereas MPC is based on dynamic linear models. It might produce inconsistences between them that affect the final result.

To cope with the uncertainty already mentioned and to drive the process to its real optimum point, there have been several developments in RTO. The first approach emerged in the late 1970s as an iterative two-stage algorithm; a parameter estimation step (to update uncertain model parameters) followed by an economic optimization that is solved to obtain new decision variables (Chen and Joseph, 1987). This formulation works well only if there is a little structural plant-model mismatch and the changing operating conditions provide sufficient excitation to estimate the uncertain parameters (Yip and Marlin, 2004). Such conditions are rarely met in practice, for this reason, the classical approach of RTO will not satisfy the necessary conditions of optimality (NCO) and the real optimum will not be reached using this method.

Later, Roberts incorporated information regarding plant gradients adding an additional modifier to the economic optimization stage that results from the difference between the gradient of the real cost and the model one (Roberts, 1979), this method was called "integrated system optimization and parameter estimation" (ISOPE).

In 2002, Tatjewski proved that the convergence to the optimum point does not depend on parameter estimation but on the equality between the output of the process and the model in each RTO iteration (Tatjewski, 2002), for this reason, he introduced a new modifier that takes into account the difference between these outputs. New modifiers were

also defined by Gao and Engell for process dependent constraints (Gao and Engell, 2005).

From these ideas, several methods have emerged; most of them require the calculation of experimental gradients, which is a difficult task.

One of these methods is called Dual modifier-adaptation (Marchetti et al., 2010) which estimates experimental gradients based on the past operating points generated by the previous RTO iterations by using the definition of directional derivative. To ensure that gradients are obtained accurately a new constraint is added to the optimization problem. This constraint represents the dual characteristic of the method: while the rest of the optimization tries to converge to the optimum of the modified model (primal objective), the dual constraint ensures that in the next RTO iteration the system will have enough energy to estimate the process gradient again (dual objective).

To avoid the calculation of experimental gradients, a recent formulation of modifier-adaptation as a nested optimization problem has been developed (Navia et al., 2013). This method uses a gradient-free algorithm, for example, the Nelder-Mead algorithm, to update the modifiers, iterating with them over the modified optimization until the optimum of the process is found, in this way, gradient estimation and the modifier calculus steps are replaced by any other method that takes into account the minimization of the cost function measured directly from the process.

The Nelder-Mead algorithm has been chosen because it requires less function evaluations per iteration, typically only one or two evaluations of the cost function, than other direct search methods. This property is very important considering that each evaluation implies changing the operation point of the real process.

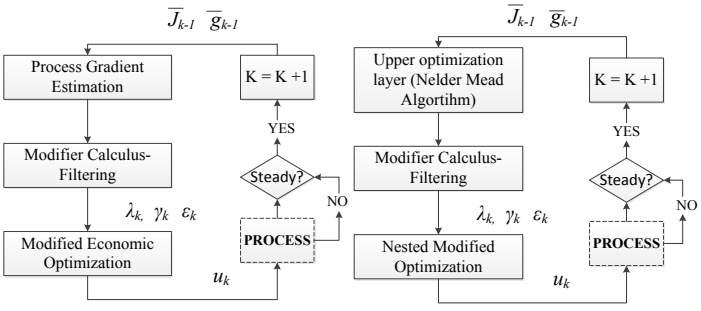

Fig.2. Dual Modifier and Nested Modifier adaptation methodology

In this paper, modifier-adaptation methodology has been applied to a distillation column simulation using a gradient based method Dual modifier-adaptation (DMA) and a gradient free method, Nested Modifier-Adaptation (NMA) to solve the problem that results from the uncertainty presents in RTO of distillation columns. In this example, uncertainties are due to the modelling mismatch between the stationary and the dynamic model of the process and also in the MPC layer that is based on linear dynamic models identified around a certain identification point and could be incorrect if the process is operated away this point. The simulated distillation column is composed by 129 differential equations and 197 algebraic which supposes a realistic simulation.

The paper is organized as follows. Section two presents the description of the case study. Section three shows the use of the stationary and dynamic models of the process. The next section presents formulation of RTO problem. Section five presents the results of the implementation of modifier-adaptation methodology in two scenarios, under noise-free and noisy conditions. Finally, section six gives some conclusions.

2. CASE STUDY

2.1 Process description

The oil refining process involves several distillation units; one of them is the separation of propane in a depropanizer column. A depropanizer is a distillation column that is used to isolate propane from a mixture containing butane and other heavy components.

Continuous distillation columns use variation of temperature and pressure conditions along the height of the column to get more volatile component at the top of the column, propane in this case, and less volatile component at the bottom of the column, that is, butane.

The control objective for the distillation column is to maintain the composition of propane in distillate and bottom streams at their desired specifications by controlling head and bottom temperatures. These temperatures are obtained by the economic optimization carried out in the RTO layer which sends the set-points to the Model Predictive Control (DMC) layer which is responsible to keep the process under control at this target manipulating the reflux to the column and the vapour boil up flow rate which are the set points of PID controllers. This control structure is shown in Fig.3.

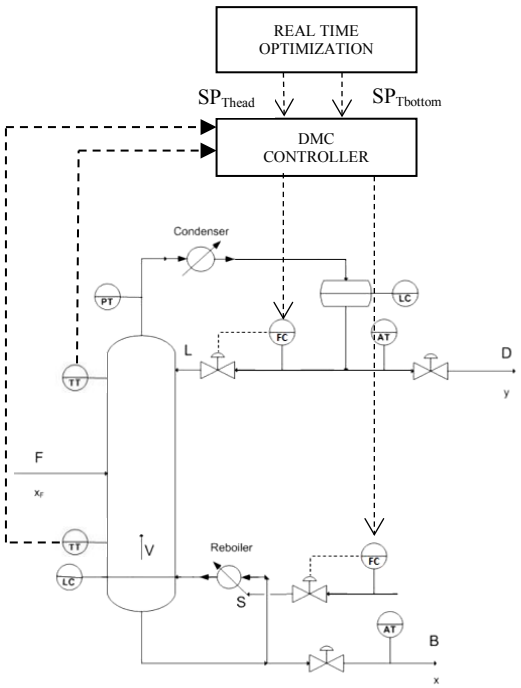

Fig. 3. Control structure of a depropanizer distillation column

The considered depropanizer is an industrial example located in Repsol YPF Tarragona Refinery (Spain), it has a total condenser, a partial reboiler, 37 equilibrium stages, and operates at 1.57 10^6 Pa. The feed mixture enters the depropanizer at stage 19 at a flow rate of 468 kmol/h and 330.42 K. The composition of the feed is 45.55 mol% propane, 44.67 mol% butane, and 9.77 mol% ethane. The main equations of the dynamic model are presented in the next section.

2.1.1Material balances

The column mass balances in each tray are given by equations (1)-(6), where *dmol/dt* is the variation of the molar flow (kmol/h), *n* is the number of tray, *l, v, f* are liquid, vapour and feed molar flow respectively (kmol/h), l_{ref} is the molar reflux flow (kmol/h) and *B* and *D* are the molar flow of bottom and distillate streams. (1) presents the overall mass balance around the n^{th} tray, whereas (2), (3), (4) and (5) show the mass balances in the feed tray, the top of the column (tray k), the bottom (tray 1)and the top accumulator where l_{acum} is the flow that comes from the condenser and $l_{overflow}$ is the excess liquid that overflows from the accumulator:

$$\frac{dmol_n}{dt} = l_{n+1} + v_{n-1} - l_n - v_n \tag{1}$$

$$\frac{dmol_{n\_feed}}{dt} = f + l_{n\_feed+1} + v_{n\_feed-1} - l_{n\_feed} - v_{n\_feed} \tag{2}$$

$$\frac{dmol_k}{dt} = l_{ref} + v_{k-1} - l_k - v_k \tag{3}$$

$$\frac{dmol_1}{dt} = l_2 + v_1 - B \tag{4}$$

$$\frac{dmol_{acum}}{dt} = l_{acum} - l_{ref} - D - l_{overflow} \tag{5}$$

Component mass balances are expressed by (6) - (8) where $x_{j,n}$ and $y_{j,n}$ are the composition of component *j* (butane, propane and ethane) in the liquid and vapour streams through n^{th} tray (º/1mol):

$$\frac{dx_{j,n}}{dt} = l_{n+1}x_{j,n+1} + v_{n-1}y_{j,n-1} - l_n x_{j,n} - v_n y_{j,n} \tag{6}$$

$$\frac{dx_{j,n\_feed}}{dt} = fz_j + l_{n\_feed+1}x_{j,n\_feed+1} + v_{n\_feed-1}y_{j,n\_feed-1} - l_{n\_feed}x_{j,n\_feed} - v_{n\_feed}y_{j,n\_feed} \tag{7}$$

$$\sum_j x_{j,n} = 1 \qquad \sum_j y_{j,n} = 1 \tag{8}$$

2.1.2 Energy balances

Energy balances around the nth tray have been modelled as steady-state model and are expressed by (9) - (14), where H_v is the vapour enthalpy (kJ/kg), h_l is the liquid enthalpy (kJ/kg) and h_j is the specific enthalpy of each component (kJ/kg) that depends on the tray temperature T_n (K):

$$H_{v,n}v_n = h_{l,n+1}l_{n+1} + H_{v,n-1}v_{n-1} - h_{l,n}l_n \tag{11}$$

$$H_{v,n\_feed}v_{n\_feed} = h_f f + h_{l,n\_feed+1}l_{n\_feed+1} + H_{v,n\_feed-1}v_{n\_feed-1} - h_{l,n\_feed}l_n \tag{12}$$

$$H_{v,n} = \sum_j y_{j,n}h_j(T_n) \tag{13}$$

$$h_{l,n} = \sum_j x_{j,n}h_j(T_n) \tag{14}$$

2.1.3 Vapour-liquid equilibrium:

The concentration of vapour in contact with liquid at equilibrium $y_{eq\ j,n}$ in each tray is often expressed by the Raoult's law (15) where the equilibrium constant $K_{j,n}$ is given by the ratio between component j vapour pressure $P_{sat,j}$ (Pa) and the total pressure in the n^{th} tray P_n (Pa):

$$y_{eq\ j,n} = K_{j,n}x_{j,n} \tag{15}$$

$$K_{j,n} = \frac{P_{sat,j}}{P_n} \tag{16}$$

4. USE OF THE MODELS

The nonlinear dynamic model described before has been used to simulate the distillation process in the system modelling and simulation software called EcosimPro. It is composed by 2056 equations (129 differential equations, 1927 algebraic equations) and 2152 variables (1887 explicit, 129 derivative, 40 algebraic and 96 boundary variables). It is also used to identify the prediction model of the DMC controller, a step response model.

A nonlinear stationary model of the process is developed from the dynamic one and it is used by the RTO layer to make decisions. It is formed by 1076 equations and 1076 variables (928 explicit, 148 algebraic and 7 boundaries).

The uncertainty presents in this process has two sources. One, is the modelling mismatch that appears between the stationary and the dynamic model. There are parameters that have been changed in the stationary model to cause this type of uncertainty, such as, equilibrium constants (-2%) , tray efficiency (+15%) and the pressure of the reboiler (+80%). On the other hand, the DMC controller is based in a linear dynamic model of the process which has been identified around a certain operating point of head and bottom temperatures (T_{head} = 322.65 K, T_{bottom}= 366.15 K) and steam and distillate mass flows of (S = 5254.32 kg/h, D = 8735.38 kg/h), far away from this point this model could not be correct, it implies more uncertainty as long as decision variables are moved from the identification point.

5. RTO PROBLEM FORMULATION

The economic objective of RTO is to maximize the profit obtained from producing distillate *D* (kg/h) with a purity specification minimizing the steam consumption *S* (kg/h). Prices P_D and P_S have been fixed for both streams, 80 €/ton for the distillate obtained and 50 €/ton for the steam consumed. The objective function is represented by the value of *J* (€/h) calculated by (17) and the constraints over the

composition of propane in distillate and bottoms g_1 and g_2 are expressed by (18):

$$\max_{\{T_{head},T_{bottoms}\}} J = P_D D - P_s S \quad (17)$$

s.t

$$g_1 = x_D(C_3H_8) \geq 0.80$$
$$g_2 = x_B(C_3H_8) \leq 0.025 \quad (18)$$

Stationary model of the process

The number of modifiers required to adapt the RTO problem n_K is given by (19) where n_u is the number of decision variables, head and bottom temperatures (T_{head}, T_{bottom}), and n_g is the number of constraints (distillate and bottoms composition) so, in our problem $n_k = 8$.

$$n_k = n_g + n_u(n_g + 1) \quad (19)$$

The modified problem is expressed by (20) and (21). The superscript "–" indicates that the variable is measured from the process and the subscript "*k-1*" is the measurement taken in the steady state before:

$$\max_{\{T_{head},T_{bottoms}\}} J = P_D D - P_s S + \lambda_1 T_{head} + \lambda_2 T_{bottom} \quad (20)$$

s.t

$$g_1 = -x_D(C_3H_8) + 0.80 + \gamma_1(T_{head} - T_{head,k-1}) + \gamma_2(T_{bottom} - T_{bottom,k-1}) + \varepsilon_{g1} \leq 0$$
$$g_2 = x_B(C_3H_8) - 0.025 + \gamma_3(T_{head} - T_{head,k-1}) + \gamma_4(T_{bottom} - T_{bottom,k-1}) + \varepsilon_{g2} \leq 0 \quad (21)$$

Stationary model of the process

Modifiers λ, γ and ε are given by (22) - (24) and represent the difference between experimental and model gradients:

$$\lambda_1 = \frac{\partial \bar{J}}{\partial lT_{head}} - \frac{\partial J}{\partial T_{head}} \qquad \lambda_2 = \frac{\partial \bar{J}}{\partial T_{bottom}} - \frac{\partial J}{\partial T_{bottom}} \quad (22)$$

$$\gamma_1 = \frac{\partial \bar{g}_1}{\partial T_{head}} - \frac{\partial g_1}{\partial T_{head}} \qquad \gamma_2 = \frac{\partial \bar{g}_1}{\partial T_{bottom}} - \frac{\partial g_1}{\partial T_{bottom}} \quad (23)$$

$$\gamma_3 = \frac{\partial \bar{g}_2}{\partial T_{head}} - \frac{\partial g_2}{\partial T_{head}} \qquad \gamma_4 = \frac{\partial \bar{g}_2}{\partial T_{bottom}} - \frac{\partial g_2}{\partial T_{bottom}}$$
$$\varepsilon_{g1} = \bar{g}_1 - g_1 \qquad \varepsilon_{g2} = \bar{g}_2 - g_2 \quad (24)$$

The NMA algorithm starts from a given value of the modifiers, obtained with any of the methods available to calculate the process gradients. After the next steady state is reached, modifiers are updated using an unconstrained gradient free algorithm, for example the Nelder Mead algorithm, that takes modifiers as their decision variables and uses the cost function measured from the process as their objective function.

However, DMA calculates the experimental gradients by using the definition of directional derivative and adding a constraint in the grade of excitation of the process to ensure sufficient information in the measurements and guarantee gradient accuracy.

4. RESULTS

A performance comparison of DMA and NMA methods in a noise-free and noisy scenario has been made. All cases start from the same operating conditions, the model optimum which corresponds to the optimum reached by the process if the RTO problem is not adapted.

4.1 *Noise- free scenario*

Fig.4 shows the evolution of the objective function applying the previously mentioned algorithms for noise-free scenario.

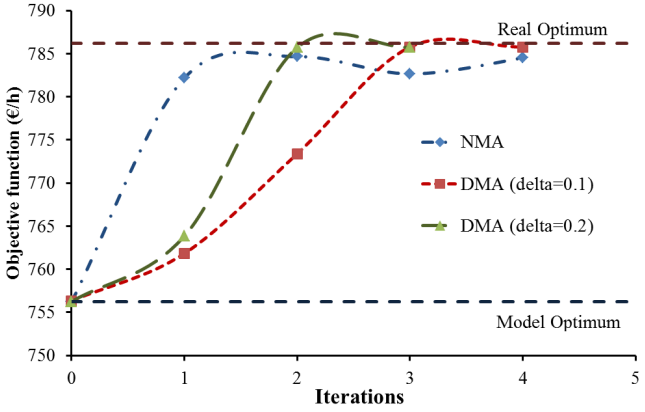

Fig.4. Evolution of the objective function for noise-free scenario

The above figure shows that the NMA method (blue diamonds) converges to the real optimum of the process after four iterations; similarly, the DMA (green triangles and red squares) reaches the same point by using four with a δ equal to 0.1 and three when δ is equal to 0.2. However, the solution of the NMA algorithm approximates faster to the optimal zone by only using one iteration.

In DMA methods is needed to take into account the grade of excitation of the process to ensure sufficient information in the measurements and guarantee gradient accuracy. This is equivalent to choose the parameter δ, which is very sensitive to the evolution to the real optimum of the process as can be noted from Fig.4. A bigger value of δ implies an increase in the excitation of the system. Table 1 presents a quantitative analysis of the performance of the different methods. Values in parentheses show the percentage of deviation respect to the real optimum.

Table 1. Comparison of results for noise-free scenario

	Real Optimum	Model Optimum	NMA	DMA (δ= 0.1)	DMA (δ = 0.2)
Steam mass flow (kg/h)	***5477.77***	5633.14 (2.84)	5399.96 (-1.42)	5444.82 (-0.60)	5475.09 (-0.05)
Reflux mass flow(kg/h)	***8976.44***	9840.60 (9.63)	8710.32 (-2.96)	8833.67 (-1.59)	8934.05 (-0.47)
Distillate mass flow (kg/h)	***11197.08***	10861.10 (-3.00)	11162.01 (-0.31)	11208.63 (0.10)	11246.07 (0.44)
Distillate composition (°/1)	***0.80***	0.82 (2.25)	0.80 (0.00)	0.80 (0.00)	0.80 (0.00)
Head Temperature (K)	***325.66***	319.03 (-2.04)	325.53 (-0.04)	325.87 (0.06)	326.37 (0.22)
Bottom Temperature (K)	***374.74***	375.70 (0.26)	374.46 (-0.07)	375.39 (0.17)	375.92 (0.32)
Cost function (€/h)	***786.21***	756.22 (-3.81)	784.51 (-0.22)	785.77 (-0.06)	785.71 (-0.06)

As can be seen in Table 1, there is an important improvement in the cost function from using RTO without modifiers to use RTO modified, saving approximately 30 €/h.

The evolution of the composition of the distillate for DMA with δ = 0.1 and NMA is shown in Fig 5. The founded solution using any of these methods is always situated in this active constraint, $X_D \geq 0.80$, as expected.

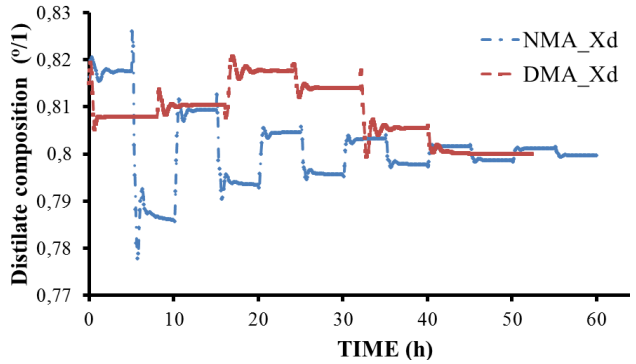

Fig.5. Evolution of the composition of propane in the distillate stream.

To reach this composition the temperatures has changed according to the references given by the RTO layer following the path shown in Fig.6.

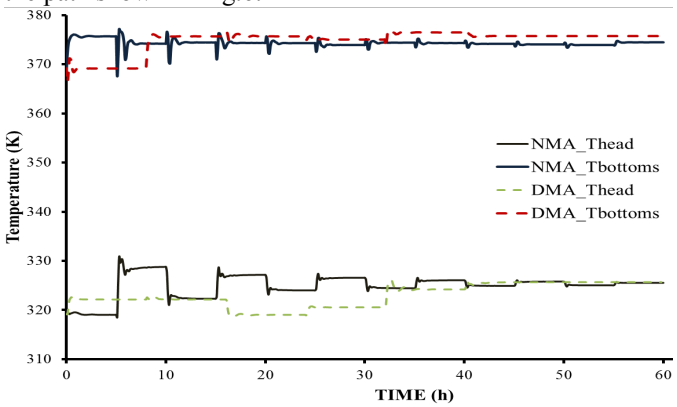

Fig.6. Variation of head and bottom temperatures in the distillation column.

The steam and reflux flows have been manipulated as Fig.7. shows:

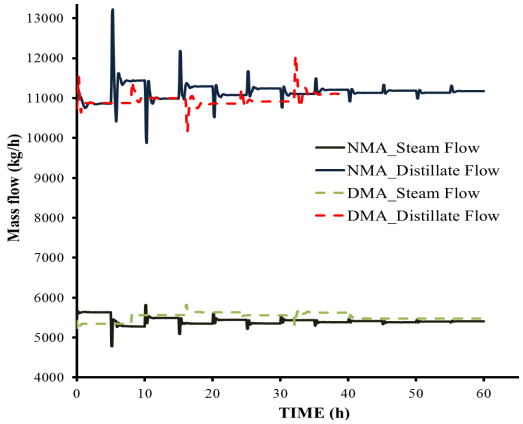

Fig.7. Variation of steam and reflux flow rates.

In both methods the number of iterations is not the same than the number of RTOs solved or steady states reached. In the case of DMA method the total of steady states that is necessary to reach the optimal solution is equal to the number of iterations plus n_u+1 previous states to calculate the gradients iterations by using the definition of directional derivative. For the NMA algorithm, the amount of steady states reached is higher because the construction of initial simplex requires n_K +1 steady states previous. In addition, each iteration of the Nelder Mead Algorithm could require several steady state evaluations. This is a disadvantage of this type of methods since processes can reach a steady state after several hours so, they take a long time before starting to work. In this example, steady states are reached every five hours when NMA is applied and six hours for DMA because the changes in temperature references are more drastic using this method.

4.2 Noisy scenario

The described algorithms have been checked under more realistic conditions by adding a white noise error in the measurements of distillate and bottoms composition of propane. The maximum amplitude was a 1% of the total range of the mole fraction so the measurement composition can be represented as $X_i \pm 0.005$. The random noise has been filtered using the average value of the last twenty measurements measured every fifteen seconds.

Fig.8 shows the evolution of the objective function applying the previously mentioned algorithms under noisy conditions.

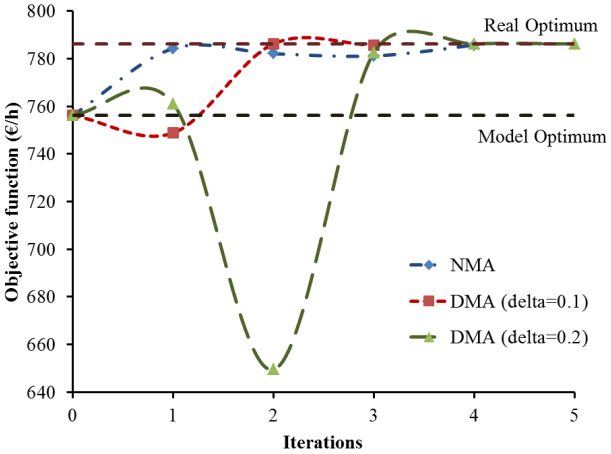

Fig.8. Evolution of the objective function under noisy conditions

The evolution of the gradient-free based method is quite similar to the previous case without noise. However, the evolution of the cost function using DMA is different under noisy conditions observing that the objective function jumps sharply from one iteration to another. This jump is bigger with a δ = 0.20 since the bigger this parameter the greater the excitation of the system and also, it drives the process to the optimum following a less optimal path.

With higher amplitude of noise the resulting operating point may be suboptimal or even infeasible; in this case, the NMA

method seems to be more robust since it does not require the calculation of process gradients (Navia, D. 2013).

Fig.9 shows the evolution of the propane composition including the noise error in the distillate applying DMA with a parameter δ equal to 0.20 and NMA. Both methods reach the active constraint $X_D \geq 0.80$.

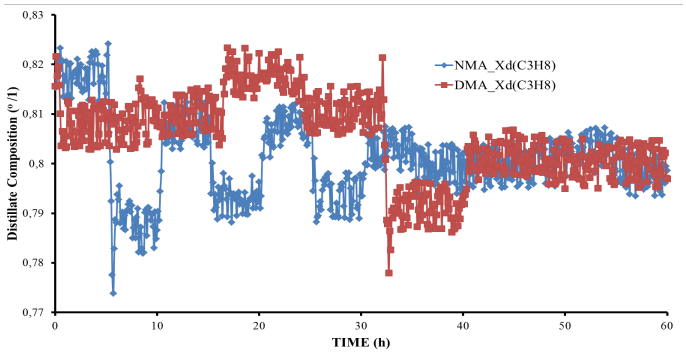

Fig.9. Variation of the composition of propane in the distillate stream under noisy conditions

Table 2 presents the results obtained with the different methods. Values in parentheses show the percentage of deviation respect to the real optimum.

Table 2. Comparison of results for noisy scenario

	Real Optimum	Model Optimum	NMA	DMA (δ= 0.1)	DMA (δ = 0.2)
Steam mass flow (kg/h)	***5477.77***	5633.14 (2.84)	5402.99 (-1.37)	5444.27 (-0.61)	5475.20 (-0.05)
Reflux mass flow(kg/h)	***8976.44***	9840.60 (9.63)	8726.91 (-2.78)	8808.38 (-1.87)	8966.54 (-0.11)
Distillate mass flow (kg/h)	***11197.08***	10861.10 (-3.00)	11155.80 (-0.37)	11240.08 (0.38)	11195.80 (-0.01)
Distillate composition (°/1)	***0.80***	0.82 (2.25)	0.80±0.005 (0.00)	0.80±0.005 (0.00)	0.80±0.005 (0.00)
Head Temperature (K)	***325.66***	319.03 (-2.04)	325.90 (0.07)	326.30 (0.20)	325.65 (0.00)
Bottom Temperature (K)	***374.74***	375.70 (0.26)	374.20 (-0.14)	375.56 (0.22)	375.70 (0.26)
Cost function (€/h)	***786.21***	756.22 (-3.81)	785.70±2 (-0.17)	785.64±8 (-0.07)	786.16±3 (-0.01)

The results presented in Table 2 show that the applied methods reach an operation point near to the real optimum being the final cost function better in the case of DMA, however, it is observed that its variability is higher than using NMA.

5. CONCLUSIONS

In this paper, two types of modifier-adaptation methodology in the context of RTO have been considered, gradient-free and gradient-based algorithms. These methods have been implemented in a realistic example as a depropanizer distillation column with a hierarchical control structure that is part of the refining process in all refineries (RTO, DMC and PID layers).

Both approaches are able to reach an operating point close to the real optimum starting from the same situation that is the model optimum, which is equivalent to solve RTO without modifiers. This ability does not change under noisy conditions, so both methods seem to be robust enough for this situation. However, NMA is less sensitive to noise during the evolution to optimal steady state since it does not require the calculation of experimental gradients.

To conclude, it has been proved that modifier-adaptation methodology work well with few decision variables but, the difficulty of these methods increase with the number of inputs because of the estimation of experimental gradients and the increase in the number of modifiers that are needed.
The application of these methods in reality is also unpractical due to the necessity of reaching a steady state in each iteration and the no guarantee of satisfying constraints during the transient states , so trying to use dynamical optimization to avoid these problems is an issue that should be considered in future work.

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