**Modifier-Adaptation approach to deal with structural and parametric uncertainty**

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**Abstract:** Real-Time Optimization (RTO) is not always able to achieve optimal process operation due to the presence of significant uncertainty about the plant models that are used to make decisions and also due to the differences between control architecture layers which operate on different time-scales and use different kind of models. To overcome these issues the economic optimization problem is modified following the Modifier Adaptation methodology to bring the process to the real optimum despite the presence of uncertainty by using plant measurements.

To deal with parametric and structural plant-model mismatch, a new approach is presented that combines the estimation of process gradients from transient and steady-state information. It speeds up the convergence of Modifier Adaptation methodology to the process optimum. The approach is illustrated through the simulated example of a depropanizer distillation column.

**Keywords:** Real-Time optimization, modifier-adaptation, uncertainty, distillation columns.

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1. INTRODUCTION

The management of large scale systems, such as many in the 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.

RTO makes decisions 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). However, optimal operation is not guaranteed since process models are inaccurate, so the optimum of the process may not be the same as the optimum computed from the model.

Several proposals have been developed to cope with the uncertainty already mentioned and to drive the process to its real optimum point. 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 little structural plant-model mismatch and the changing operating conditions provide sufficient excitation to estimate the uncertain parameters (Yip and Marlin, 2004).

Later on, 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 outputs of the process and the model at each RTO iteration (Tatjewski, 2002). For this reason, he introduced a new modifier that takes into account the differences between these outputs. New modifiers were also defined by Gao and Engell for process dependent constraints (Gao and Engell, 2005).

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**Fig.1. General formulation of Modifier Adaptation methodology (MA).**

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From these ideas, several methods have emerged; most of them requiring the computation of experimental gradients, which is a difficult task.
One of these methods is called Dual Modifier Adaptation (DMA) (Marchetti et al., 2010) which estimates experimental gradients based on 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 excitation to estimate the process gradient adequately (dual objective). This approach has been implemented on the case study shown in this paper.

To avoid the direct calculation of experimental gradients, a formulation called Nested- Modifier Adaptation (NMA) has been developed (Navia et al., 2013). This method uses a nested optimization architecture with a gradient-free optimization algorithm, 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, the process gradient estimation is replaced by other methods that take into account the minimization of the cost function measured directly from the process.

Both methods, NMA and DMA, were successfully implemented and compared in a realistic example as a depropanizer distillation column (Rodríguez-Blanco et al., 2015).

One of the main disadvantages of MA is the necessity of waiting for the steady state of the process for each adaptation of modifiers. In many real applications, such as the operation of distillation columns, this state could be achieved after several hours, so the convergence of MA would be very slow and the real optimum could be achieved after several days of operation. During this period of time operating conditions or differences between process and model may change and the method will not converge to the real optimum. This issue makes the application of this methodology unpractical in these cases.

To overcome this problem, a MA approach that uses transient measurements can be applied (François et al., 2014). This method consists of using transient measurements to estimate the steady-state values of the gradients that are required to compute the modifiers, allowing convergence to the plant optimum within a single steady-state. In that way waiting for the steady state at each iteration is not necessary so the MA approach is sped up. Nevertheless, this method presents also strong limitations such as:

- The method works well only if there is parametric uncertainty or little structural plant model mismatch.
- The optimum is achieved but may be not following a feasible path.
- The number of output measurements must be at least equal to the number of uncertain parameters \( n_y \geq n_\theta \)

To overcome the first limitation mentioned above a new methodology is presented that combines MA by using transient measurements with the traditional methodology which estimates process gradients from steady state information.

The paper is organized as follows. Section two presents a short description of MA using transient measurements. The next section presents a MA approach to deal with both, parametric and structural uncertainty. Section four describes the case study and the stationary and dynamic models of the process. The following section presents formulation of RTO problem. Section six presents the results of the implementation of different modifier-adaptation approaches. Finally, the paper ends with some conclusions and references.

2. MODIFIER ADAPTATION USING TRANSIENT INFORMATION

This method consists of using transient measurements to estimate the steady-state value of plant gradients and therefore the value of modifiers, thus allowing convergence to the steady-state plant optimum within a single iteration. For this purpose, measurements at each optimization instant (during the transient) are used to estimate the modifiers of the optimization problem, the solution of which provides the new set of constant inputs \( u \) to be applied to the plant until the next optimization instant.

The philosophy behind this framework is inspired from Neighbouring- Extremal techniques, which use transient information for steady-state optimization. The main difference is that the control update is not obtained by computing a control law but, rather, by solving a modified optimization problem.

Consider the following static optimization problem:

\[
\min_u J(u) = \phi(x,u,\theta) \\
\text{s.t} \quad F(x,u,\theta) = 0
\]

(1)

Where \( J \) is the cost to be minimized and \( \phi \) is a smooth function that represents the cost depending on the unknown parameters \( \theta \). The model includes the output equation (2):

\[
y = H(x,u,\theta)
\]

(2)

Here the variables \( x, u, \) and \( y \) represent the states, inputs, and outputs at steady state.

From the analysis of the first order variations of necessary optimality conditions (NCO), considering the parametric variations \( \delta \theta \) around the nominal values of the parameters, \( \theta_{\text{nom}} \), the gradient condition of the Lagrangian for optimality \( g_{\text{opt}} \) can be expressed as (3) (François et al., 2014):

\[
g_{\text{opt}} = A\delta u + B\delta \theta = 0
\]

(3)

With

\[
A = \nabla^2 \phi \quad B = \nabla^2 \phi
\]

\[
\delta \phi = \delta u + P\delta \theta
\]

(4)

Output variables can be linearized with respect to \( x, u \) and \( \theta \):

\[
\delta y = Q\delta u + P\delta \theta
\]

(5)
With
\[ Q = \frac{\partial y}{\partial u} \quad P = \frac{\partial y}{\partial \theta} \]  
(6)

Let us assume \( ny \geq n\theta \), that is, there are at least as many output measurements as there are uncertain parameters. Using (5), the parametric variations \( \partial \theta \) can be inferred from \( \partial y \) and \( \partial u \) as follows:
\[ \partial \theta = D(\partial \dot{y} - Q\partial \dot{u}) \]  
(7)

where \( D \) is a pseudoinverse of \( P \).

Equation (3) provides a first-order approximation to the cost gradient, which can be estimated from \( \partial y \) and \( \partial u \) upon using (7) to eliminate \( \partial \theta \):
\[ g(t) = G_y \partial \dot{y}(t) + G_u \partial \dot{u}(t) = \frac{\partial \phi}{\partial u} \]  
(8)

\[ G_y = BD = \frac{\partial^2 \phi}{\partial u \partial \theta} \left( \frac{\partial y}{\partial \theta} \right)^{-1} = \frac{\partial^2 \phi}{\partial u \partial y} \]  
(9)

\[ G_u = A - BDQ = \frac{\partial^2 \phi}{\partial u \partial y} \]  
(10)

Considering that \( \Delta u \) has the same value for the model and the process, that is \( u_{to} = u \), RTO modifiers \( \lambda \) can be expressed by the following equation being \( g_p \) the process cost gradient, \( y_p \) output measurement from the process and \( y_{nom} \) the model output for the nominal solution (RTO without modifiers):
\[ \lambda = g_p - g = G_y \partial \dot{y}_p + G_u \partial \dot{u}_p - (G_y \partial \dot{y} + G_u \partial \dot{u}) \]  
(11)

\[ \partial \dot{y}_p = y_p - y_{nom} \]  
(12)

\[ \partial \dot{y} = y - y_{nom} \]  
(13)

The main advantage of this method is that the process cost gradient is estimated only by using the model offline, through expression for \( G_y \) (9) and \( \partial \dot{y}_p \) measured from the process.

3. MODIFIER ADAPTATION APPROACH TO DEAL WITH PARAMETRIC AND STRUCTURAL UNCERTAINTY

One idea to speed up the convergence of MA methodology is to combine the use of transient measurements with the traditional methodology which estimates process gradients waiting for the steady state. In that way one could deal with both, parametric and structural plant-model mismatch.

This methodology consists of two steps:

1) First MA is applied by using transient measurements to overcome the parametric uncertainty between the process and the model used in RTO layer applying the method described in the previous section.

2) Once, the steady-state is achieved, the method based on transient measurements won’t be able to find a more optimal operating point, for this reason, static MA is applied at the end of the transient to deal with the structural plant-model mismatch, computing the process gradients from steady state information applying the DMA methodology.

4. CASE STUDY

4.1 Process description

The petro refining process uses many distillation units, in particular, depropanizers are distillation columns used to isolate propane from a mixture containing butane and other heavy components.

Continuous distillation columns use variations 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, among them, butane.

The control objective for the depropanizer column considered in this paper is to maintain the composition of propane in the distillate stream at the desired specification by manipulating the reflux to the column and the vapour boil up flow rate. The control structure and the associated RTO are shown in Fig.2.

Fig.2. Control structure of a depropanizer distillation column.

The considered depropanizer corresponds to an industrial example located in the Repsol Tarragona Refinery (Spain), comprising a total condenser, a partial reboiler, 37 equilibrium stages, and operates at 1.57 \( 10^8 \) 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.

4.2 Material and energy balances

The column mass balances in each tray are given by equations (14)-(18), where \( dmol/dt \) is the accumulation 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. (14) presents the overall mass balance around the \( n^{th} \) tray, whereas (15), (16), (17) and (18) show the mass balances in the feed tray, the top of the
column (tray k), the bottom (tray 1) and the top accumulator where $l_{\text{sum}}$ is the flow that comes from the condenser and $l_{\text{overflow}}$ is the excess liquid that overflows from the accumulator:

$$\frac{dl_{n}}{dt} = l_{n+1} + v_{n-1} - l_{n} - v_{n}$$  
(14)

$$\frac{dl_{n, \text{feed}}}{dt} = f + l_{n, \text{feed}+1} + v_{n-1} - l_{n, \text{feed}} - v_{n, \text{feed}}$$  
(15)

$$\frac{dl_{k}}{dt} = l_{\text{ref}} + v_{k-1} - l_{k} - v_{k}$$  
(16)

$$\frac{dl_{\text{accum}}}{dt} = l_{\text{accum}} - l_{\text{ref}} - l_{\text{overflow}} - D$$  
(18)

Component mass balances are expressed by (19) - (21) 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 nth tray ($\text{mol/m}^3$):

$$\frac{dx_{j,n}}{dt} = l_{n+1}y_{j,n+1} + v_{n-1}y_{j,n-1} - l_{n}x_{j,n} - v_{n}y_{j,n}$$  
(19)

$$\frac{dx_{j,n, \text{feed}}}{dt} = f_{j} + l_{n, \text{feed}+1}y_{j,n, \text{feed}+1} + v_{n-1}y_{j,n, \text{feed}-1} - l_{n, \text{feed}}x_{j,n, \text{feed}} - v_{n, \text{feed}}y_{j,n, \text{feed}}$$  
(20)

$$\sum_{j} x_{j,n} = 1 \quad \sum_{j} y_{j,n} = 1$$  
(21)

Energy balances around the nth tray have been modelled as steady-state model and are expressed by (22) - (25), 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):

$$H_{v,n} = h_{n+1} + H_{v,n-1} - h_{n}$$  
(22)

$$H_{v,n, \text{feed}} = h_{f} + l_{n, \text{feed}+1} + v_{n-1} - l_{n, \text{feed}}$$  
(23)

$$H_{v,n} = \sum_{j} y_{j,n}h_{j}(T_{n})$$  
(24)

$$h_{n} = \sum_{j} x_{j,n}h_{j}(T_{n})$$  
(25)

4.4 RTO model and uncertainty

The nonlinear dynamic model described before has been used to simulate the distillation process in the system modelling and simulation software 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).

The nonlinear stationary model of the process to be used in the RTO is developed from the dynamic one with structural and parametric differences. It is formed by 1076 equations and 1076 variables (928 explicit, 148 algebraic and 7 boundaries).

The uncertainty affecting this process has two main sources. One is the modelling mismatch that appears between the stationary RTO model and the dynamic process, since parameters have been modified on purpose to cause this type of uncertainty, for instance, tray efficiency $E_{f}$ (+20%) that affects the vapour-liquid equilibrium (26). On the other hand, the structural uncertainty since the steady-state model considers that pressure is constant along the distillation column, that is, there is no pressure drop across the column and finally significant energy losses $E_{\text{lost}}$ in each tray are considered in the model used by RTO layer as a function of the difference between tray temperature $T_{\text{tray}}$ and ambient temperature $T_{\text{amb}}$ multiplied by a global heat transfer coefficient $U$. This term has been considered in the steady-state model because it is easier to modify the RTO model than the model describing the real process:

$$E_{\text{lost}} = U(T_{\text{tray}} - T_{\text{amb}})$$  
(28)

The real process is considered to be perfectly insulated so there are not energy losses to the environment.

5. RTO PROBLEM FORMULATION

The economic objective of RTO is to maximize the profit obtained from producing distillate $D$ (kg/h) with a given purity specification minimizing the steam consumption $S$ (kg/h) (Porru et al., 2015). Prices $P_{D}$ and $P_{S}$ have been fixed for both streams, 50 €/ton for the steam consumed and 80 €/ton for distillate above propane composition specification, below this target, the price decreases as a function of the composition. The objective function is represented by the value of $J$ (€/h) calculated by (29) and the constraint over the composition of propane in distillate stream $g$ is expressed by (30):

$$\max J = P_{D}(x_{D}(C_{j}H_{j}g))D - P_{S}S$$  
(29)

s.t

Stationary model of the process

$$g = x_{D}(C_{j}H_{j}g) \geq 0.80$$  
(30)

The number of modifiers required to adapt the RTO problem $n_{K}$ is given by (31) where $n_{h}$ is the number of decision variables which are reflux and steam flows ($l_{\text{ref}}, S$), and $n_{g}$ is the number of constraints (distillate composition) so, in our problem $n_{h} = 5$.

$$n_{h} = n_{g} + n_{u}(n_{g} + 1)$$  
(31)
The modified problem is given by (32) and (33). The subscript “p” indicates that the variable is measured from the process and the subscript “k-l” is the measurement taken in the previous steady state:

\[ \max J = P_D D - P_r S + \lambda_I l_{ref} + \lambda_S S \]  
\[ \text{s.t.} \]

Stationary model of the process

\[ g = x_g(C_{H_2}) + 0.80 + \gamma_I (l_{ref} - l_{ref}) + \gamma_S (S - S_{ref}) + \varepsilon \leq 0 \]

Modifiers \( \lambda, \gamma \) and \( \varepsilon \) are given by (34) - (36) and represent the difference between experimental and model gradients:

\[ \lambda_I = \frac{\partial J}{\partial l_{ref}} - \frac{\partial J}{\partial l_{ref}} \]

\[ \gamma_I = \frac{\partial g}{\partial l_{ref}} - \frac{\partial g}{\partial l_{ref}} \]

\[ \varepsilon = g_{ref} - g \]

6. RESULTS

6.1 Modifier Adaptation using transient information

MA methodology using transient measurements is not useful for the case where structural uncertainty is present. This can be observed when this approach is applied in the case study described before which presents both, parametric and structural uncertainty.

In this case RTO is executed every half an hour so that the modifiers are also updated every this period of time covering 4 hours. Fig.3 and Fig.4 show the evolution of the decision variables, steam flow and reflux flow in this case, while the evolution of the constraint on propane composition in distillate stream is shown in Fig.5.

Fig.3. Evolution of the Set Point steam flow controller.

Fig.4. Evolution of the Set Point reflux flow controller.

Fig.5. Evolution of the distillate composition (%).

Comparing the values at steady state with the ones of the real optimum in Table 1, the previous graphs show that the MA approach using transient measurements is not able to achieve the real optimum of the process when a structural uncertainty has been considered or even satisfy the process constraint on the propane composition (≥0.80) in steady state. Table 1 includes also results of other approaches, in particular direct RTO without modification (under Model optimum), which provides the worst value of the cost function and also violates the constraint.

6.2 Static Modifier Adaptation

The static approach DMA (Marchetti et.al, 2010) has been implemented on the depropanizer distillation column. RTO is executed every 6 hours that is the time required for the process to achieve a new steady state.

Fig.6 and Fig.7 show the evolution of the RTO decision variables, steam flow and reflux flow, with the evolution of the constraint on propane composition in distillate stream shown in Fig.8.

Fig.6. Evolution of the Set Point steam flow controller.

Fig.7. Evolution of the Set Point reflux flow controller.

Fig.8. Evolution of the distillate composition (%).

In view of the results, static Modifier adaptation is able to achieve the real optimum but after two days of operation (54 hours, 2.25 days), it involves nine steady states, 7 optimization solved plus \( n_u \) initial steady states required to estimate the gradients. This long period of time can result in loss of optimality since operating conditions and plant-model mismatch could change and the method would not converge to the process optimum.

|   | Real optimum | Model optimum | Static MA | Transient MA | New approach |
|---|--------------|---------------|-----------|--------------|--------------|
| Steam flow (Kg/h) | 5558.20 | 5473.42 | 5562.31 | 5679.83 | 5590.26 |
| Reflux flow (Kg/h) | 9389.67 | 8549.26 | 9402.92 | 9753.26 | 9523.33 |
| \( x_d \) (C\(_{3}H_8\)) | 0.80 | 0.76 | 0.80 | 0.78 | 0.80 |
| \( J \) (€/h) | 783.19 | 491.36 | 783.15 | 577.66 | 783.17 |
6.3 Modifier Adaptation approach to deal with parametric and structural uncertainty

Modifier adaptation using transient measurements is applied until this method is not able to find a better operating point, in this case 4 hours, then, a step of traditional modifier adaptation from steady state information is implemented until the real optimum is achieved as seen in Table 1.

The optimum operating point is achieved after 22 hours which means a considerable time reduction compared to the traditional static MA. This period of time involves eight RTO during the transient and only one RTO executed during the steady state. However, three steady states are required, two to estimate process and model gradients and one steady state that is achieved after applying the obtained RTO solution.

7. CONCLUSIONS

In this paper, different Modifier Adaptation approaches have been implemented in a realistic example as a depropanizer distillation column of a refining process.

Static Modifier Adaptation is able to achieve the real optimum of the process, but it takes a long time in the case of processes with long settling time. The use of transient measurements for the gradient estimation speeds up the convergence of MA but it is only valid in the case of parametric uncertainty, so, the process optimum is not reached if structural plant-model mismatch is present. For this reason these two methodologies have been combined showing good performance, reducing the time required to achieve the real optimum of the process by a 60%.

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