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Distributed Stochastic Optimization of a Process Plant Start-up

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Abstract: This paper presents a decentralized solution to the stochastic optimization problems that appear when uncertainty is considered explicitly using a set of scenarios in model based control and optimization. In particular, the paper deals with two-stage optimization problems, where the first-stage solution has to fulfil the constraints for all multiple scenarios simultaneously. To deal with the large size of the problem, a reformulation has been performed solving the optimization in parallel for as many deterministic problems as scenarios are, and coordinating their solutions in order to force a common decision for all of them, using a price-driven methodology followed by a sensitivity-based update. The methodology is illustrated with an example involving the optimal start-up of a hydrodesulphurization plant.

1. INTRODUCTION

One of the main problems associated to the industrial application of model based control and optimization is related to the uncertainty of process behaviour or unreliable measurements. The sources of the variability are diverse, but the effects are similar: model-process gaps leading to prediction errors so that what one computes with the model as optimum, maybe does not corresponds to the real process optimum. Of course, control is a good way of dealing with uncertainty. In control systems, integral action of the controllers and estimators can bring the controlled output to the set point in spite of certain disturbances or model errors. But in this case the target is clearly defined.

Nevertheless, more and more, economic optimization is being used combined with control, either as a two layer structure where the upper level of Real-Time Optimization (RTO) computes steady optimal set points for the underlying dynamic control system according to an economic criterion, or as a combined problem where the dynamic control is calculated in the framework of MPC with a direct economic target (Engell *et al*., 2007) (Gonzalez *et al*., 2001). In these cases, when the model is used to compute the optimal operating point and bringing the process to it, there is no reference to follow and errors or disturbances can lead to wrong decisions. So, it is important to take into account explicitly these sources of errors in the optimization in order to avoid them.

Description of the uncertainty can adopt several formats. Among them, one natural approach is to consider some of the variables intervening in the process as stochastic ones, with a certain probability distribution. This leads to stochastic models and, consequently, to stochastic control and optimization problems that must be solved on-line in the economic MPC.

A general formulation of a stochastic optimization problem is given by:

$$\begin{aligned} &\min_{\mathbf{u}} \ J(\mathbf{x},\mathbf{u},\xi,t_f) \\ &\text{s.t.} \\ &\mathbf{h}(\dot{\mathbf{x}},\mathbf{x},\mathbf{u},\xi,t)=0 \quad \mathbf{x}(t_0)=\mathbf{x}_0 \\ &\mathbf{g}(\mathbf{x},\mathbf{u},\xi,t)\le 0 \\ &\mathbf{x}\in X, \quad \mathbf{u}\in U, \quad \xi\in \Xi, \quad t\in[t_0,t_f] \end{aligned} \tag{1}$$

Where $\boldsymbol{x}$ is the vector of states, $\boldsymbol{u}$ are the decision variables, t is time and ξ represents a random variable that belong to a probability space with a certain probability distribution function (PDF). The process model is given by the set of equations $\boldsymbol{h}$, and the cost function to be minimized is represented by J, while $\boldsymbol{g}$ denotes the constraints on the model variables.

A direct solution of a stochastic dynamic optimization problem cannot be obtained most of the times, so, in practice, the continuous probability distributions characterizing the stochastic variables are discretized, giving rise to a set of scenarios (Birge *et al*., 1997). The optimization is then carried on considering all possible values of these scenarios, over time and solving the problem so that some statistic of the outcomes for all scenarios is minimized satisfying the constraints. If we assume that the random variables can take different values over a certain period of time, the problem is known as multi-stage. Solving these problems requires a lot of computation due to the large number of combinations of scenarios that may appear (Dupacová J., 2002). Nevertheless, in certain cases, it is possible to consider that the information we have about the unknown variables is different over time, as a result of possible measurements or the nature of the problem. For instance, in the start-up of a process unit, it is possible that measurements for some variables are not

available, but, after some period of time, the lab can provide values for them. In these situations, an optimal decision problem can be formulated as a two-stage optimization where in the first stage a single decision has to be made without any other knowledge than the probability distribution of some variables, but considering that its value will be known in the future second–stage (Sahinidis, N. V.,2004). Even so, depending in number of scenarios, the size of the problem can be large enough to require formulations allowing an acceptable degree of parallelization of the solution. The purpose of this paper, and its main novelty, is to present an approach that combines two-stage stochastic optimization with price-coordination methods in order to allow parallel computation of the optimization of each scenario, while maintaining the global constraints of the problem. Price coordination is one of the most promising approaches in distributed control and optimization (Cheng *et al*. 2007), (Martí *et al*. 2013) specially indicated for optimization problems where the global constraints are given by shared resources among the participant components. The method is illustrated with an application to the start-up of a hydrodesulphurization plant of the petrol refining industry.

The paper is organized as follows: after the introduction, a summary of the two-stage stochastic optimization problem is given in section 2, presenting also the main associated problems. Then, section 3 explains the price coordination approach and its application to the solution of two-stage optimization. Next, in section 4 the operation of a hydrodesulphurization plant is explained as well as the application of the method to its start-up, followed in section 5 by the results obtained and a conclusions section.

2. TWO-STAGE STOCHASTIC OPTIMIZATION

As mentioned before, in two-stage problems, the information available about the stochastic variables is considered to be different in both stages: in the first one (stage 0) only their PDF is known, so that one must consider all possible values of these variables, or scenarios, in order to compute the optimal decisions satisfying the constraints. Nevertheless, in the second stage (stage 1) their realizations have taken place so that the uncertain variables are assumed to be known and constant until the end of the prediction horizon. From the point of view of the decision variables, a single decision $\boldsymbol{u}_0(\xi)$ must be computed in the first stage, taking into account all possible values of the uncertainty, while in the second stage several ones $\boldsymbol{u}_1(\xi_1)$ will be computed, corresponding to each of the possible particular values ξ_1 of the stochastic variable in the future. The first stage value $\boldsymbol{u}_0(\xi)$ is the one that will be implemented in the process, according to a receding horizon policy in the framework of MPC. Fig.1 illustrates this scheme, where t_0 is current time and t_1 corresponds to the starting time of the second stage. In mathematical terms, the optimization problem can be stated as:

$$\begin{aligned}
&\min_{\mathbf{u}_0,\mathbf{u}_1} \mathrm{E}[\mathrm{J}_0(\mathbf{u}_0,\mathbf{x}_0(\xi),\xi)+\mathrm{J}_1(\mathbf{u}_1(\xi),\mathbf{x}(\xi),\xi)]\\
&\text{s.t.}\\
&\mathbf{h}_0(\dot{\mathbf{x}}_0(\xi),\mathbf{x}_0(\xi),\mathbf{u}_0,\xi,\mathrm{t})=0 \quad \mathbf{x}_0(\mathrm{t}_0,\xi)=\mathbf{x}_{0\mathrm{i}}\\
&\mathbf{h}_1(\dot{\mathbf{x}}_1(\xi),\mathbf{x}_1(\xi),\mathbf{u}_1(\xi),\xi,\mathrm{t})=0 \quad \mathbf{x}_{1\mathrm{i}}(\xi)=\mathbf{x}_1(\mathrm{t}_1,\xi)\\
&\mathbf{g}_0(\mathbf{x}_0,\mathbf{u}_0,\xi)\le 0, \quad \mathbf{g}_1(\mathbf{x}(\xi_1),\mathbf{u}_1(\xi_1),\xi_1)\le 0\\
&\mathbf{x}\in\mathrm{X}, \quad \mathbf{u}\in\mathrm{U}, \quad \xi,\xi_1\in\Xi, \quad \mathrm{t}\in[\mathrm{t}_0,\mathrm{t}_\mathrm{f}]
\end{aligned} \tag{2}$$

Where the sub-indexes 0 and 1 are referred to the first and the second stage and *E* stands for the expected value of the cost function over the scenarios. Notice that the variables can take several values over time according to a certain parameterization in each stage, but the notation (and figures) has been shortened to only one for simplicity.

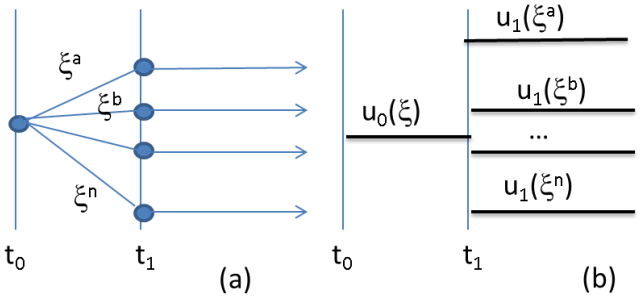

Fig.1. (a) Values of a stochastic variable over time and (b) decisions to be considered in the optimization problem

A solution method of this type of problems considers a set of n scenarios or possible realizations of the stochastic variables $\{\xi^a, \xi^b, \ldots \xi^n\}$, taken from a discretization of its joint probability distribution, and solves (2) as an optimization problem where the cost function is computed as a weighted sum of the costs corresponding to every scenario according to their probabilities while the model and constraints must be satisfied for all scenarios. Hence, the size of the problem is very large because of the simultaneous consideration of all scenarios. Nevertheless, it is possible to exploit the structure of the problem to facilitate parallelization, noticing that the full problem can be split in a set of sub-problems like (2) for each scenario, but with one shared constraint to all of them: the optimal decision u_0 in the first stage must be the same for all scenarios, called the non-anticipativity constraint.

3. PRICE COORDINATION METHODS

Developed with the purpose of facilitating the solution of large scale optimization problems by distributing the computation among several coordinated sub-problems, price coordination methods apply to problems with a structure similar to (3), where the optimization problem is formulated as an aggregation of n sub-problems that have their own local variables $\boldsymbol{x}_j$ and $\boldsymbol{u}_j$ but sharing common constraints R_T. Here the index *j* refers to each of the sub-problems.

$$\begin{aligned}
&\min_{\mathbf{u}_j, j=1,..,n} J = \sum_{j=1}^{n} J_j(\mathbf{x}_j, \mathbf{u}_j) \\
&\mathbf{h}_j(\dot{\mathbf{x}}_j, \mathbf{x}_j, \mathbf{u}_j) = 0 \quad \forall\ j = 1,..,n \\
&\mathbf{g}_j(\mathbf{x}_j, \mathbf{u}_j) \le 0 \quad \forall\ j = 1,..,n \\
&\sum_{j=1}^{n} R_j(\mathbf{u}_j) \le R_T
\end{aligned} \tag{3}$$

In these cases, it is possible to find an equivalent solution using a two level structure as in Fig.2.

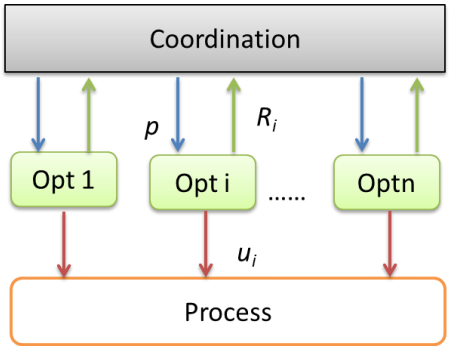

Fig.2. Schematic of price coordination method, with the coordination layer and the modified sub-problems.

Here, in the lower level, *n* modified sub-problems like (4) are solved in parallel independently:

$$\begin{aligned}
&\min_{\mathbf{u}_j} \mathrm{J}_j + \mathbf{p}\mathrm{R}_j \\
&\mathrm{st}: \quad \mathbf{h}_j(\dot{\mathbf{x}}_j, \mathbf{x}_j, \mathbf{u}_j) = 0 \\
&\qquad \mathbf{g}_i(\mathbf{x}_j, \mathbf{u}_j) \le 0
\end{aligned} \tag{4}$$

Notice that every cost function includes a term that depends on its own contribution to the global cost function J_j and on the price $\boldsymbol{p}$ and local use of the shared resources R_j. In the upper coordination level, prices $\boldsymbol{p}$ are computed (one per global constraint) in order to enforce the global constraints and the optimality conditions of the problem (5) (Jose and Ungar, 1998).

$$\begin{aligned}
&\sum_{j=1}^{n} \mathrm{R}_j(\mathbf{u}_j) - \mathrm{R}_T \le 0 \\
&\mathbf{p}\left(\sum_{j=1}^{n} \mathrm{R}_j(\mathbf{u}_j) - \mathrm{R}_T \right) = 0 \quad \mathbf{p} \ge 0
\end{aligned} \tag{5}$$

Several policies can be applied to select $\mathbf{p}$, among them the one based on Newton's method (Cheng, R. et al, 2007), which, for the case of *N* global constraints R_{Ti}, reads as:

$$\begin{aligned}
&\mathbf{p}_{[k+1]} = \mathbf{p}_{[k]} - \alpha \mathbf{Q}^{-1} \mathbf{T}_{[k]} \quad \mathbf{p}^T = [p_1,\ p_2,\ \ldots,\ p_N] \\
&\mathbf{T} = \left[\sum_{j=1}^{n} R_{1j}(u_{1j}) - R_{T1}, \ldots, \sum_{i=1}^{n} R_{Nj}(u_{Nj}) - R_{TN} \right]^T
\end{aligned} \tag{6}$$

Here the index *k* denotes the iteration step, α is the step size in Newton's method and $\boldsymbol{Q}$ is the sensitivity matrix with respect to $\mathbf{p}$ of dimension *N* x *N*. The proposed price-adjustment scheme adaptively updates $\mathbf{p}$, unless the global constraints are fulfilled. $\boldsymbol{Q}$ can be calculated as:

$$\mathbf{Q} = \frac{d \sum_{i=1}^{n} R_{ji}(u)}{d\mathbf{p}}_{[k]} = \sum_{i=1}^{n} \frac{dR_{ji}}{du_{ji}} \frac{du_{ji}}{d\mathbf{p}}_{[k]} \tag{7}$$

The parametric sensitivities d$\boldsymbol{u}$/d$\boldsymbol{p}$ are needed to calculate $\boldsymbol{Q}$ and the general approach of (Ganesh and Biegler, 1987) for a NLP problem will be used to obtain them.

3.1 Sensitivity analysis and changing active set

For the general NLP problem (8) with objective function φ, constraints $\boldsymbol{g}(\cdot)$, decision variables $\boldsymbol{u}$ and $\boldsymbol{p}$ a set of parameters:

$$\begin{aligned}
&\min_{\mathrm{u}} \varphi(\mathbf{u}, \mathbf{p}) \\
&\text{s.t. } \mathbf{g}(\mathbf{u}, \mathbf{p}) \le 0 \\
&\text{with Lagrangean } \mathrm{L}(\mathbf{u}, \mathbf{p}, \boldsymbol{\lambda}) = \varphi(\mathbf{u}, \mathbf{p}) + \boldsymbol{\lambda}^{\mathrm{T}} \mathbf{g}(\mathbf{u}, \mathbf{p})
\end{aligned} \tag{8}$$

At the optimal solution, $\boldsymbol{u}^*$, $\boldsymbol{\lambda}^*$ for a given $\boldsymbol{p}^*$, the constraints $\boldsymbol{g}$ are divided into active constraints $\boldsymbol{g}^{\mathrm{a}}$ and inactive ones $\boldsymbol{g}^{\mathrm{ina}}$ of dimensions n_g^{a} and $n_g - n_g^{a}$, respectively. The corresponding Lagrange multipliers $\boldsymbol{\lambda}^*$ can be divided into $\boldsymbol{\lambda}^{*\mathrm{a}}$ and $\boldsymbol{\lambda}^{*\mathrm{ina}}$. Assuming that φ and $\boldsymbol{g}$ are at least twice continuously differentiable in $\boldsymbol{u}$, the first order necessary conditions of optimally (NCO) of (8) are:

$$\begin{aligned}
&\mathbf{L}_{\mathrm{u}}\left(\mathbf{u}^*, \mathbf{p}^*, \boldsymbol{\lambda}^*\right) = 0, \\
&\mathrm{g}_{\mathrm{i}}^{\mathrm{a}}\left(\mathbf{u}^*, \mathbf{p}^*\right) = 0; \quad \lambda_{\mathrm{i}}^{*\mathrm{a}} > 0; \mathrm{i} = 1,..., \mathrm{n}_{\mathrm{g}}^{\mathrm{a}}, \\
&\mathrm{g}_{\mathrm{j}}^{\mathrm{ina}}\left(\mathbf{u}^*, \mathbf{p}^*\right) < 0; \quad \lambda_{*,\mathrm{i}}^{\mathrm{ina}} = 0; \quad \mathrm{j} = 1,..., \mathrm{n}_{\mathrm{g}}^{\mathrm{ina}}
\end{aligned} \tag{9}$$

with $\boldsymbol{L_u}$ the partial derivative of $\boldsymbol{L}$ respect to $\boldsymbol{u}$. Assuming that the NCO holds at $\boldsymbol{u}^*$, $\boldsymbol{\lambda}^*$ with strict complementarity, the sensitivity of the optimal solution with respect of the parameter $\boldsymbol{p}$, $(\partial \boldsymbol{u}^*/\partial \boldsymbol{p})$ can be obtained deriving equation (9) (Fiacco, 1983), provided the functions $\boldsymbol{u} = \mathbf{u}(\boldsymbol{p})$ and $\boldsymbol{\lambda}^{\mathrm{a}} = \boldsymbol{\lambda}^{\mathrm{a}}(\boldsymbol{p})$ are at least once differentiable in $\boldsymbol{p}$, which leads to:

$$\begin{bmatrix} \mathbf{L}_{\mathbf{uu}} & -\mathbf{g}_{\mathbf{u}}^{\mathrm{a}}(\cdot) \\ \mathbf{g}_{\mathbf{u}}^{\mathrm{a}}(\cdot) & 0 \end{bmatrix} \begin{bmatrix} \dfrac{\partial \mathbf{u}}{\partial \mathbf{p}} \\ \dfrac{\partial \boldsymbol{\lambda}}{\partial \mathbf{p}} \end{bmatrix} = - \begin{bmatrix} \mathbf{L}_{\mathbf{up}}(\cdot) \\ \mathbf{g}_{\mathbf{p}}^{\mathrm{a}}(\cdot) \end{bmatrix} \tag{10}$$

Equation (10) can then be used to obtain the sensitivities when a perturbation $\Delta\boldsymbol{p}$ does not cause a change in the active set. Nevertheless, even for a moderate perturbation $\Delta\boldsymbol{p}$, the set of active constraints can change. The problem can be avoided reformulating equation (10) as a QP problem, to take into account the scenario of change in the active set:

$$\begin{aligned}
&\min_{\Delta \mathbf{u}} \frac{1}{2} \Delta \mathbf{u}^{\mathrm{T}} \mathbf{L}_{\mathbf{uu}} \Delta \mathbf{u} + \Delta \mathbf{p}^{\mathrm{T}} \mathbf{L}_{\mathbf{up}}^{\mathrm{T}} \Delta \mathbf{u} + \frac{\partial \varphi^{\mathrm{T}}}{\partial \mathbf{u}} \Delta \mathbf{u} \\
&\text{s.t} \\
&\mathbf{g}_{\mathbf{u}}(\cdot) \Delta \mathbf{u} \ge -\mathbf{g}_{\mathbf{p}}(\cdot) \Delta \mathbf{p} - \mathrm{g}(\cdot)
\end{aligned} \tag{11}$$

Where all functions are evaluated at $\boldsymbol{u}^*, \boldsymbol{p}^*, \boldsymbol{\lambda}^*$. It is easy to see that the NCO conditions of (11) correspond to (10), so, its solution provides the required sensitivities with the advantage that it does not require specifying the active set as (10) does. For a constant small $\Delta\boldsymbol{p}$ selected by the user, the solution of this QP problem (11) gives the optimal $\Delta\boldsymbol{u}$ (as well as the corresponding active set). Therefore, $\partial\boldsymbol{u}/\partial\boldsymbol{p}$ can be approximated as $\Delta\boldsymbol{u}/\Delta\boldsymbol{p}$.

3.1 Implementation of the price coordination distributed optimization

The two-stage stochastic optimization can be carried on in a distributed way combining the optimization for each scenario with an upper layer of price coordination that enforces the non-anticipativity global constrains of stage one. If the problem is formulated in the framework of MPC, the implementation of the coordinator can be made following the steps of Fig.3 each sampling time.

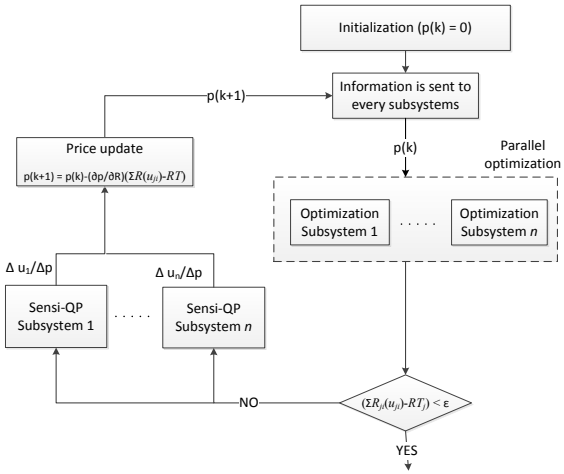

Fig.3. Price-driven coordination algorithm with sensitivity analysis

1. Initialization: The coordination sets up an initial price vector $\boldsymbol{p}(k)$, typically zero, and sends that information to every subsystem.

2. Optimization performed by each subsystem: Based on the price given by the coordinator, each subsystem solves its own optimization problem and calculates the resource $R_j(\boldsymbol{u}_j)$. In addition, each subsystem solves its QP problem in order to determine $\Delta\boldsymbol{u}/\Delta\boldsymbol{p}$ (11). This information is sent back to the coordinator.

3. Price update: The coordinator gathers the information from each subsystem, it calculates $\Sigma R_j(\boldsymbol{u}_j) - R_T$ and $\boldsymbol{Q}$ given by (7). Then, the coordinator updates the price vector $\boldsymbol{p}(k)$ using equation (6). The new price vector is sent to each subsystem.

4. Iteration until convergence: Step (2)-(3) are repeated until convergence is achieved, that is, when the global constraints are satisfy: $\Sigma R_j(\boldsymbol{u}_j)-R_T < \varepsilon$, being ε a tolerance error. If fulfilled initially, $\mathbf{p}$ is set to zero and no update is required.

4. STOCHASTIC NMPC OF A HDS PLANT

4.1 Process description

In order to illustrate the approach, the problem of the optimal start-up of a hydrodesulphurization (HDS) plant has been considered. In petroleum refineries, the HDS process is used to remove sulphur from the hydrocarbons to fulfil environmental regulations. To do this, hydrogen is put in contact with the corresponding hydrocarbon in bed reactors with a specific catalyst. The optimal management of the hydrogen provided is very important in order to operate efficiently: If the quantity of hydrogen supplied is less than the minimum required, then the catalysts can suffer important damage, while if the supply is in excess, economic losses will be experienced (Sarabia et al., 2009).

Fig. 4 shows a simplified structure of a HDS plant. Hydrogen comes from three sources named H4, H3 and LP. H4 and H3 are collectors transporting hydrogen produced in especially dedicated production units. Each unit produces hydrogen at different purity levels. On the other hand, the LP source is a recirculated stream of excess hydrogen with low and variable hydrogen concentration. The mixture that goes through the compressor (C1) must have its hydrogen purity within a range being fed with the hydrocarbon stream (FC), to the packed bed reactors (R1, R2). The products of the reaction (F7) are sent to a separation unit (T1). One part of the excess hydrogen fed is recirculated to the reactors (F11) while the rest (F10) is purged in order to eliminate impurities.

To ensure that enough hydrogen is available for the desulphurization, and the purities are within their limits in the reactor, the operators can modify F1, F2 and F10. On the other hand, a pressure controller manipulates F3 to close material balances. As there are different ways to provide the same amount of hydrogen that the reactor is consuming, the operational target is to supply the required hydrogen to the reactor, using the best combination of the sources from an economic point of view, satisfying the set of operational constraints.

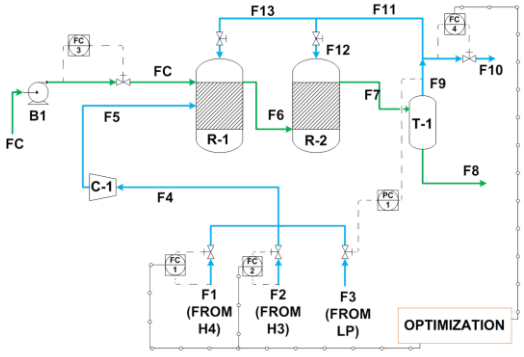

Fig.4. Schematic of the HDS plant

Several problems are related to the hydrogen management that are worth to mention; among them, the lack of reliable information about many streams and compositions, and the uncertainty of the hydrogen consumption in the reactors. Regarding the first one, the uncertainty comes fundamentally in the hydrogen composition of the LP stream since it

depends on the operation of other units. Regarding the reactors, the hydrogen consumption depends on the composition of the hydrocarbon stream being treated in the HDS plants, which is an uncertain variable since its value is linked to the type of oil crude or to production policies. This value changes every 2-3 days, generating a transient lasting some hours after which the uncertain variables can be estimated from measurements. Hence, it is necessary to implement a supervisory layer in the HDS, capable of computing the optimal trajectories of the manipulated variables in order to perform the transition minimizing the total cost of hydrogen, respecting operation constraints and taking into account the main sources of uncertainty previously mentioned: the specific hydrogen demand in the reactors and the hydrogen purity of stream F3.

4.2 NMPC based on stochastic optimization

Assuming that both sources of uncertainty are denoted as ξ_1 and ξ_2 respectively, the optimal stochastic optimization problem using a two-stage approach is summarized in (12), where the objective function is the cost of pure fresh hydrogen weighted with the probabilities of different scenarios of the uncertain variables obtained from a probability distribution assumed to be known. Table 1 summarizes the nomenclature employed.

$$\min_{\{F^j_{1,k},F^j_{2,k},F^j_{10,k}\}} \sum_{k=\{0,1\}}\sum_{j=1}^{N_{Sc}} \Pr^j \left\{ \int_{t_k}^{t_{k+1}} C_{H4}x_1F^j_{1,k} + C_{H3}x_2F^j_{2,k}dt \right\}$$

s.t.:

$$\left.\begin{aligned}
&h_1 := F^j_{1,k}x_1 + F^j_{2,k}x_2 + F^j_3\xi^j_2 = F^j_5x^j_5\\
&h_2 := F^j_{1,k} + F^j_{2,k} + F^j_3 = F^j_5\\
&h_3 := F^j_5 - F^j_{10,k} - F^{H_2,j}_X = 0\\
&h_4 := \frac{VP}{ZRT}\left[\dot{x}^j_{H2}\right] = F^j_5x^j_5 - F^j_{10,k}x^j_{10} - F^{H_2,j}_X x^j_{H2},\\
&\quad x^j_{H2}(t_0) = x_{H2,0}\\
&h_5 := \tau\dot{F}^j_X + F^j_X = F_{HC}\xi^j_1, \quad F^j_X(t_0) = F_{X0}\\
&g_1 := x^j_5 \geq x^{LO}_5,\\
&g_2 := x^j_{H2} \geq x^{LO}_{H2}\\
&g_3 := F^{LO}_m \leq F^j_{m,k} \leq F^{UP}_m, \quad m = \{1,2,10\}\\
&\xi^j_1, \xi^j_2 \in \Xi\\
&t \in [t_k, t_{k+1}], \; t_f = t_2
\end{aligned}\right\} \begin{array}{l} j = 1\ldots N_{Sc} \\ k = \{0,1\} \end{array} \quad (12)$$

$$h_6 := F^j_{m,0} = F^i_{m,0},\ j = 1\ldots N_{Sc},\ i = 1\ldots N_{Sc},\ j \neq i,\ m = \{1,2,10\}$$

The model implemented in (12) is based on mass balances applied in: a) the mixing point (h_1 and h_2) and b) the control volume composed by R-1, R-2 and T-1 (h_3 and h_4). h_5 represents an approximated first-order dynamics of the hydrogen consumption inside the reactor. Inequality constraints g_1 and g_2 avoid damages in the catalyst inside the reactor. On the other hand, g_3 refers to the capacity constraints of the collectors. In both inequalities, superscript LO and UP denotes the lower and the upper bounds of the variables respectively. Finally, h_6 is the non-anticipativity constraint to force that all the control actions implemented in the first stage must be the same for all the scenarios. The super-index j refers to each of the N_{Sc} scenarios considered for the stochastic variables and k to the stage, 0 or 1, of the two-stage optimization

Table 1. Nomenclature

Variable	Meaning
$F^j_{m,k}$	Molar flow of stream m=1,2,10, in scenario j at stage k (Decision variables)
F^j_m	Molar flow of stream m= 3, 5, and inside the reactor m=X
x^j_m	Molar percentage of hydrogen in stream m=1,2,3,5,10 and inside the reactor m=$H2$
ξ^j_1, ξ^j_2	Stochastic variables representing the hydrogen consumption inside the reactor, and the hydrogen purity of F_3 respectively
$\Pr^j$	Probability of occurrence of scenario j
C_w	Cost of 1 mole of hydrogen in unit w = H3, H4
T, P, V	Temperature, pressure and volume of the reactor
R, Z	Universal constant of gases and compressibility factor

4.3 Solving the two-stage problem by price coordination

As mentioned before, in order to facilitate the solution of the large scale problem (12), the price coordination approach of section 3 can be used, solving a set of N_{Sc} sub-problems with cost function:

$$\min_{\{F^j_{1,k},F^j_{2,k},F^j_{10,k}\}} \sum_{k=\{0,1\}} \Pr^j \left\{ \int_{t_k}^{t_{k+1}} C_{H4}x_1F^j_{1,k} + C_{H3}x_2F^j_{2,k}dt \right\} + p\sum_{m=[1,2,10]}(F^j_{m,0} - F_{m,0})^2 \quad (13)$$

and the whole set of equality and inequality constraints of (12) for a given j, except the non-anticipativity one h_6, formulated as

$$\sum_{m=[1,2,10]}(F^j_{m,0} - F_{m,0})^2 \leq 0 \quad (14)$$

Equation (14) must be enforced by the upper coordination level by proper choice of the prices $\boldsymbol{p}$, following the scheme of Fig.3. The Price-Coordinated method was developed to solve global inequality constraints, how to transform global quality h6 to the inequality constraints (14) is shown in (Cheng *et al*. 2007) and (Martí *et al*. 2013).

5. RESULTS

For simplicity, results corresponding to three scenarios (ξ^1={12.554 0.85}, ξ^2={13.238 0.85} and ξ^3={12.554 0.875}) for the two uncertain variables and a simple parameterization of the three decision variables F_1, F_2 and F_{10} in each stage are shown. In addition, to prevent the exponential growth of the decision variables, the scenario tree has been branched in the first stage and the horizon of the stages has been chosen to be equal to one sampling time (De Lucia and Engell, 2013).

In Fig.5, the constrained purities using centralized (12) and coordinated (13) schemes are compared. Both approaches are applied on the same process for a given set of uncertain parameters (ξ_1 = 13.238 and ξ_2 = 0.85). The centralized optimization problem has 18 decision variables and 21

equations, while using coordinated scheme each optimization problem (12) has been reduced to 6 decision variables and 5 equations (13) that can be solved in parallel. The computational time is reduced by 69.31% each sampling time. The different trajectories show that the solutions obtained using centralized and coordinated approaches have similar behaviour. Therefore, coordinated multi-stage NMPC will be useful to avoid computational explosion when a huge scenario tree with many uncertainties appears. On the other hand, the cost of operating the centralized scheme is 122.45 €, while the coordinated one achieves an operating cost of 123.12 €. The difference being due to tolerance error selected as stop criteria.

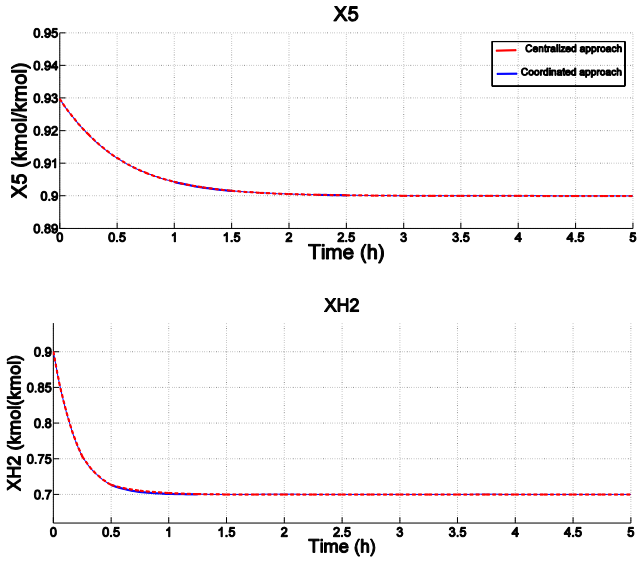

Fig.5. Simulation of multi-stage NMPC using centralized and coordinated approach.

Fig. 6 shows the same purity constraints of coordinated multi-stage NMPC designed in the previous section when it is applied to the process under uncertainties, using different values of $\xi \in \{ \xi^1, \xi^2, \xi^3 \}$ in the model of process (dashed red lines corresponds to ξ^1, solid blue line corresponds to ξ^2 and dashed black line corresponds to ξ^3), always satisfying the 0.7 and 0.9 lower bounds. As it can be seen, coordinated multi-stage NMPC automatically implements a security gap that can prevent the constraints violations minimizing the operations cost.

6. CONCLUSIONS

This work presents an alternative to manage the computational explosion associated to stochastic optimization using two–stage scenario formulation, with a Price-driven coordination scheme to facilitate parallelization of the solution.

The results and the advantages of the coordinated approach are evaluated using a simulated hydrodesulphurization unit that shows that the approach provides a real-time implementable robust controller of the nonlinear process with the same results than the centralized scheme.

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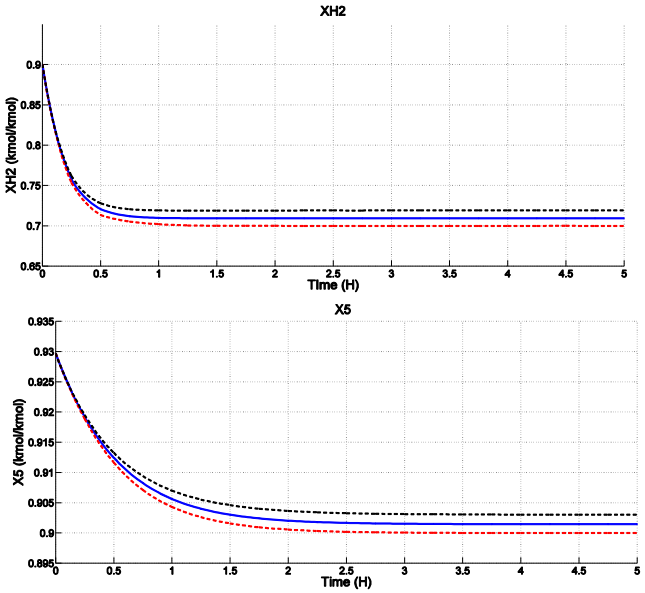

Fig.6. Simulation of coordinated multi-stage NMPC for different values of the uncertain parameters.

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