STOCHASTIC OPTIMIZATION IN A HYDROGEN DISTRIBUTION NETWORK

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Abstract

This paper is about the stochastic optimization in a hydrogen distribution network which feeds a desulfuration plant, using multistage formulation. The network has two hydrogen production units with different levels of purity and one recirculated low purity stream from an adjacent process. The source of uncertainty is the hydrogen consumption in the desulfuration unit, and is correlated with a discrete probability distribution function. The results obtained shows that no matter the values that the random variable can have, the variables are always within a safety-quality range. The cost that must be paid for manage the uncertainties is 4% in average respect deterministic optimization.

Keywords: stochastic programming, multistage, scenario, hydrogen distribution network

I. INTRODUCTION

In a petroleum refinery the desulfuration process is where the sulfur is removed from the hydrocarbon using hydrogen, reducing the acid rain occurrence [1]. The hydrogen is produced, and transported to the desulfuration units in hydrogen distribution networks (HDN's). The optimal management of HDN's is critical: if the quantity of hydrogen transported is less than the minimum required, then the fuel will be out of the emission policies, and if is much more than the required, important losses will be experimented, see [2] for more information. Therefore an optimization in the hydrogen production can be formulated, but the demands of this gas in the desulfuration unit depend on the fuel loaded, which generally is a mixture, so there is uncertainty in this parameter, consequently an appropriate management of these uncertainties is required by using stochastic optimization.

In the classical approach of optimization, the equations and the parameters are considered totally known, but when the solution is applied into the reality, frequently the value of the objective function is worse than the expected and/or the constraints are violated systematically [3]. These problems can be attributed to the uncertainty that affect the system, related with parameters that connect the system with the exterior (e.g. market demands) [4]. Usually, the behavior of these parameters can be described using a random variable ξ that belongs in to a probability space correlated with a probability distribution function (PDF).

For solving this kind of problem, we can assume that there are n stages of decision (k). Each stage can be solved knowing only partial information about the random variable, which is known as multistage formulation. So in the first stage of decision the initial conditions and the PDF of the random variable is known, once that this variable is realized in time, i.e. has a concrete value, we can make a second decision considering: the first one, the value for the random variable in the first stage and the PDF of the random variable in the second stage, and so on with the following stages [5]. Therefore the decision variables in each stage will depend of the value of the random variables in the previous stages. If ξ_k is the random variable in the stage k, the general problem of multistage approach can be formulated as [3]:

$$\begin{aligned}
&\min_u f_0(u_0) + E_{\xi_1}\left[f_1\left(u_1(\xi_1)\right) + E_{\xi_2}\left[u_2(\xi_1,\xi_2) + \dots \right.\right. \\
&\left.\left. E_{\xi_{n-1}}\left[f_{n-1}\left(u_{n-1}(\xi_1,\xi_2,\dots,\xi_{n-1})\right)\right]\dots \right]\right] \\
&s.t.: h_0\left(u_0, x_1(\xi_1)\xi_1\right) \geq 0 \\
&\cdots h_{n-1}\left(u_0,\dots,u_{n-1}(\xi_0,\dots,\xi_{n-1}), x_1(\xi_1),\dots,\right. \\
&\left. x_n(\xi_0,\dots,\xi_n),\xi_n\right) \geq 0
\end{aligned} \tag{1}$$

Being E_{ξ_k} the estimated value of f_k respect to the random variable ξ. The problem in (1), is in the space of probabilities Ξ. If the PDF has only a discrete number of values q, each of them with a determined probability of occurrence π_k^q, the problem in (3), can be reformulated in its

deterministic equivalent by using the scenario approach [6, 7].

In this work we'll use multistage formulation for minimize the production cost of hydrogen in a simplified HDN solving it with scenario approach.

II. Problem Formulation

Let's consider a simplified structure of a HDN represented in Figure 1 that has one desulfuration unit (HD3), two hydrogen production units that produces with different levels of purities (H4 and H3), one low purity recirculated stream that came from other process (UNI), and collectors connecting the production and recirculation units with the desulfuration ones (CH4, CH3 and CBP).

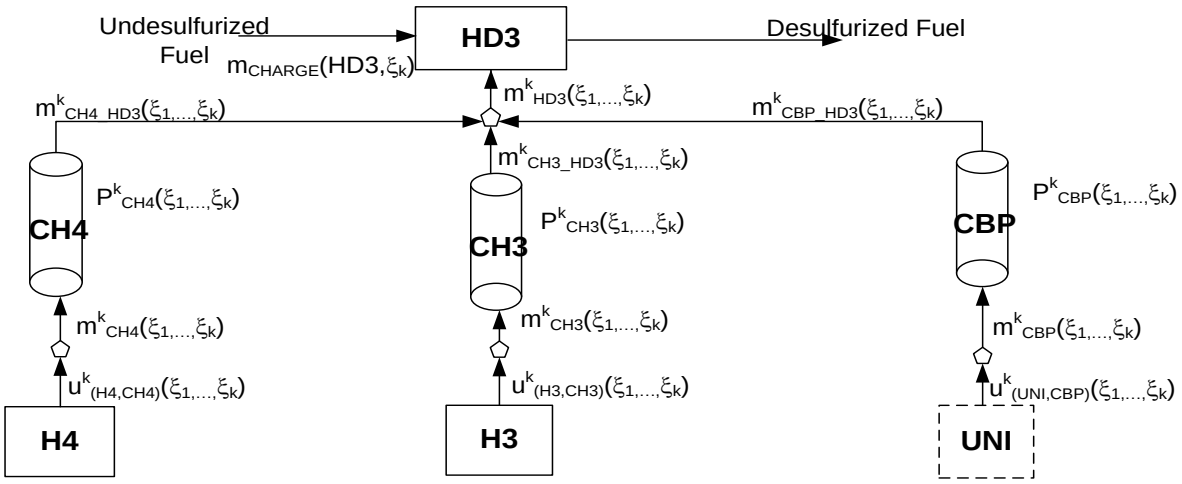


Fig. 1: Process flow sheet for a simplified HDN

The HDN works in stationary state because is a continuous process, but due the uncertainties that affect the system, the problem formulation will be pseudo-stationary i.e.: for each decision stage, the hydrogen demand can change according to its PDF.

Defining the following elements for the optimization:

Sets

PU : Production and recirculation units.

CU : Consumption units.

CL : Hydrogen Collectors.

STR : Process streams.

ξ_k : Random variable in each decision stage: $k = 1,\ldots,n$.

$OPU(PU, CL)$: Process streams that comes out from PU to CL.

$OCL(CL, STR)$: Process streams that come out from CL to CU.

$ICU(CU, STR)$: Process streams that come into CU.

Parameters

$Q_{PU}^{LOW}, Q_{PU}^{UP}$: Lower and Upper hydrogen molar flow production in each PU

x_{PU} : Available hydrogen purity in each PU

C_{PU} : Cost of produce hydrogen in each PU

x_{CU}^{LOW} Minimal mole fraction allowed for the desulfuration process.

P_{CL}^0 : Initial pressure in CL.

$P_{CL}^{LOW}, P_{CL}^{UP}$: Minimal and maximal pressures allowed respectively in each CL.

V_{CL}, T_{CL} : Volume and temperature of the collectors.

Uncertain Parameter

$m_{CHARGE}^k(CU, \xi_k)$: Flow of hydrogen needed for the desulfuration in each stage.

Positive Variables

x_{STR} Hydrogen mole fraction in process streams.

$m_{STR}^k(\xi_1,\ldots,\xi_k)$: Molar flow in process streams, upstream collectors, in stage $k = 1,\ldots,n$.

$u_{(PU,CL)}^k(\xi_1,\ldots,\xi_k)$: Molar flow produced in each PU to CL, in the stage $k = 1,\ldots,n-1$.

$u_{(PU,CL)}^0$: Molar flow produced in each PU to CL in the first decision stage.

x_{CL} Hydrogen mole fraction in CL.

$m_{CL}^k(\xi_1,\ldots,\xi_k)\cdot$: Molar flow that come into each CL, in the stage $k = 1,\ldots,n-1$.

m_{CL}^0: Molar flow that come into each CL, in the first decision stage.

$P_{CL}^k(\xi_1,\ldots,\xi_k)$: Pressure in CL at the end of the stage $k=1,\ldots,n$.

$x_{CU}^k(\xi_1,\ldots,\xi_k)$: Hydrogen mole fraction of the stream that come into CU, in the stage $k=1,\ldots,n$

$m_{CU}^k(\xi_1,\ldots,\xi_k)\cdot$: Molar flow of the stream that come into CU, in the stage $k=1,\ldots,n$.

Free Variables

$A_{CL}^k(\xi_1,\ldots,\xi_k)$: Mole accumulation in each CL, in stage $k=1,\ldots,n$

$\Delta n_{CL}^k(CL,\xi_1,\ldots,\xi_k)$: Quantity of mole accumulated in each CL, in stage $k=1,\ldots,n$

Equations

Mole balance at the entrance of the collector: the molar flow entering in the collector is equal to the sum of molar flows that come from production units.

$$\sum_{UP\in OPU} u_{(PU,CL)}^k(\xi_1,\ldots,\xi_k)=m_{CL}^k(CL,\xi_1,\ldots,\xi_k)$$
$$\sum_{CL\in OPU} u_{(PU,CL)}^0=m_{CL}^0(CL),\quad \forall CL,\quad k=1,\ldots,n-1 \tag{2}$$

Mole balance in the collector: due the different values that the random variable can have, the mole balance in this unit is pseudo-stationary and the difference between the flows produced and consumed is the mole accumulation.

$$m_{CL}^k(\xi_1,\ldots,\xi_k)-\sum_{STR\in OCL} m_{STR}^{k+1}(\xi_1,\ldots,\xi_{k+1})=$$
$$=A_{CL}^{k+1}(\xi_1,\ldots,\xi_{k+1})$$
$$m_{CL}^0-\sum_{STR\in OCL} m_{STR}^1(\xi_1)=A_{CL}^1(\xi_1),\quad \forall CL,$$
$$k=1,\ldots,n-1 \tag{3}$$

The mole accumulation formulated in (6) affects the pressure inside the collectors. The change in this variable is proportional to accumulation time Θ and the difference between inner and outer flows. Ideal Gas Law is used (in operational conditions implies a maximal error of 2.5% [8]).

$$m_{CL}^k(\xi_1,\ldots,\xi_k)-\sum_{STR\in OCL} m_{STR}^{k+1}(\xi_1,\ldots,\xi_{k+1})=$$
$$=\frac{V_{CL}}{\Theta RT_{CL}}\left[P_{CL}^{k+1}(\xi_1,\ldots,\xi_{k+1})-P_{CL}^k(\xi_1,\ldots,\xi_k)\right]$$
$$m_{CL}^0-\sum_{STR\in OCL} m_{STR}^1(\xi_1)=\frac{V_{CL}}{\Theta RT_{CL}}\left[P_{CL}^1(\xi_1)-P_{CL}^0\right],$$
$$\forall CL,\quad k=1,\ldots,n-1 \tag{4}$$

Pressure bounds: For safety reasons, the pressure inside the collector must be bounded.

$$P_{CL}^{LOW}\le P_{CL}^k(\xi_1,\ldots,\xi_k)\le P_{CL}^{UP},\quad \forall CL,\quad k=1,\ldots,n \tag{5}$$

Mole Balance at the entrance of the consumption unit:

$$\sum_{STR\in ICU} m_{STR}^k(\xi_1,\ldots,\xi_k)=m_{CU}^k(\xi_1,\ldots,\xi_k)\quad \forall CU$$
$$k=1,\ldots,n \tag{6}$$

Hydrogen balance at the entrance of the consumption unit:

$$\sum_{STR\in ICU} m_{STR}^k(\xi_1,\ldots,\xi_k)\,x_{STR}(STR)=$$
$$m_{CU}^k(\xi_1,\ldots,\xi_k)\,x_{CU}^k(\xi_1,\ldots,\xi_k),\quad \forall CU,\quad k=1,\ldots,n \tag{7}$$

Minimal purity allowed in the consumption units: The mole fraction of the stream that enters into the consumption unit must be at least grater than a lower bound.

$$x_{CU}^k(\xi_1,\ldots,\xi_k)\ge x_{CU}^{LO},\quad \forall CU,\quad k=1,\ldots,n \tag{8}$$

Minimal hydrogen flow in the consumption units: The hydrogen flow that enters into the desulfuration unit, must be at least the one required for the desulfuration.

$$m_{CU}^k(\xi_1,\ldots,\xi_k)\,x_{CU}^k(\xi_1,\ldots,\xi_k)\ge m_{CHARGE}^k(CU,\xi_k),$$
$$\forall CU.\quad k=1,\ldots,n \tag{9}$$

Purity relationships:

$$x_{PU}=x_{CL},\quad \forall(CL,PU)\in OPU$$
$$x_{CL}=x_{STR},\quad \forall(CL,STR)\in OCL \tag{10}$$

Lower and upper production: operational constraint about production capacity

$$Q_{PU}^{LOW}\le\sum_{CL\in OPU} u_{PU}^k(\xi_1,\ldots,\xi_k)\le Q_{PU}^{UP}$$
$$Q_{PU}^{LOW}\le\sum_{CL\in OPU} u_{PU}^0\le Q_{PU}^{UP},\quad \forall PU,\ldots k=1,\ldots,n \tag{11}$$

Cost of production: the cost of hydrogen production is calculated by using the estimated value for each scenario in every decision stage, just like the expressed in (1) .

$$Cost=\sum_{(PU,CL)}\left[u_{(PU,CL)}^0 x_{PU}C_{PU}\right]+$$
$$+E_{\xi_1}\left[\sum_{(PU,CL)} u_{(PU,CL)}^1(\xi_1)\,x_{PU}C_{PU}+\cdots+\right.$$
$$\left.+E_{\xi_{n-1}}\left[\sum_{(PU,CL)} u_{(PU,CL)}^{n-1}(\xi_1,\ldots,\xi_{n-1})\,x_{PU}\,C_{PU}\right]\ldots\right] \tag{12}$$

So the stochastic optimization problem can be summarized as: minimize (12), subject to (2) to (11).

III. RESULTS AND DISCUSSION

The model was programmed using 3 stages of decision in GAMS™, with CONOPT™ as NLP solver in a computer with Intel Pentium Dual™ T2080 1.73Ghz processor and 2Gb RAM memory. The CPU time was 0.059s with 23 variables and 24 constraints. The optimization was solved using the values of the parameters given in Table 1, and the DPDF of the random variable represented in fig. 2. The lower bound for the purity in the consumption unit was 0.971 in mole fraction.

In stochastic optimization, the idea is ensure a feasible operation having in to account the possible changes in the random variable; in particular we will focus our attention in two constraints: the pressure in collectors and the purity at the entrance of HD3: the pressure is a safety constraint and always must be bounded and the hydrogen purity is a quality constraint that guaranties a good performance of the desulfuration unit.

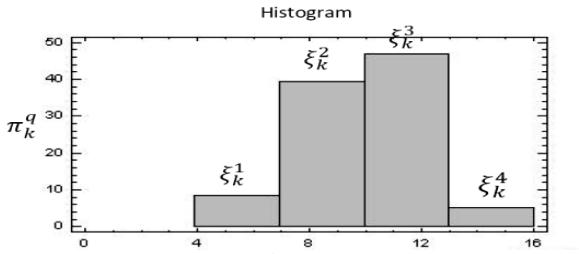


Fig. 2: Discrete PDF for hydrogen consumption

Table 1

Some values of the parameters used in the stochastic optimization

PU	$H4$	$H3$	UNI
$Q_{PU}^{LO}\left(\frac{kmol}{h}\right)$	0	0	0
$Q_{PU}^{UP}\left(\frac{kmol}{h}\right)$	32245	14300	468.77
x_{PU}	0.991	0.94	0.8
$C\left(\frac{€}{\text{MmolH}_2}\right)$	88.1	77	0
CL	$CH4$	$CH3$	CBP
$P_{CL}^{LO}\left(bar\right)$	19	19	19
$P_{CL}^{UP}\left(bar\right)$	21	21	21
$V\left(m^2\right)$	50	50	50
$T\left(K\right)$	300	300	300

Fig. 3 shows the values of purity at the entrance of the desulfuration unit. It can be see that for each possible value that the random variable can have according to its PDF, the purity is greater than the lower bound.

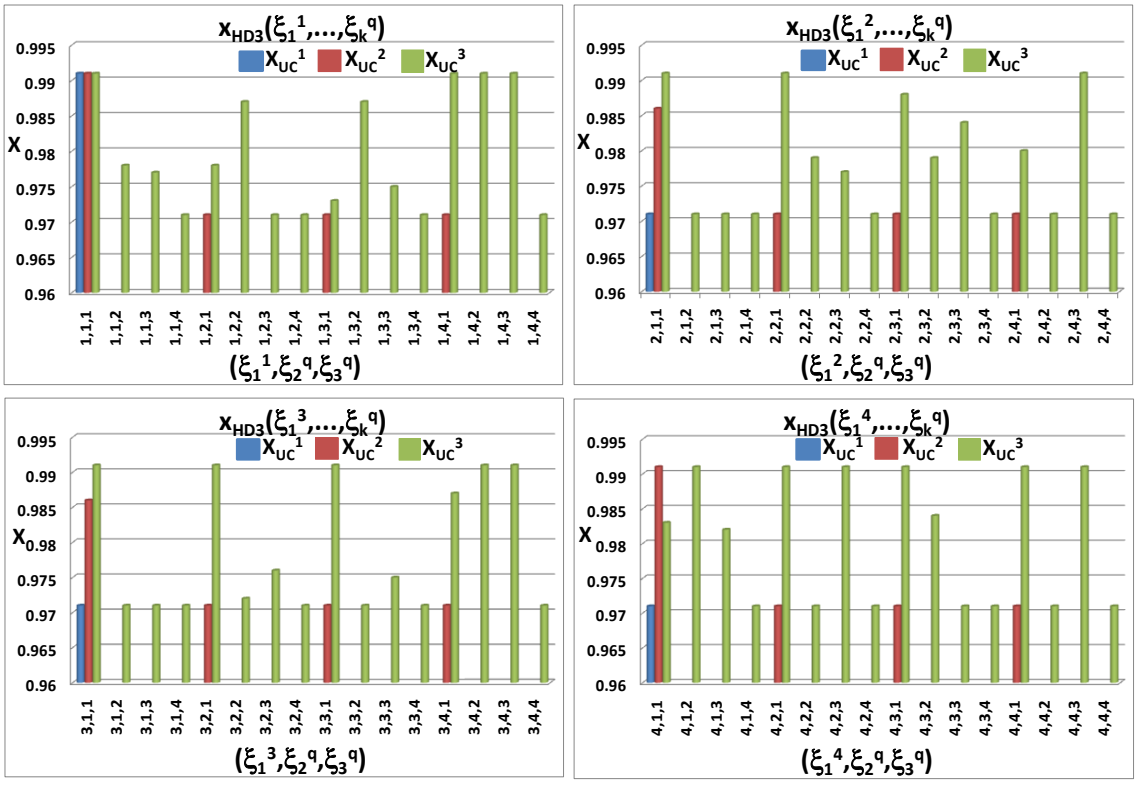
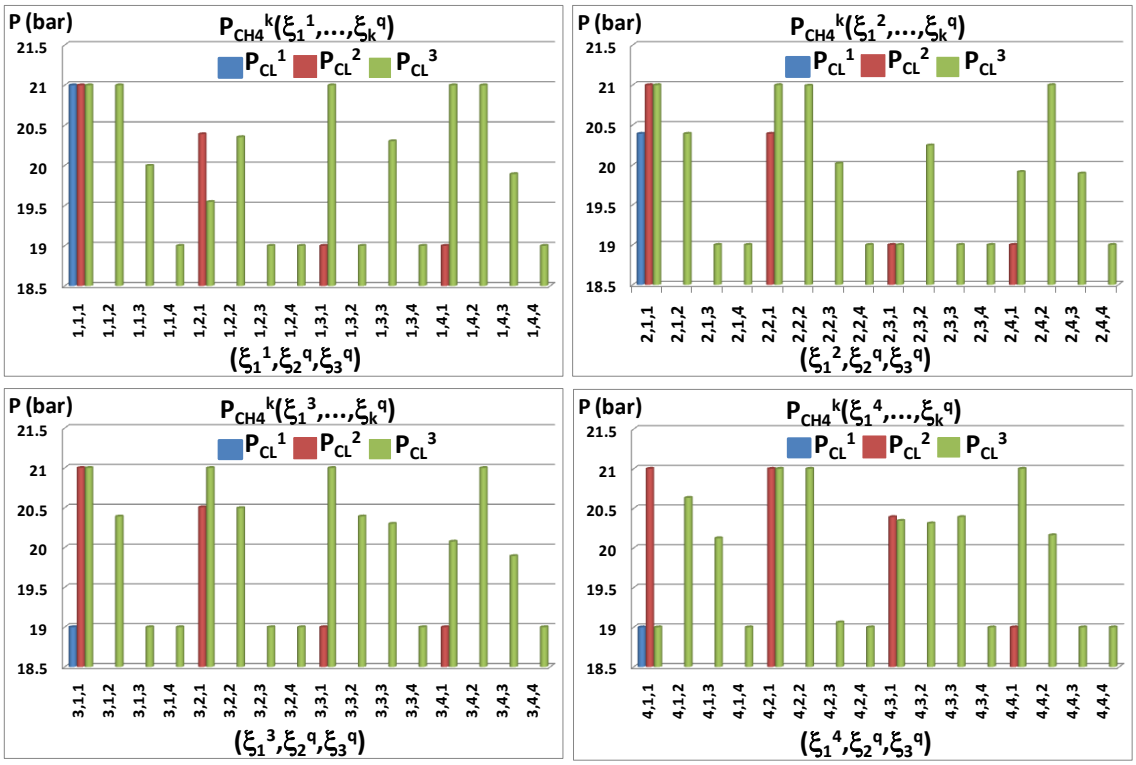


Fig. 3: Evolution of the purity at the entrance of the Consumption unit, for each stage

Fig. 4 shows the evolution of the pressure for CH4 and CH3 in every decision stage (CBP is irrelevant, because for all stages m_{CBP_HD3} is in the upper bound). For every possible value that the hydrogen demand can have, the pressure is always within the safety operational range.



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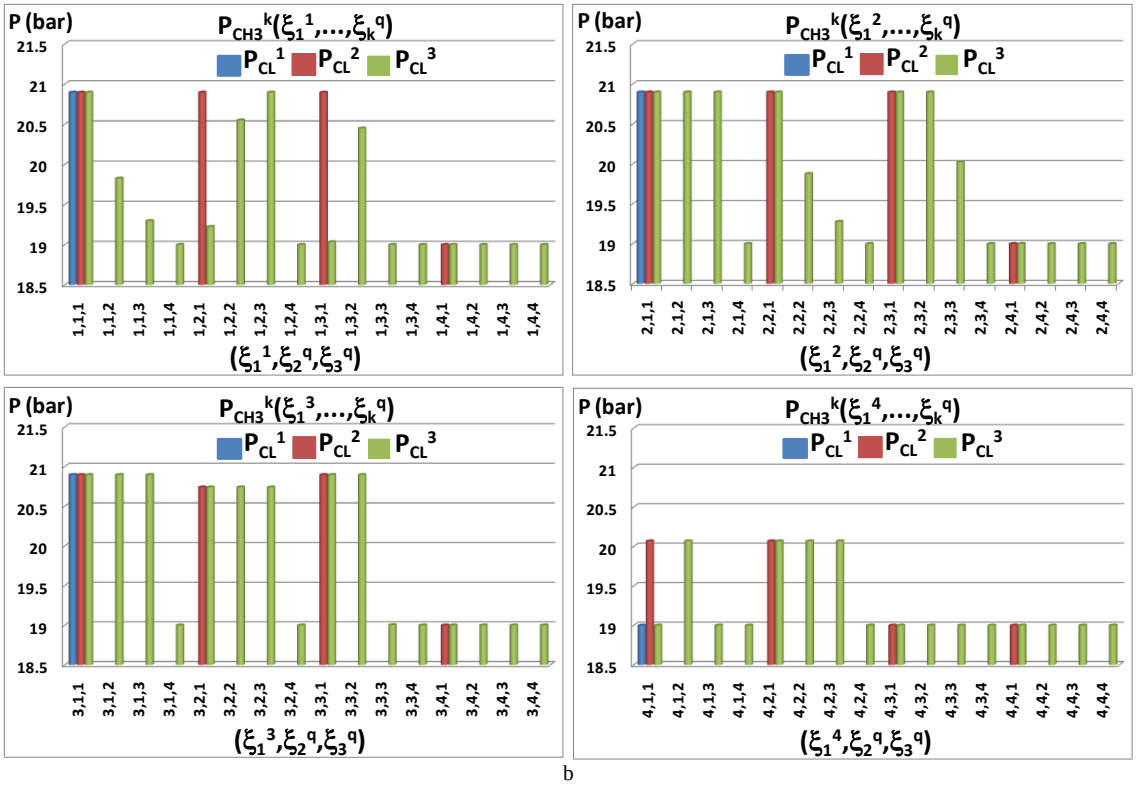

b

Fig. 4: Evolution of the Pressures inside the collectors (a) CH4 and (b) CH3, for each stage

It's important to mention that the feasible operation is only ensured for the values considered in discrete PDF because the scenario formulation.

Finally, Table 2 lists the estimated value of the hydrogen production cost obtained with stochastic approach and the one calculated by deterministic optimization using the expected value of the hydrogen demand. It can be seen that the estimated value of the objective function in stochastic optimization is 4% in average greater than the deterministic result for all the stages considered, which can be understood as the cost that must be paid to manage the uncertainties.

Table 2
Costs obtained with stochastic and deterministic optimization

	Stage	Est. Cost		Cost (€/h)
Stochastic	0	878.04	Deterministic	821.47
	1	810.71		
	2	810.24		

IV. CONCLUSIONS

The use of discrete PDF allows solving the stochastic problem like a deterministic one, but we can guarantee a feasible operation respect to critical variables in a simplified model of HDN (collector pressure and hydrogen purity) only for the values considered. If the solution must be more robust, then more values in the PDF have to be considered, with the corresponding rise in computational effort. The average cost that must be paid for handle the uncertainties is 4% respect to the deterministic optimization.

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