# Data reconciliation and real-time optimization of the hydrogen network in a refinery

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# Outline

- Hydrogen networks, problems and aims
- Plant wide optimization strategy
  - Data reconciliation / Gross errors
  - Optimal hydrogen distribution
  - Hydrogen shortages
- Implementation
- Results
- Conclusions

# Hydrogen in petrol refineries

Hydrogen is used in modern refineries in processes that have two main purposes:

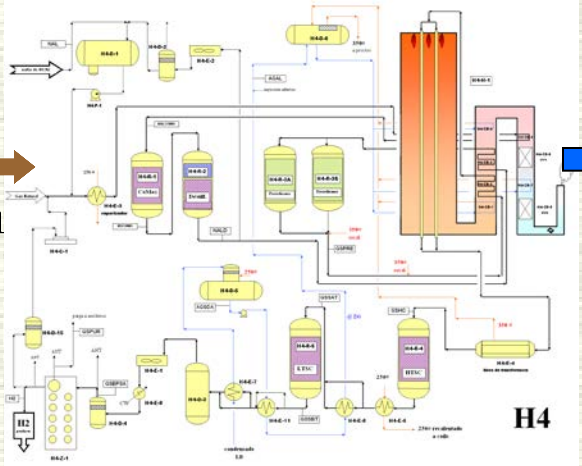
✓Increase the value of the hydrocarbons (platformers, hydrocraking, etc.)

✓Reduce the sulphur content of the products, (HDS),..

# Hydrogen plants (producers / consumers)

HC

Steam



$H_2$

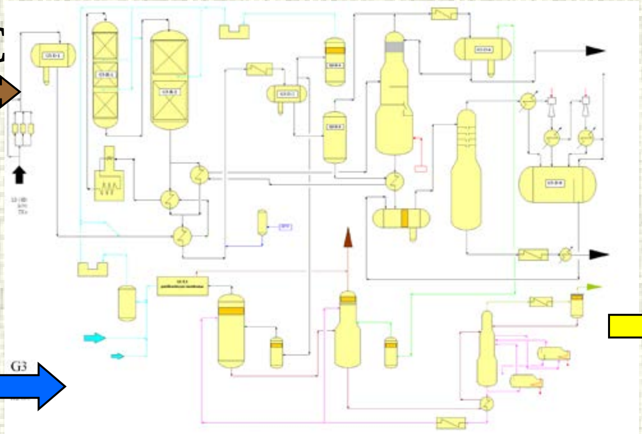
Flow

Purity

Hydrogen producer plant

catalytic hydrotreating reactions

HC



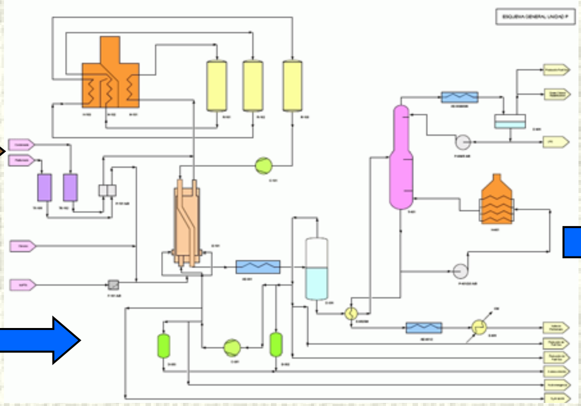
S

$H_2$

Hydrodesulphurization plant HDS

Hydrocrakers

HC

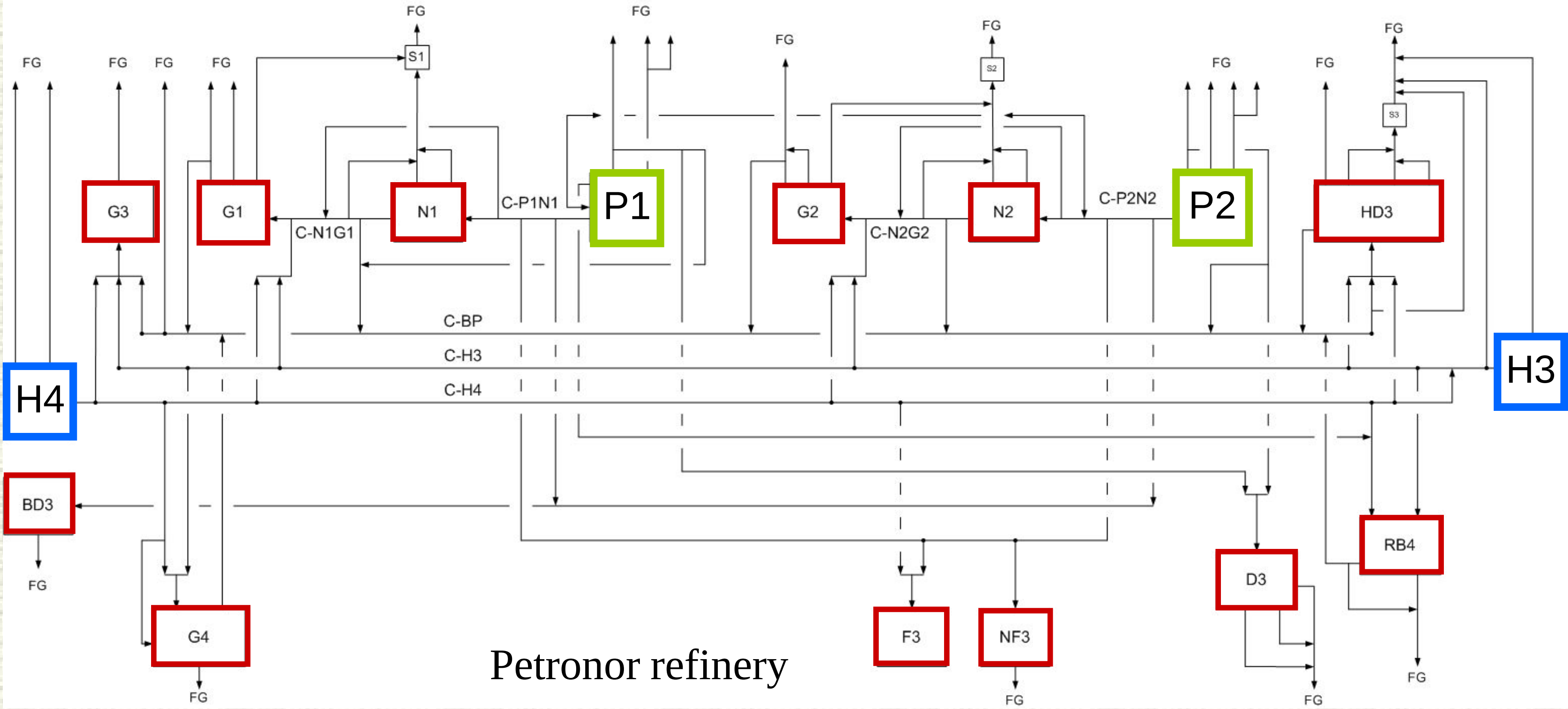


$H_2$

Low purity $H_2$ obtained as a by-product

Platformer

# Distribution network

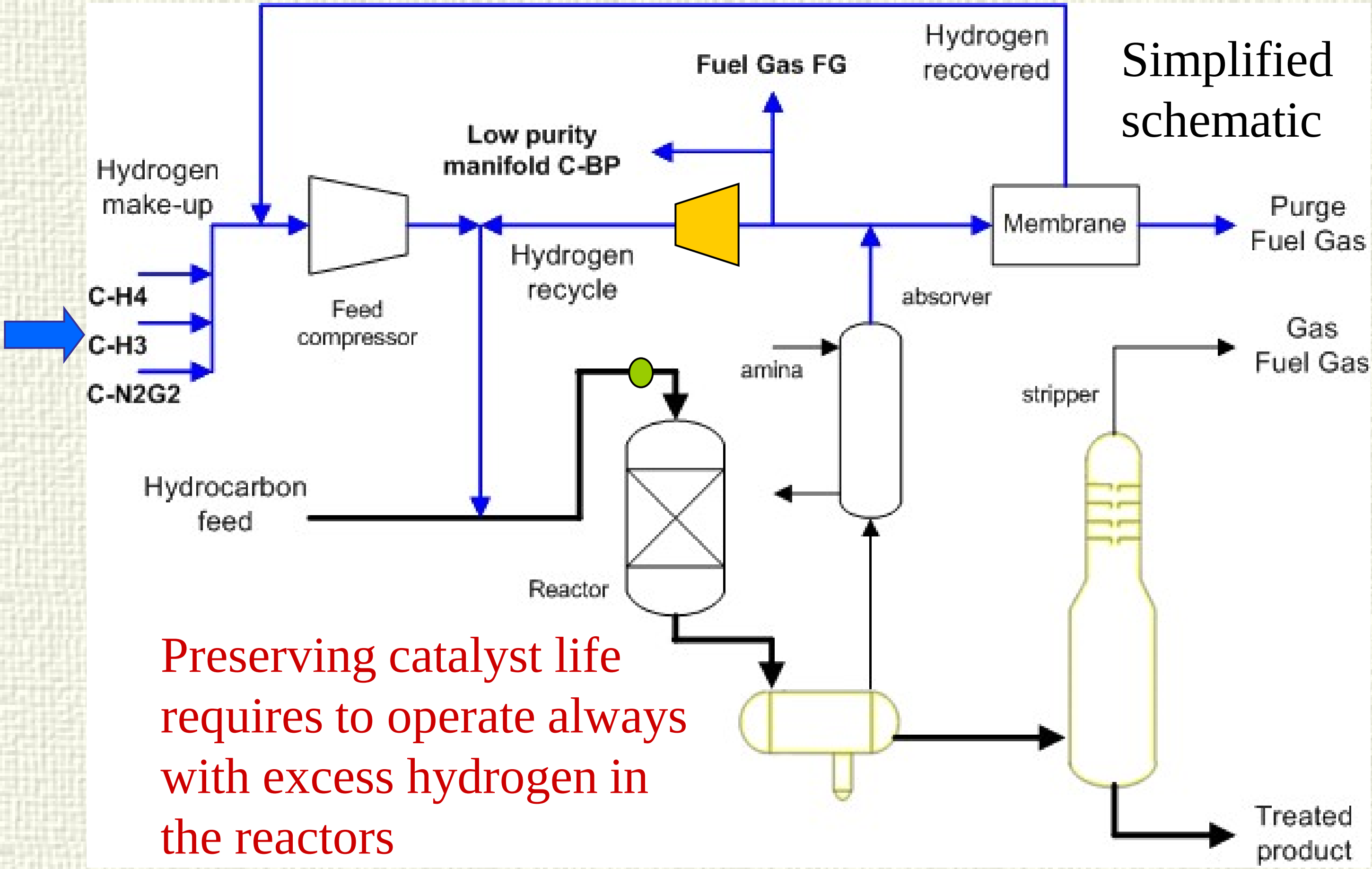


Petronor refinery

- 🟦 $H_2$ production units (2)
- 🟩 $H_2$ production units as by product (2)
- 🟥 $H_2$ consuming units (12)

Sub-networks with different pressures and purities / several supply sources

# HDS



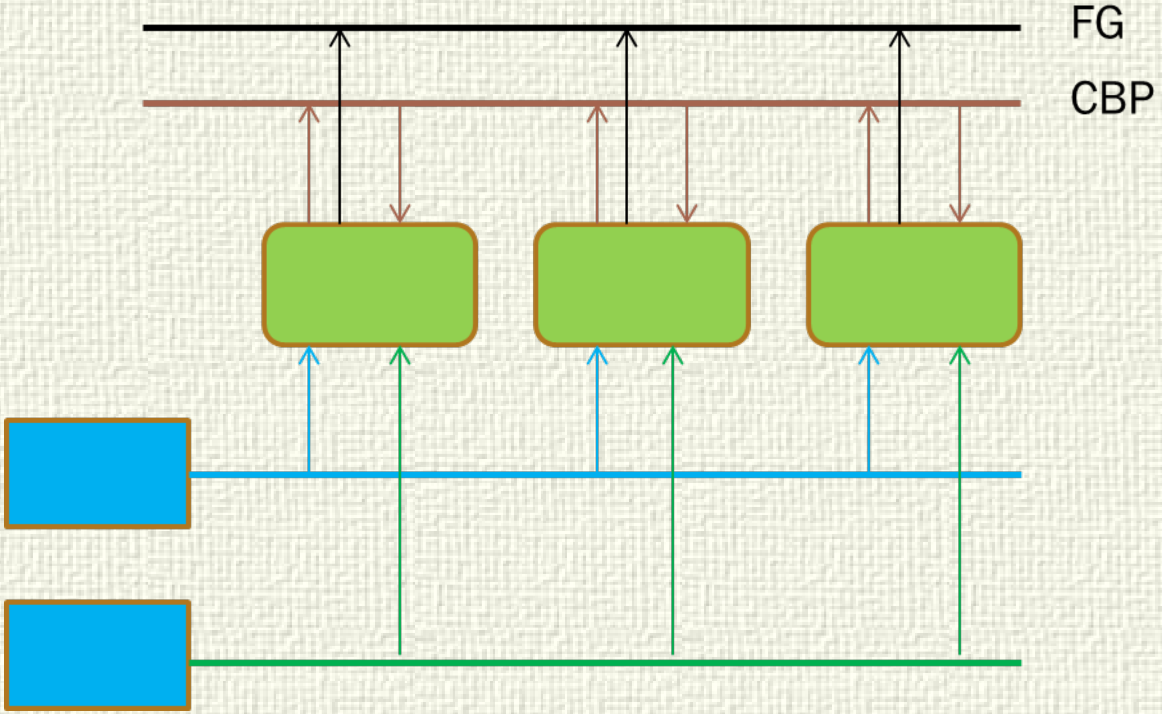
Simplified schematic

Preserving catalyst life requires to operate always with excess hydrogen in the reactors

Variable hydrogen demand according to the type and flow of the hydrocarbon to be treated

The excess hydrogen is partly recycled, partly sent to the fuel-gas FG or CBP networks to prevent accumulation of impurities

# Networks

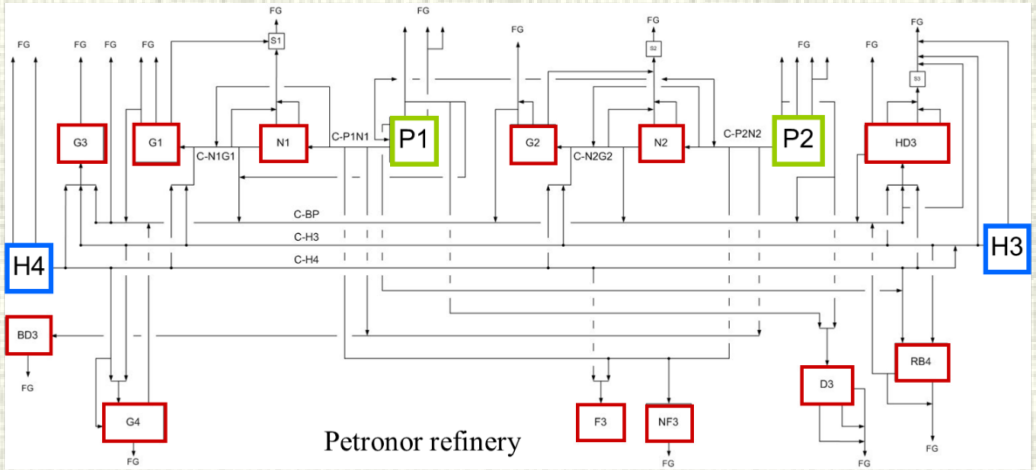


Burnt
Recycled

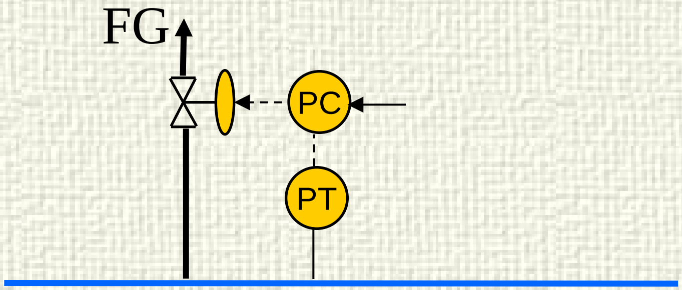
Consumer plants can be supplied from different networks with different purities: fresh hydrogen or recycled and some hydrogen is release to the FG network.

Constraints affect to pressure and purity

# Network operation



Petronor refinery



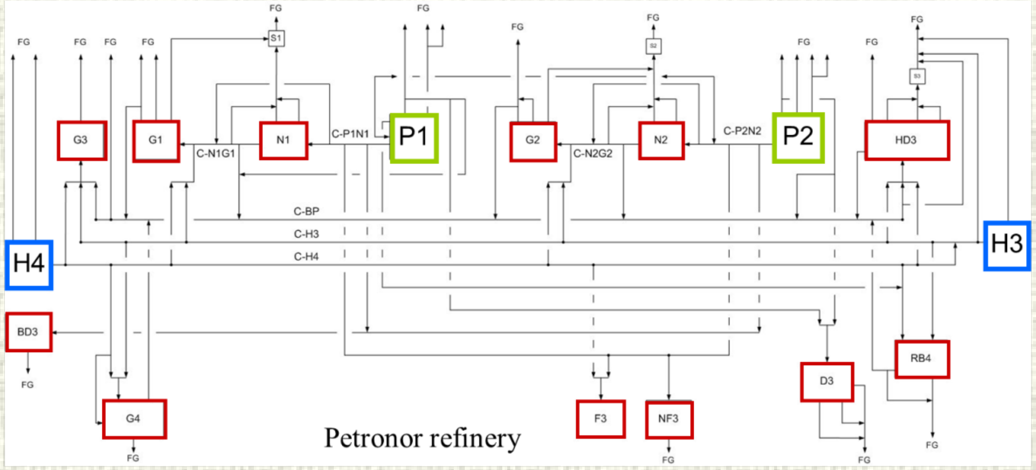
Hydrogen is an expensive product

Variable hydrogen demands

No significant $H_2$ accumulation in the network

In order to guarantee that enough hydrogen is available to the HDS when they need it, a surplus must be maintained in the collectors, the excess being released by the pressure controllers to the fuel-gas network.

# Optimal operation of the network



Petronor refinery

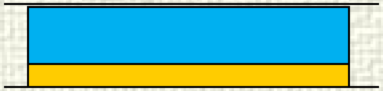
✓The problem can be formulated as of balancing the hydrogen that is being produced and consumed in the refinery and distribute it through the existing pipeline network in such a way that an economic target is optimized, while satisfying a set of operational constraints.

# Optimal operation of the network

- ✓ Many possible economic targets:
  - – Minimizing the production of fresh $H_2$, maximizing the profits, minimizing the flow of $H_2$ to the fuel gas network, maximizing the use of low purity $H_2$, etc.
- ✓ Main difficulties:
  - – Lack of reliable information about many streams and compositions / Uncertainty of demands
  - – The large scale of the system / size and time scales

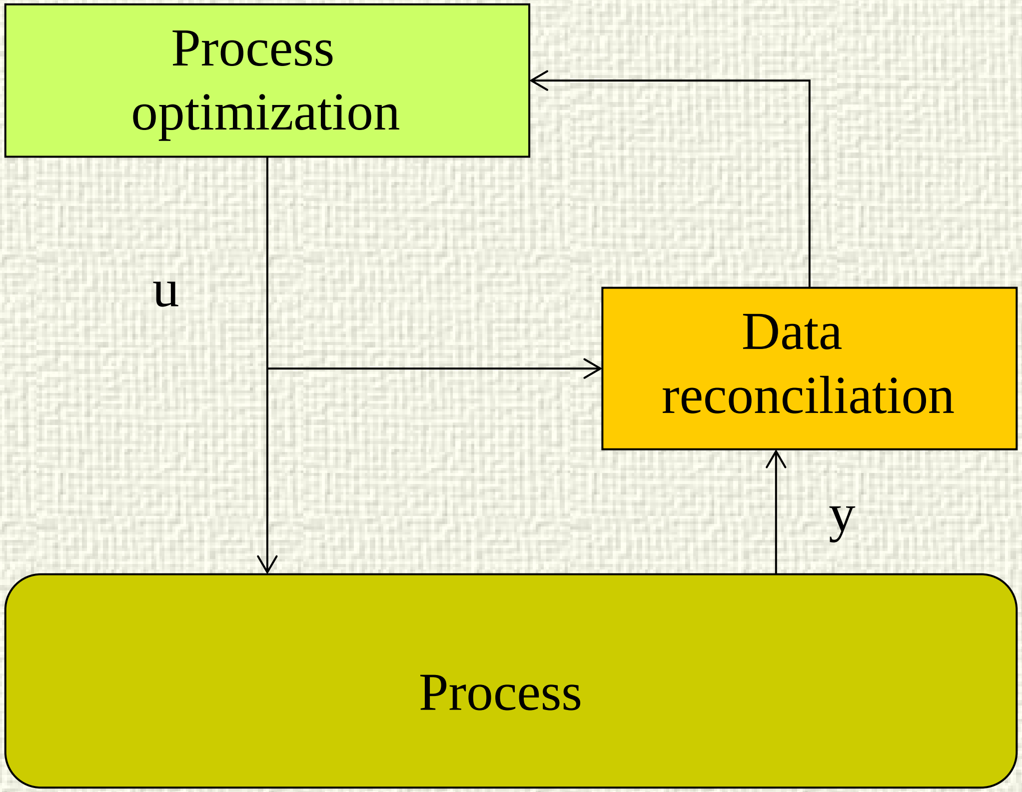
# Uncertainty

- ✓ Variable hydrogen demands from the consumer units
- ✓ Volumetric flow measurements that must be compensated to obtain massflows. Pressure, temperature and molecular weight are required
- ✓ Hydrogen purity is not always available. Moreover, the gas stream contains impurities of unknown and changing molecular weight.



- ✓ Due to the low molecular weight (2) of hydrogen, a stream with purity 90%, where one half of the impurities change composition, for instance, from methane to propane, can change the molecular weight of the stream in 41%.
- ✓ Compensated flows and purities are not always reliable.

# RTO



Process optimization

u

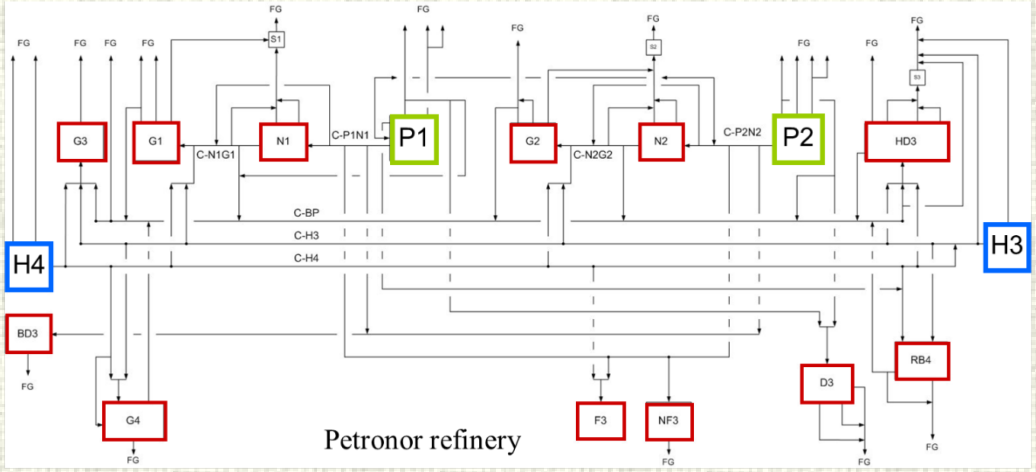
Data reconciliation

y

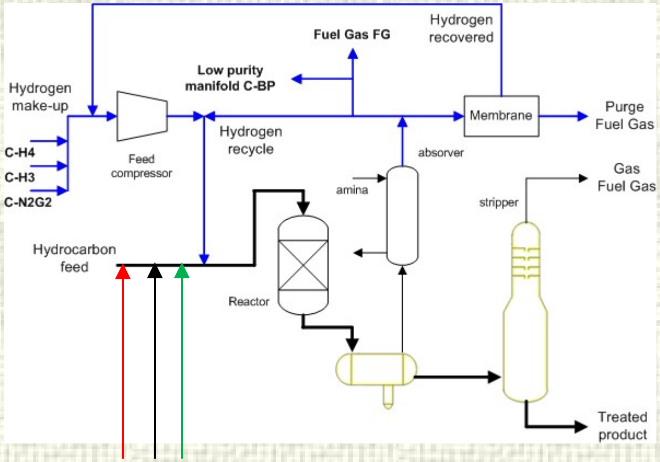
Process

# Approach

- ✓ The large scale of the system imposes computational barriers for a global dynamic solution of the problem
- ✓ HC changes that takes place every 2-3 days, impose a different approach at the times of change

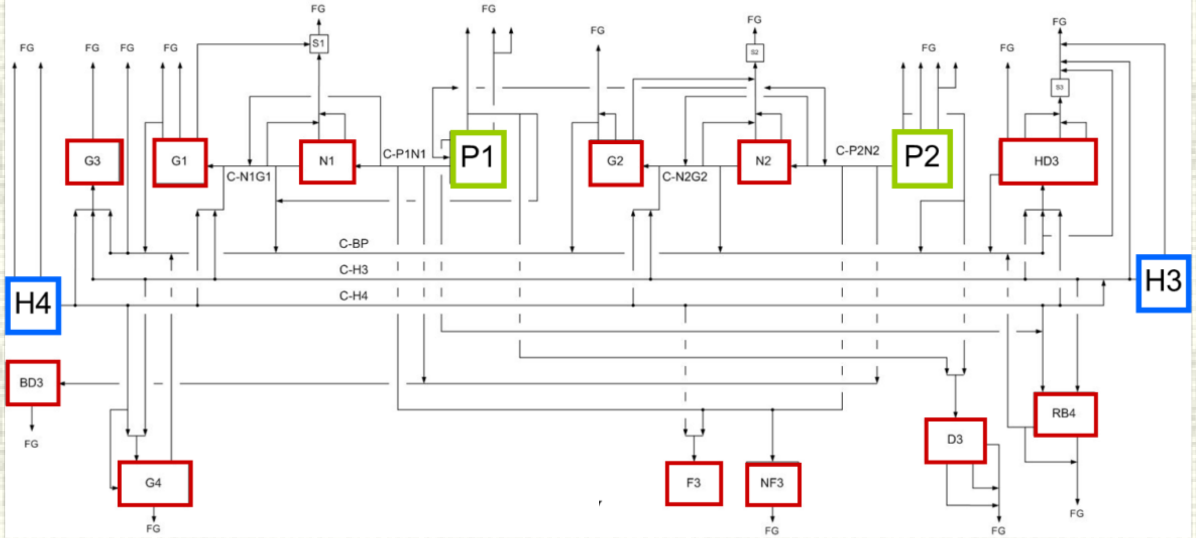


Separate the period when a HC change takes place from the rest



HC from different sources and compositions

# Decomposition



The network has much faster dynamics and can be considered static in relation to the slower producer and consumer units.

Centralized static approach

- ✓Uncertainty has been considered by using data reconciliation
- ✓Additional benefit: Information, KPI

# Distribution network model

Mass balances at every node of the network, including those inside the units

$$\xcancel{\frac{T_N \pi R^2 L}{P_N T}\frac{d(P)}{dt}} = \sum_{j,in} F_j - \sum_{i,out} F_i$$

$$X^{H2}\sum_{i,out} F_i = \sum_{j,in} X_j^{H2} F_j$$

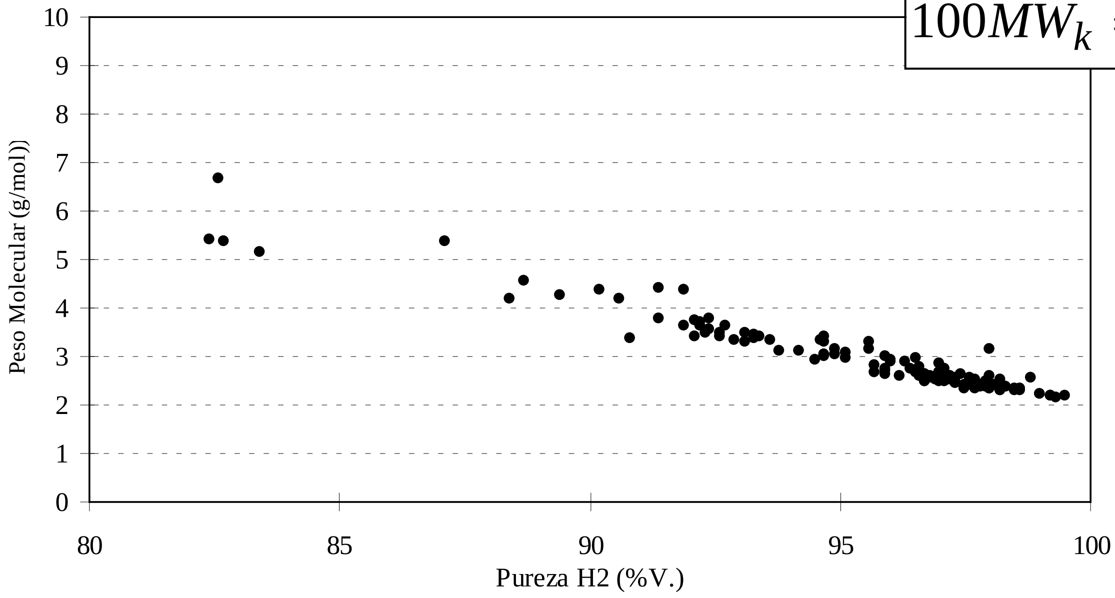
$$MW\sum_{i,out} F_i = \sum_{j,in} MW_j F_j$$

| | |
|---|---|
| **$F_j$ [Nm3/h]** | Normalized volumetric flows |
| **$X_j^{H2}$ [% vol.]** | Purity of hydrogen in each stream |
| **$MW_j$ [g/mol]** | Molecular weight of each stream |

Each stream *j* is an ideal mixture of Hydrogen ($MW^{H2}$ = 2 g/mol) and impurities with a generic molecular weight **$MW_j^I$**

$$100MW_j = MW^{H2}X_j^{H2} + (100 - X_j^{H2})MW_j^I$$

## Molecular weight vs $H_2$ purity

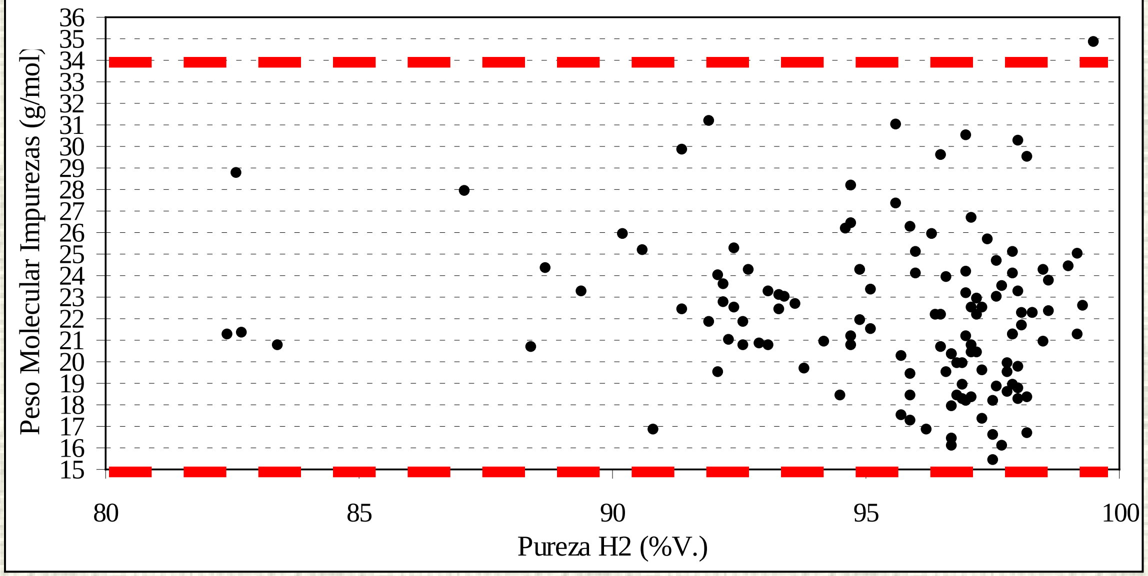


$$100MW_k = MW^{H2}X_k^{H2} + (100 - X_k^{H2})MW_k^I$$

Molecular weights of impurities will be additional variables in the data reconciliation problem

Historical data of lab analysis provide their lower and upper bounds

## Molecular weight of impurities ($MW^I_k$)



# Compensated flow measurements

Orifice plates provides measures of flows $F_{med}$ at a certain design conditions:

- Pressure ($P_d$), temperature ($T_d$) and molecular weight ($MW_d$)

To obtain the value of the flow F in other conditions, it is necessary to compensate the measured flow by a factor (β) depending on:

- **Pressure, temperature and molecular weight of operation (ope)**

$$F_{compensated} = F_{med} \times \beta \qquad where \qquad \beta = \sqrt{\frac{T_d + 273}{(P_d + 1)MW_{ope}}}\sqrt{\frac{(P_{ope} + 1)MW_d}{T_{ope} + 273}}$$

→ **Pressure and temperature of operation are available in the process for each stream**

→ **Molecular weights of operation will be estimated with the model**

# Data reconciliation

## Minimizing the quadratic error between calculated and measured data

$$\min_{\{F_i, X_i, PM_i\}} J = \sum_{i=1}^{caudales} \frac{w_i}{span_i \sigma_i}\left(F_i/\beta_i - F_{i,med}\right)^2 + \sum_{i=1}^{purezas} \frac{w_i}{span_i \sigma_i}\left(X_i - X_{i,med}\right)^2 + ..$$

$$\beta_i(PM_i) = \sqrt{\frac{T_d + 273}{(P_d + 1)PM_i}}\sqrt{\frac{(P_{ope} + 1)PM_d}{T_{ope} + 273}}$$

$$F_{i,min} \le F_i \le F_{i,max}$$

$$X_{i,min} \le X_i \le X_{i,max}$$

$$MW_{i,min}^{imp} \le MW_i^{imp} \le MW_{i,max}^{imp}$$

$$\sum_{i,sale} F_{N,i} = \sum_{j,entra} F_{N,j}$$

At each node j

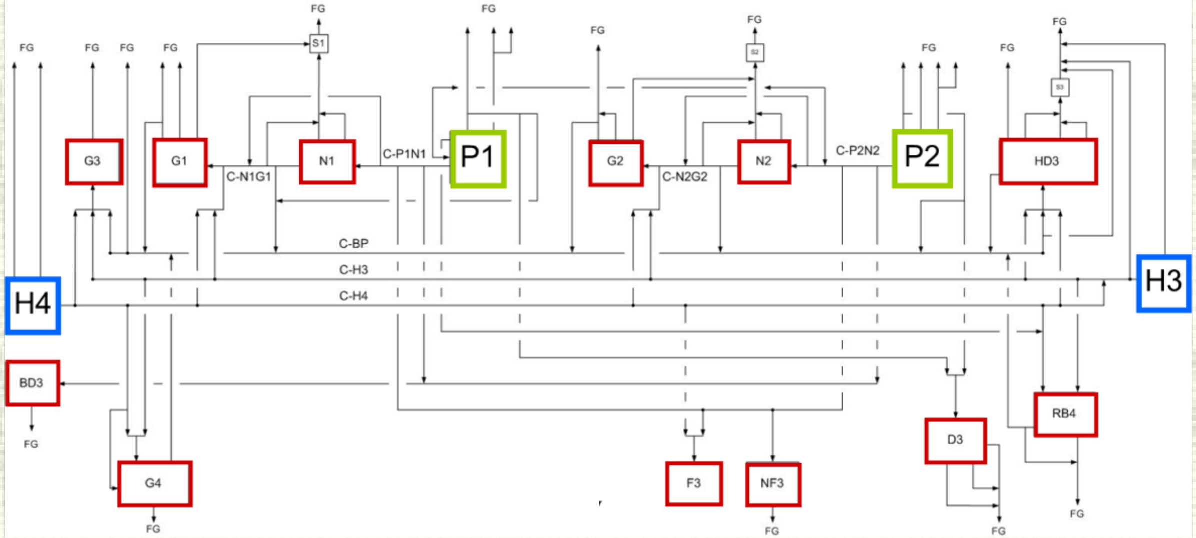
$$X^{H2} \sum_{i,sale} F_{N,i} = \sum_{j,entra} X_j^{H2} F_{N,j}$$

$$PM \sum_{i,sale} F_{N,i} = \sum_{j,entra} PM_j F_{N,j}$$

$$100 PM_k = PM^{H2} X_k^{H2} + (100 - X_k^{H2}) PM_k^I$$

The model includes other balances in the reactors and equilibrium in separation units plus additional equations for the membranes and compressors as well as slack variables for feasibility.

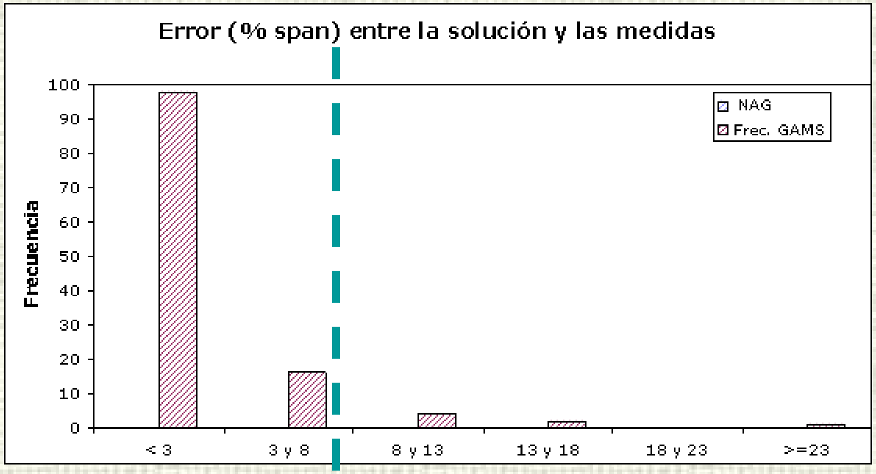
# Variable structure



The model can be reconfigured prior to the optimization according to the operational state of the plant: Plants in operation, use of collectors, ….

# Experimental results

**Number of sigma (σ) between reconciled data (optimal solution) and measures**



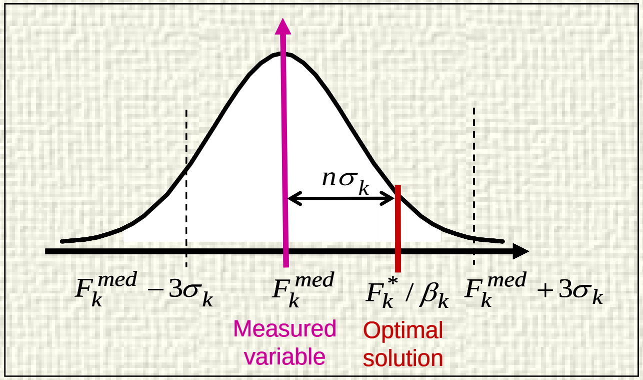
**Flows:**

$$n\sigma_k = \frac{(F_k^* / \beta_k - F_k^{med})}{\sigma_k}$$

**Purities:**

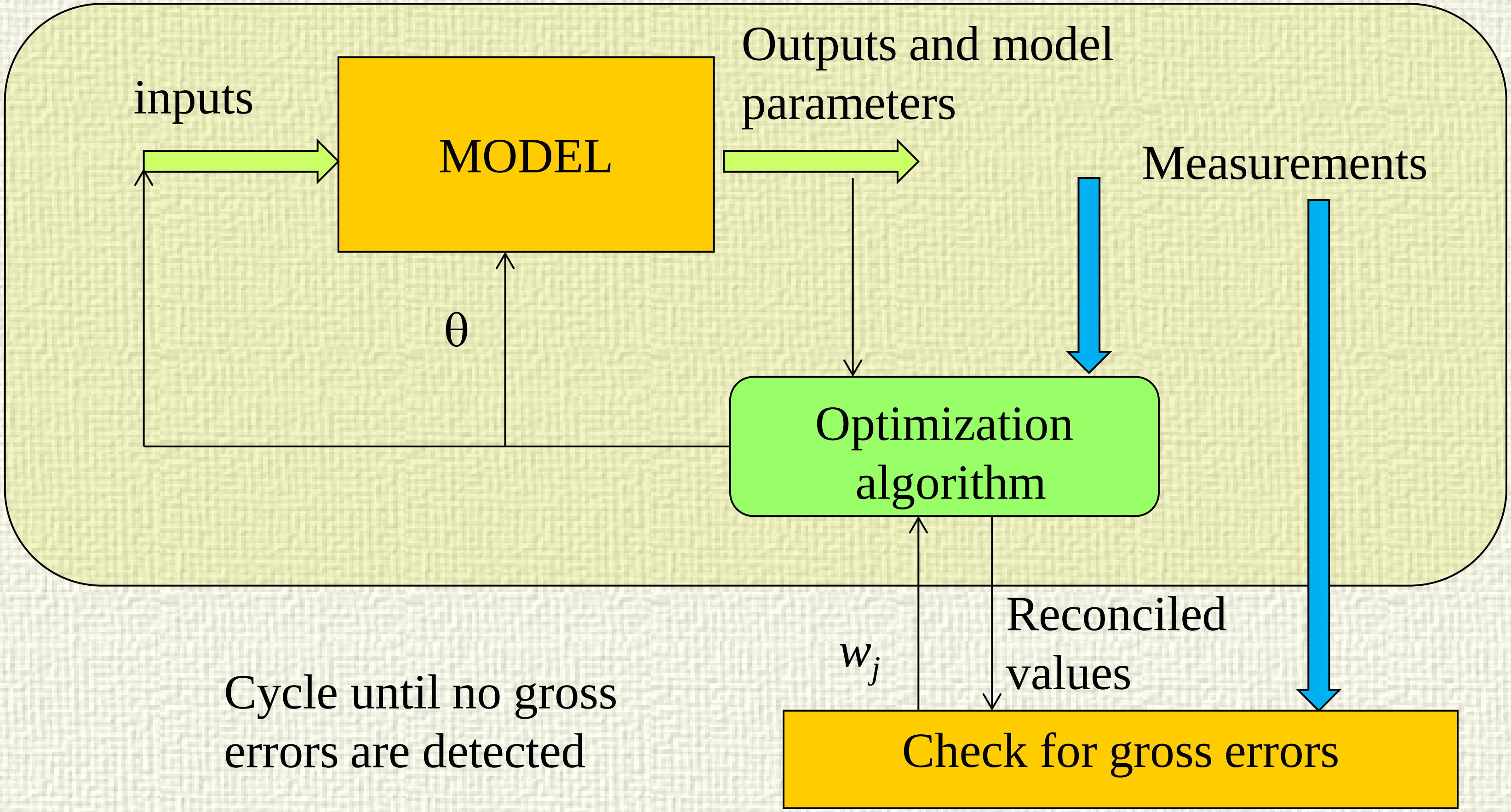
$$n\sigma_k = \frac{(X_k^* - X_k^{med})}{\sigma_k}$$

**166 measured data**



Eliminate the wrong data from the cost function and repeat the DR

# Data reconciliation



inputs

MODEL

Outputs and model parameters

Measurements

$\theta$

Optimization algorithm

$w_j$

Reconciled values

Check for gross errors

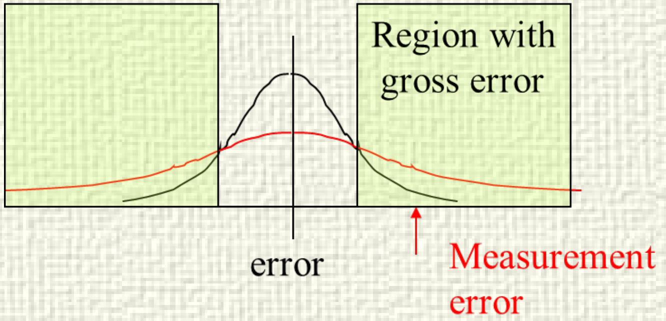
Cycle until no gross errors are detected

# Gross error detection

- ✓ Gross errors can be detected by a combination of rule base, variance and cyclic solution of the optimization problem.

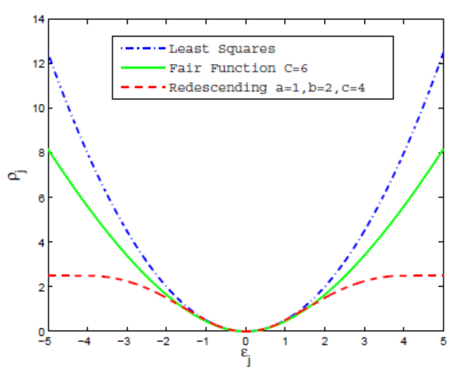
- ✓ Bivariate error distribution

$$\min_{x,p,b}[-\log L] = \min_{x,p,b,\sigma,\theta} \sum_i \left[ (1-p)\frac{\exp\left[\frac{-(x_i-x_{mi})^2}{2\sigma^2}\right]}{\sqrt{2\pi}} + p\frac{\exp\left[\frac{-(x_i-x_{mi})^2}{2(\sigma b)^2}\right]}{b\sqrt{2\pi}} \right] + \sum_i \log\sigma$$



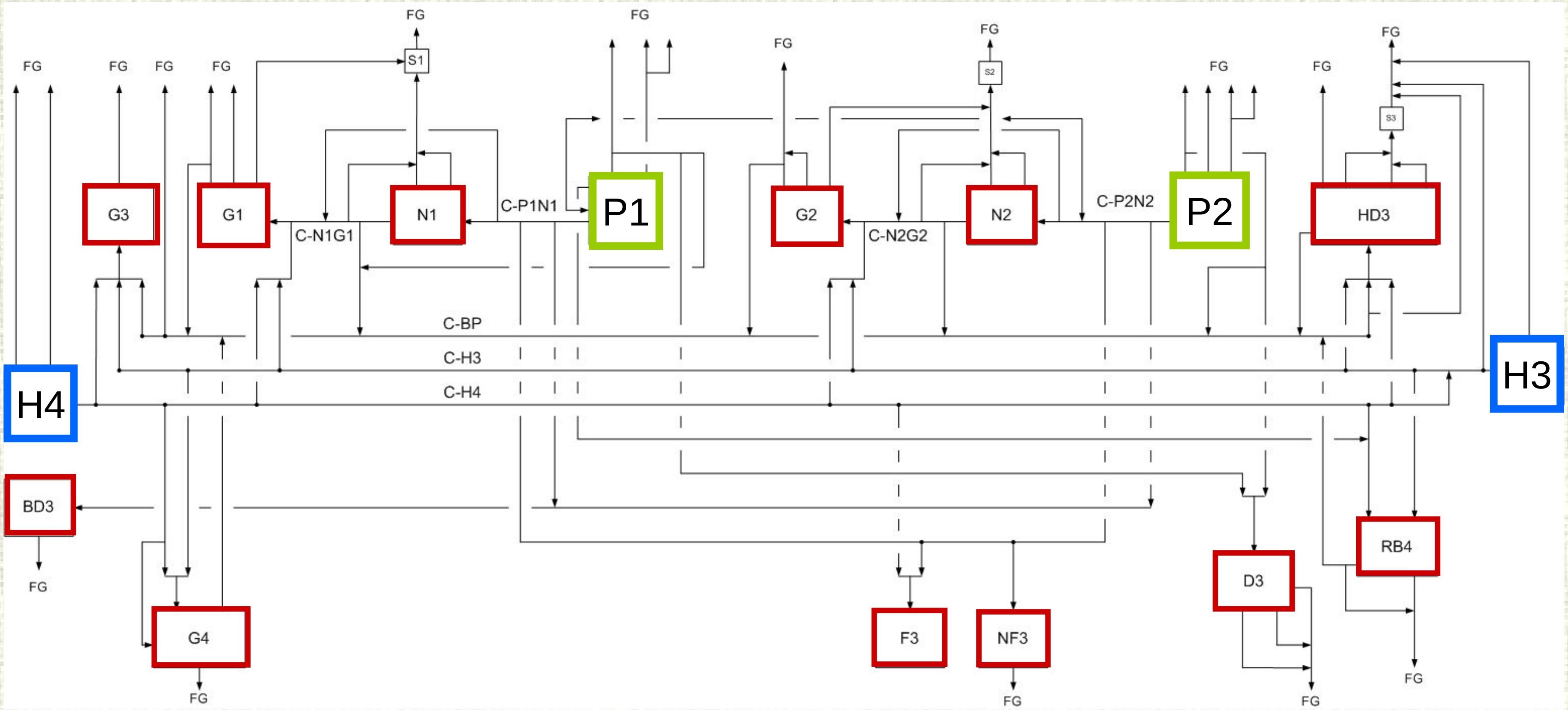
- ✓ Robust estimators

$$\boxed{F_j = c^2\left[\frac{|\varepsilon_j|}{c} - \log\left(1+\frac{|\varepsilon_j|}{c}\right)\right]}$$



Fair function, Redescending, tuning

# Optimal hydrogen management



🟦 $H_2$ production units (2)

Hydrogen distribution

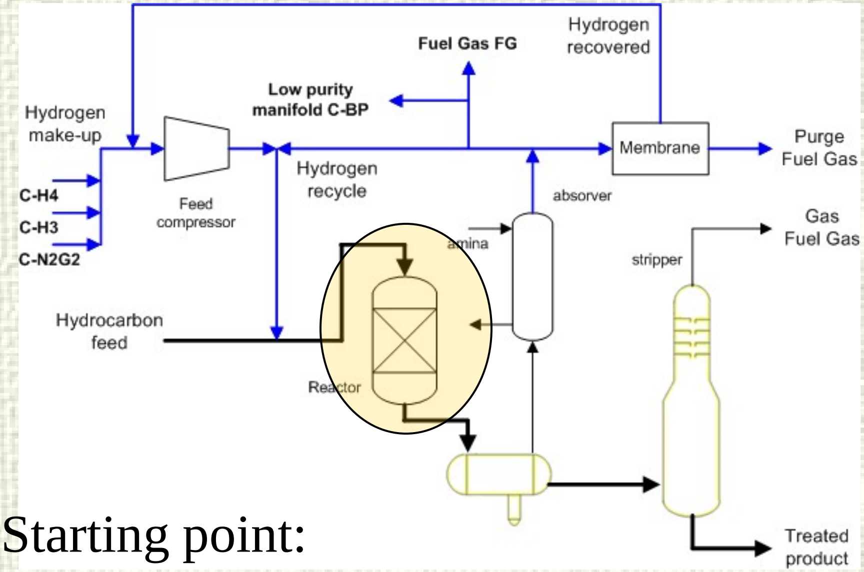
# Optimal hydrogen management

Optimize an economic target:

$$\min_{\{F_i, X_i\}} J_{opt} = \sum_i p_{pro} F_{pro} X_{pro} - \sum_j p_{fuel} F_{fuel} X_{fuel} + \sum_k p_k F_k$$

Producers Fuel-gas Compressors

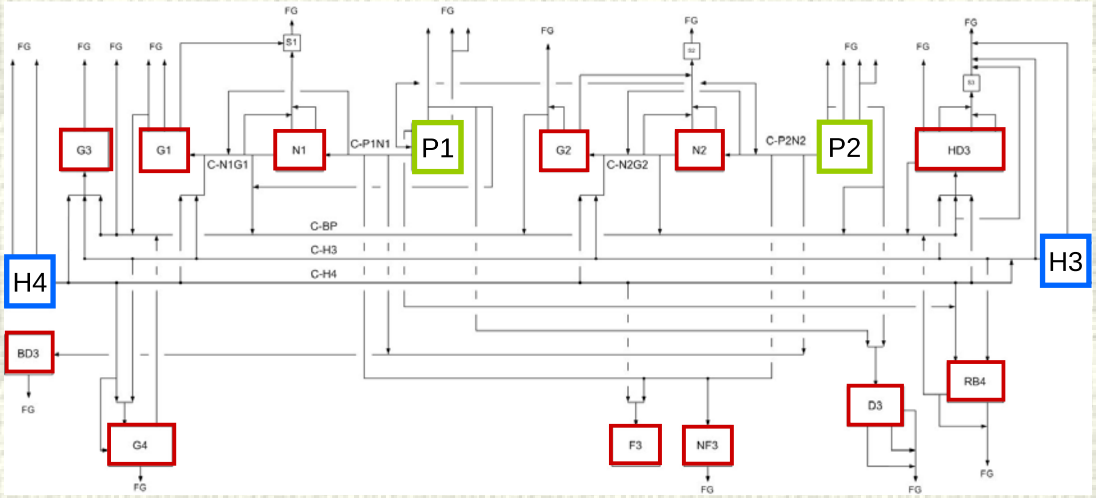
- Satisfying the model
- Under constraints imposed by the process operation (ranges, $H_2$/HC, compressors capacity and maximum purity,…)
- And with additional constraints that guarantees that the operation of the reactors is not affected (hydrogen consumption, impurities generation + load ratio). Other internal flows may change



Starting point: reconciled values

# Hydrogen shortages

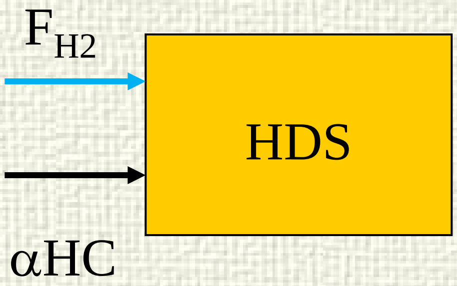
The problem has been enlarged to include reaction to hydrogen shortages that can take place due to several reasons (breakdown of equipment, failures in the platformer plants, etc.)



Two new variables are added by consumer plant:

$0 \leq \alpha_j \leq 1$ load reduction factor

$y_j$ (0,1) indicates if a plant is working or not



Some plants must reduce their hydrocarbon load or be stopped

# Hydrogen shortages

$$\min_{\{F_i, X_i, \alpha_i, y_i\}} J_{opt} = \sum_i p_{pro} F_{pro} X_{pro} - \sum_j p_{fuel} F_{fuel} X_{fuel} + \sum_k p_k F_k + \sum_l (1-\alpha_l) w_l$$

Same model and constraints as before except:

$$0 \leq \alpha_j \leq 1$$

$$F_{min} y_j \leq F_{i,j} \leq F_{max} y_j$$

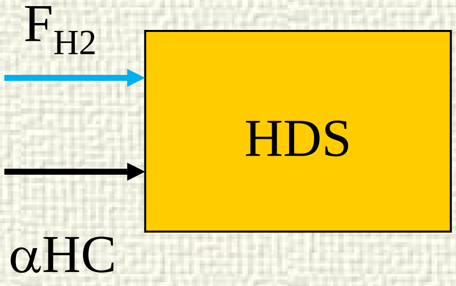
$$HC_{min} y_j \leq HC_j \alpha_j \leq HC_{max} y_j$$

$$F_{H2,j} \geq r\ HC_j\ \alpha_j$$

Mix integer problem MINLP

$w_l$ weihgts reflecting priorities

Range of operation between a minimum and a maximum capacity

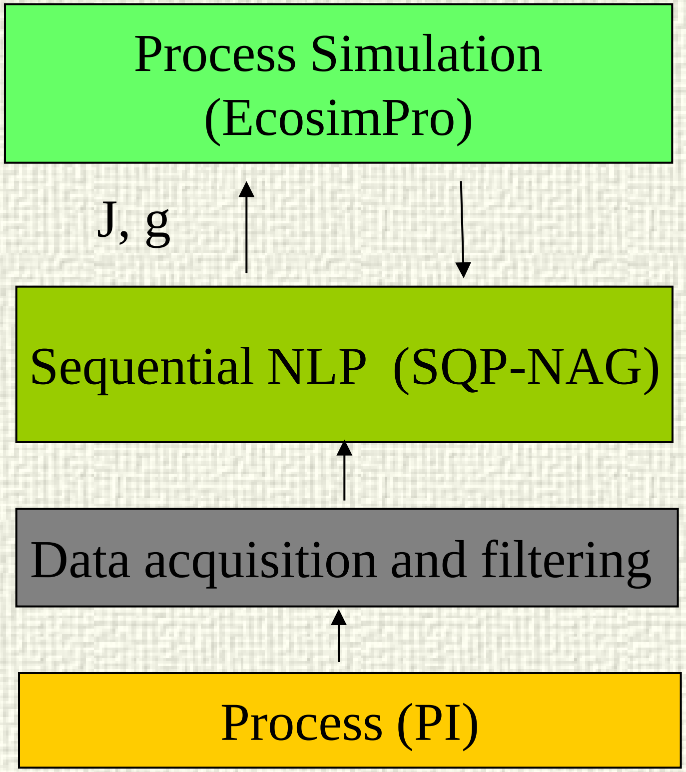


$F_{H2}$

HDS

$\alpha$HC

# Two solutions



Process Simulation
(EcosimPro)

J, g

Sequential NLP (SQP-NAG)

Data acquisition and filtering

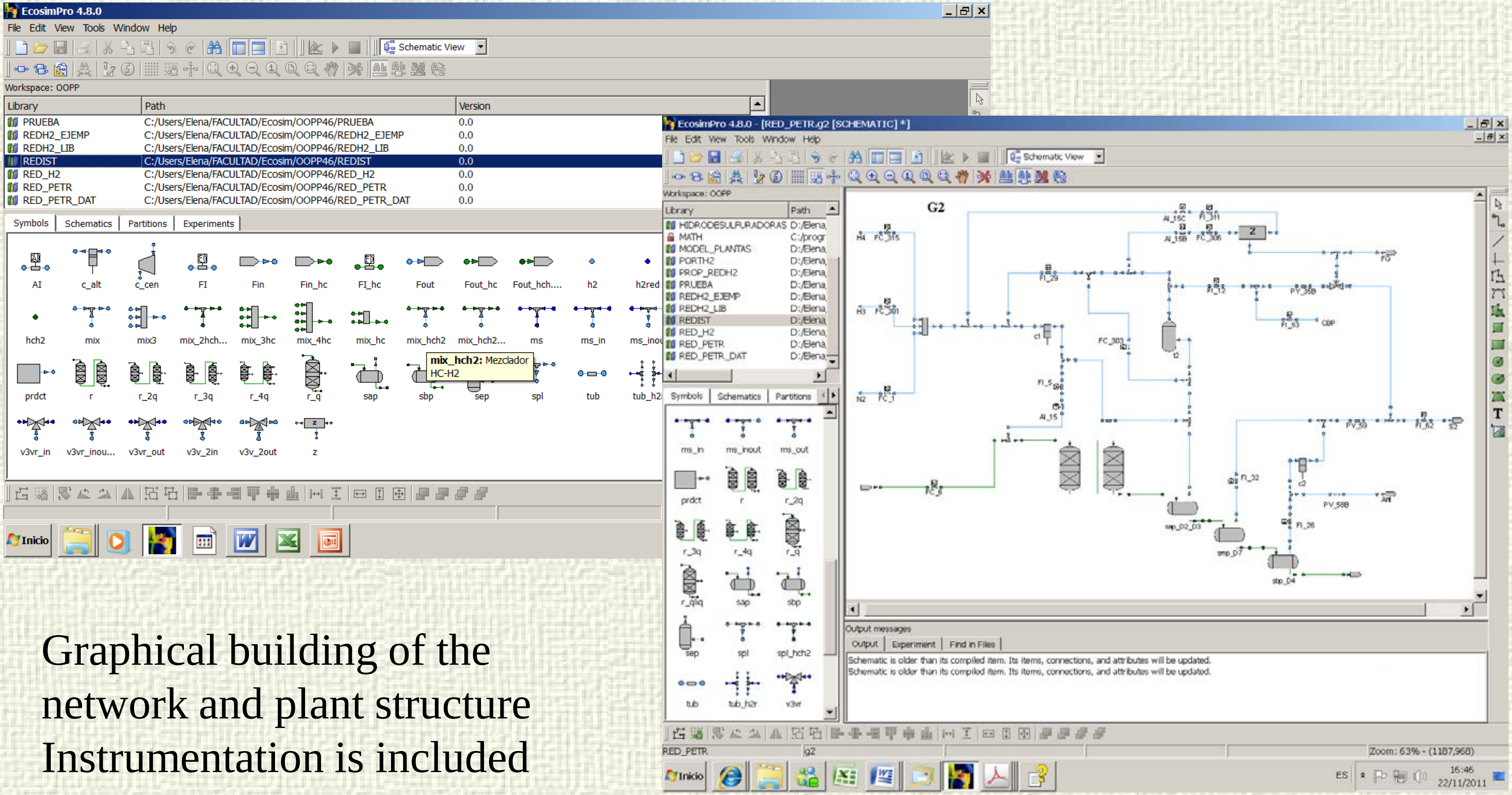
Process (PI)

Simultaneous NLP
(GAMS)

922 variables from 220 streams, 14 reactors, membranes, separators,.. Slack variables included to obtain feasible solutions totalling 1667 variables in 1631 equality and inequality equations

166 process measurements

# Modelling tools



| Library | Path | Version |
|---|---|---|
| PRUEBA | C:/Users/Elena/FACULTAD/Ecosim/OOPP46/PRUEBA | 0.0 |
| REDH2_EJEMP | C:/Users/Elena/FACULTAD/Ecosim/OOPP46/REDH2_EJEMP | 0.0 |
| REDH2_LIB | C:/Users/Elena/FACULTAD/Ecosim/OOPP46/REDH2_LIB | 0.0 |
| REDIST | C:/Users/Elena/FACULTAD/Ecosim/OOPP46/REDIST | 0.0 |
| RED_H2 | C:/Users/Elena/FACULTAD/Ecosim/OOPP46/RED_H2 | 0.0 |
| RED_PETR | C:/Users/Elena/FACULTAD/Ecosim/OOPP46/RED_PETR | 0.0 |
| RED_PETR_DAT | C:/Users/Elena/FACULTAD/Ecosim/OOPP46/RED_PETR_DAT | 0.0 |

```
Schematic is older than its compiled item. Its items, connections, and attributes will be updated.
Schematic is older than its compiled item. Its items, connections, and attributes will be updated.
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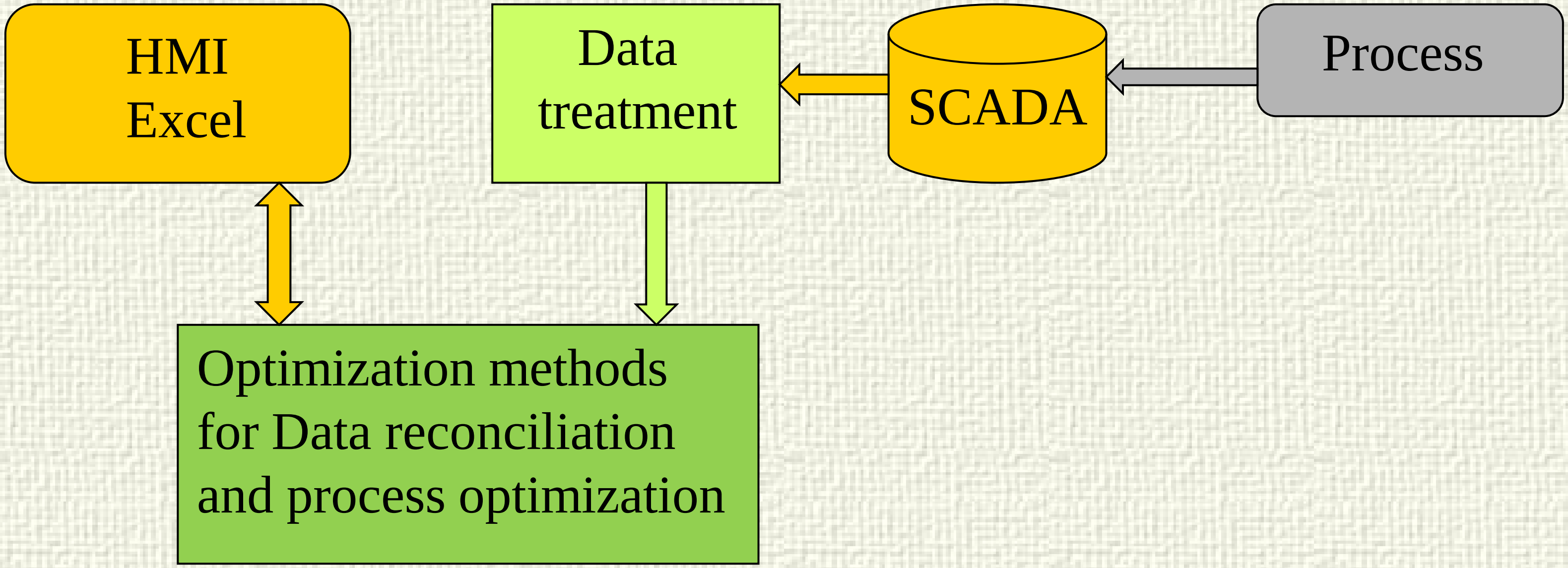
Graphical building of the network and plant structure

Instrumentation is included

Automatic partition generation

# DSS



HMI
Excel

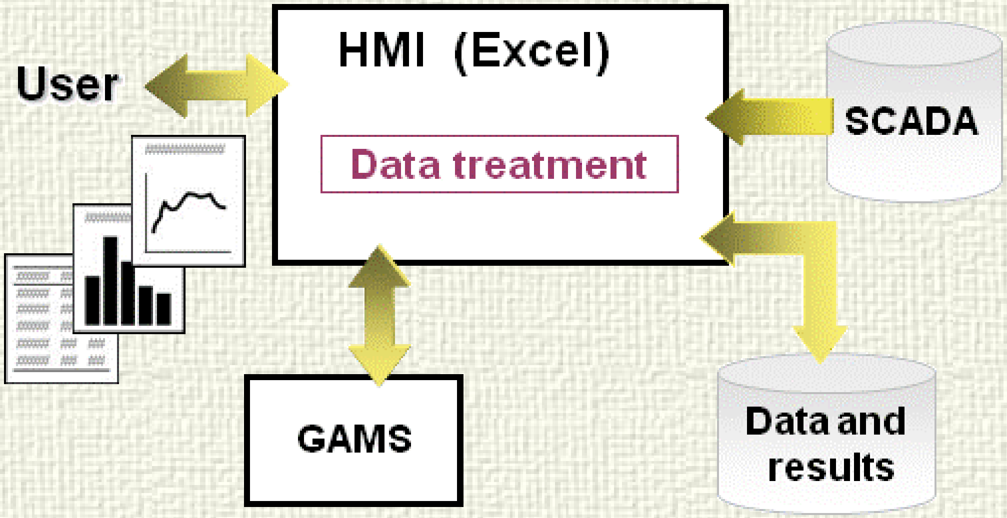
Data
treatment

SCADA

Process

Optimization methods
for Data reconciliation
and process optimization

# Decision Support System

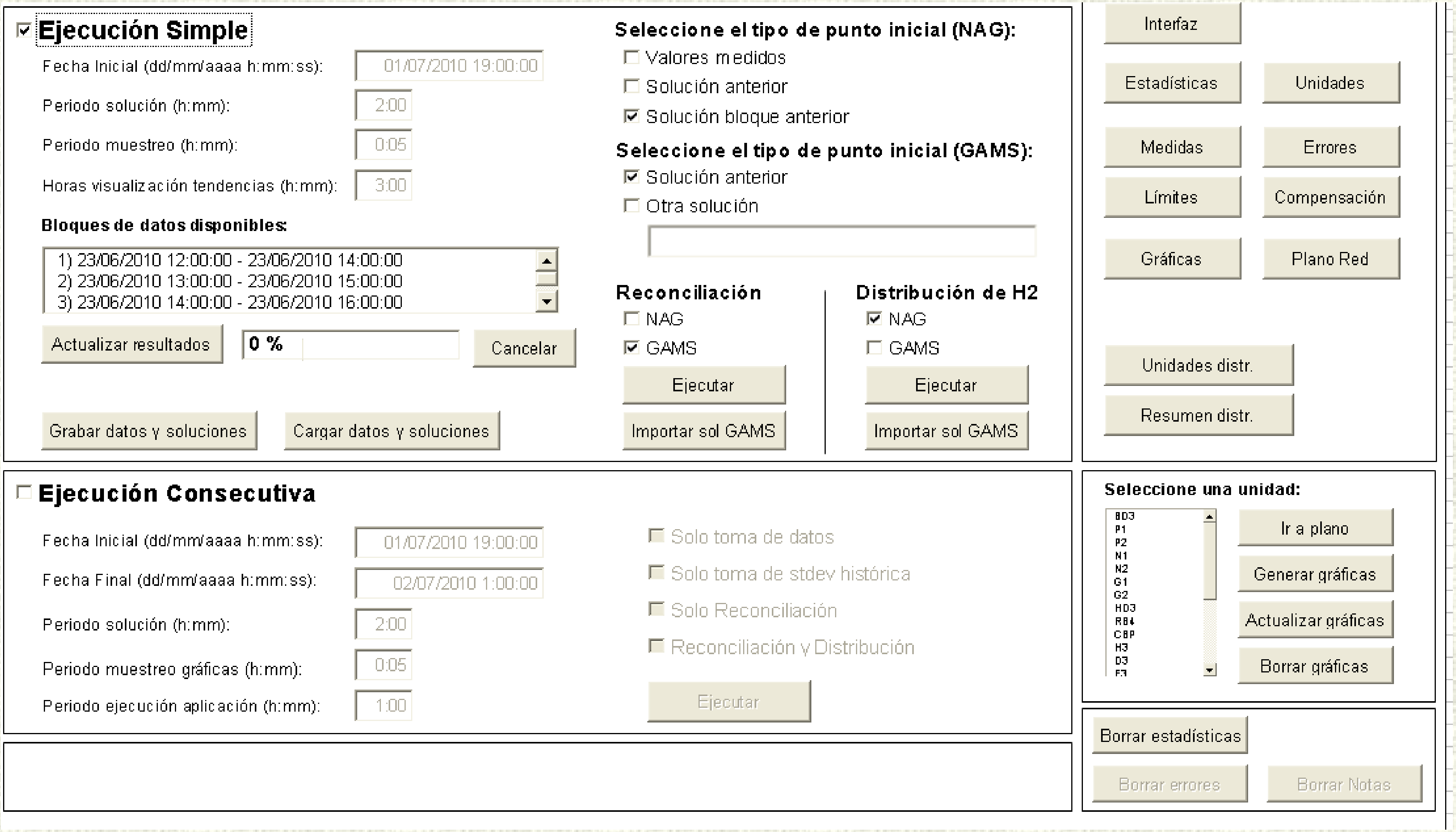


Key role played by the data treatment in the success of the application in the refinery. If data from the SCADA system are not analyzed and filter previously to their use in the numerical methods, there are no chances to obtain good results

This layer is composed of a set of rules that detect faults and information inconsistences in the raw data and decides which options are the most adequate ones

To deal with big changes, the network is formulated as a superstructure that allows to remove groups of equations depending on the value of binary variables that represent the state of the plants.

# Decision Support System



## ☑ Ejecución Simple

Fecha Inicial (dd/mm/aaaa h:mm:ss): 01/07/2010 19:00:00

Periodo solución (h:mm): 2:00

Periodo muestreo (h:mm): 0:05

Horas visualización tendencias (h:mm): 3:00

**Bloques de datos disponibles:**

1) 23/06/2010 12:00:00 - 23/06/2010 14:00:00
2) 23/06/2010 13:00:00 - 23/06/2010 15:00:00
3) 23/06/2010 14:00:00 - 23/06/2010 16:00:00

0 %

**Seleccione el tipo de punto inicial (NAG):**

☐ Valores medidos
☐ Solución anterior
☑ Solución bloque anterior

**Seleccione el tipo de punto inicial (GAMS):**

☑ Solución anterior
☐ Otra solución

**Reconciliación**

☐ NAG
☑ GAMS

**Distribución de H2**

☑ NAG
☐ GAMS

## ☐ Ejecución Consecutiva

Fecha Inicial (dd/mm/aaaa h:mm:ss): 01/07/2010 19:00:00

Fecha Final (dd/mm/aaaa h:mm:ss): 02/07/2010 1:00:00

Periodo solución (h:mm): 2:00

Periodo muestreo gráficas (h:mm): 0:05

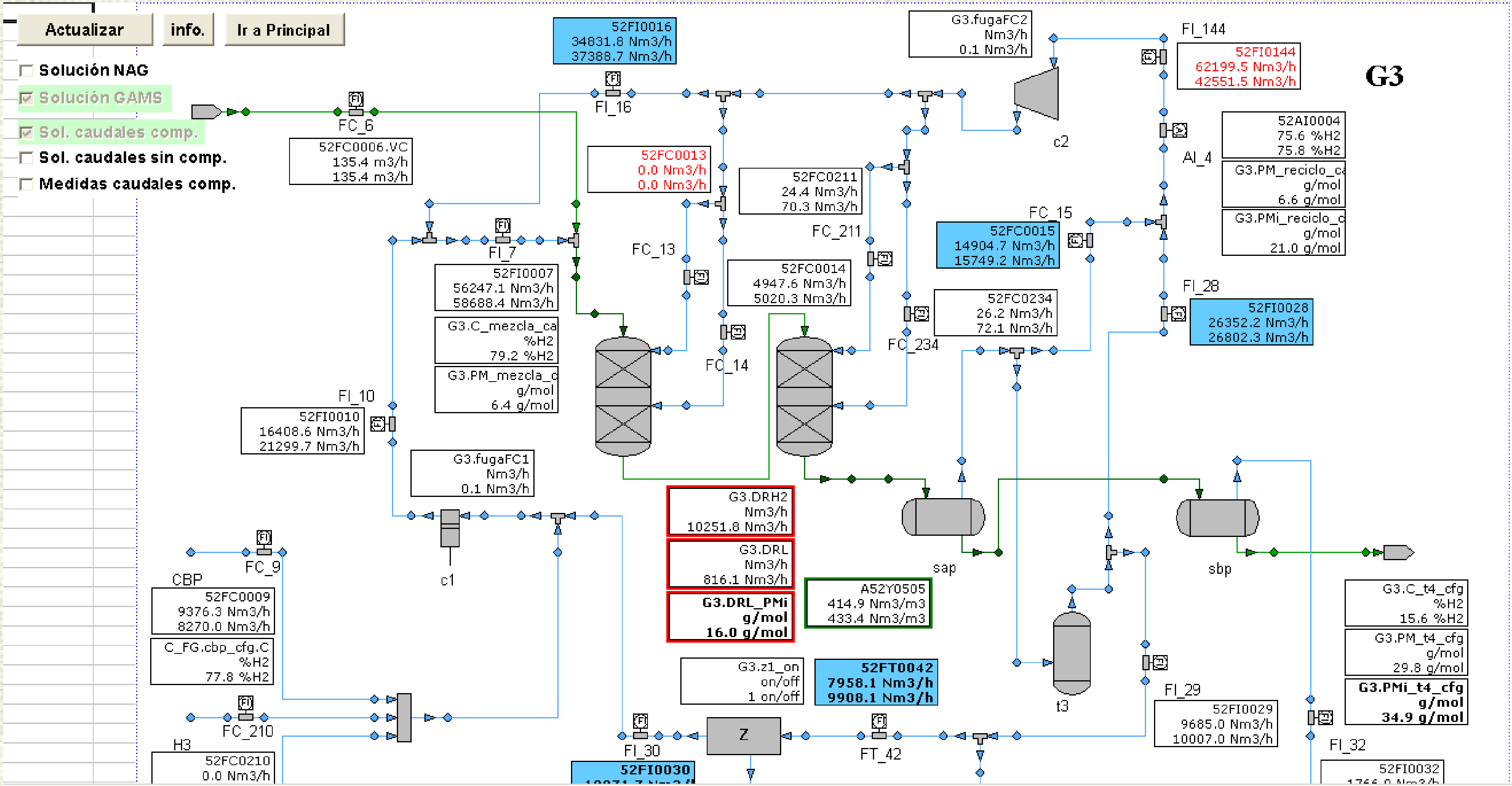
Periodo ejecución aplicación (h:mm): 1:00

☐ Solo toma de datos
☐ Solo toma de stdev histórica
☐ Solo Reconciliación
☐ Reconciliación y Distribución

**Seleccione una unidad:**

BD3
P1
P2
N1
N2
G1
G2
HD3
RB4
CBP
H3
D3

# DSS



☐ **Solución NAG**
☑ **Solución GAMS**
☑ **Sol. caudales comp.**
☐ **Sol. caudales sin comp.**
☐ **Medidas caudales comp.**

52FI0016
34831.8 Nm3/h
37388.7 Nm3/h

G3.fugaFC2
Nm3/h
0.1 Nm3/h

52FI0144
62199.5 Nm3/h
42551.5 Nm3/h

52FC0006.VC
135.4 m3/h
135.4 m3/h

52FC0013
0.0 Nm3/h
0.0 Nm3/h

52FC0211
24.4 Nm3/h
70.3 Nm3/h

52AI0004
75.6 %H2
75.8 %H2

G3.PM_reciclo_ca
g/mol
6.6 g/mol

G3.PMi_reciclo_c
g/mol
21.0 g/mol

52FC0015
14904.7 Nm3/h
15749.2 Nm3/h

52FI0007
56247.1 Nm3/h
58688.4 Nm3/h

52FC0014
4947.6 Nm3/h
5020.3 Nm3/h

52FC0234
26.2 Nm3/h
72.1 Nm3/h

52FI0028
26352.2 Nm3/h
26802.3 Nm3/h

G3.C_mezcla_ca
%H2
79.2 %H2

G3.PM_mezcla_c
g/mol
6.4 g/mol

52FI0010
16408.6 Nm3/h
21299.7 Nm3/h

G3.fugaFC1
Nm3/h
0.1 Nm3/h

G3.DRH2
Nm3/h
10251.8 Nm3/h

G3.DRL
Nm3/h
816.1 Nm3/h

**G3.DRL_PMi**
**g/mol**
**16.0 g/mol**

A52Y0505
414.9 Nm3/m3
433.4 Nm3/m3

52FC0009
9376.3 Nm3/h
8270.0 Nm3/h

C_FG.cbp_cfg.C
%H2
77.8 %H2

G3.z1_on
on/off
1 on/off

**52FT0042**
**7958.1 Nm3/h**
**9908.1 Nm3/h**

52FI0029
9685.0 Nm3/h
10007.0 Nm3/h

G3.C_t4_cfg
%H2
15.6 %H2

G3.PM_t4_cfg
g/mol
29.8 g/mol

**G3.PMi_t4_cfg**
**g/mol**
**34.9 g/mol**

52FC0210
0.0 Nm3/h

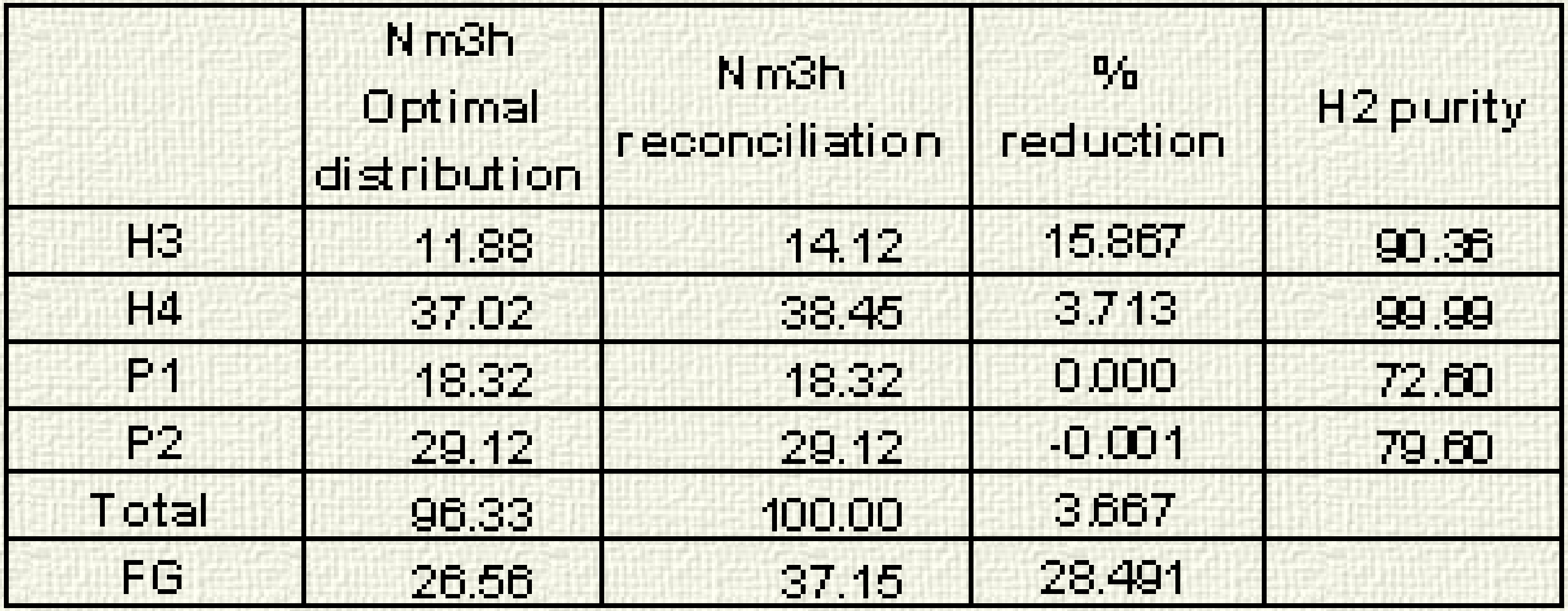
**52FI0030**

52FI0032

# Typical results

15 out of 16 plants were in operation

numbers in % H4 cheaper than H3

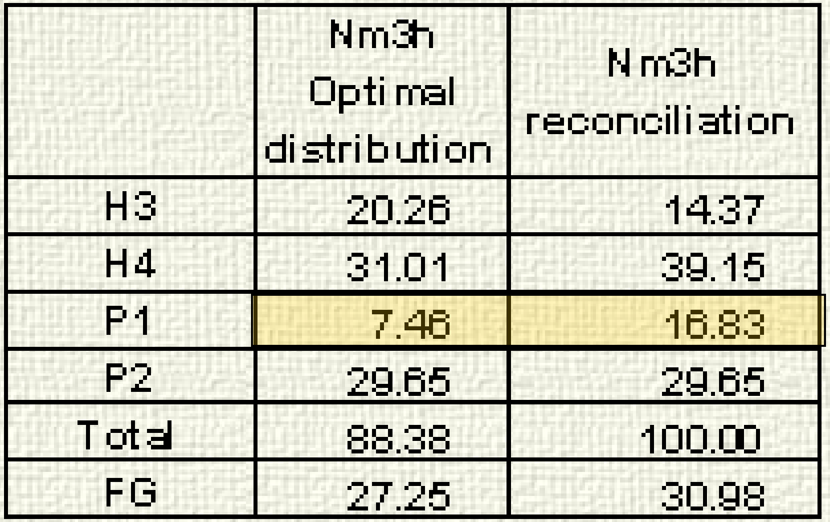


| | Nm3h Optimal distribution | Nm3h reconciliation | % reduction | H2 purity |
|---|---|---|---|---|
| H3 | 11.88 | 14.12 | 15.867 | 90.36 |
| H4 | 37.02 | 38.45 | 3.713 | 99.99 |
| P1 | 18.32 | 18.32 | 0.000 | 72.60 |
| P2 | 29.12 | 29.12 | -0.001 | 79.60 |
| Total | 96.33 | 100.00 | 3.667 | |
| FG | 26.56 | 37.15 | 28.491 | |

A reduction of about 3.7% over total use, or 7% over total fresh hydrogen production (H3 plus H4) and 28.5% of gases sent to the fuel gas network can be obtained by better management

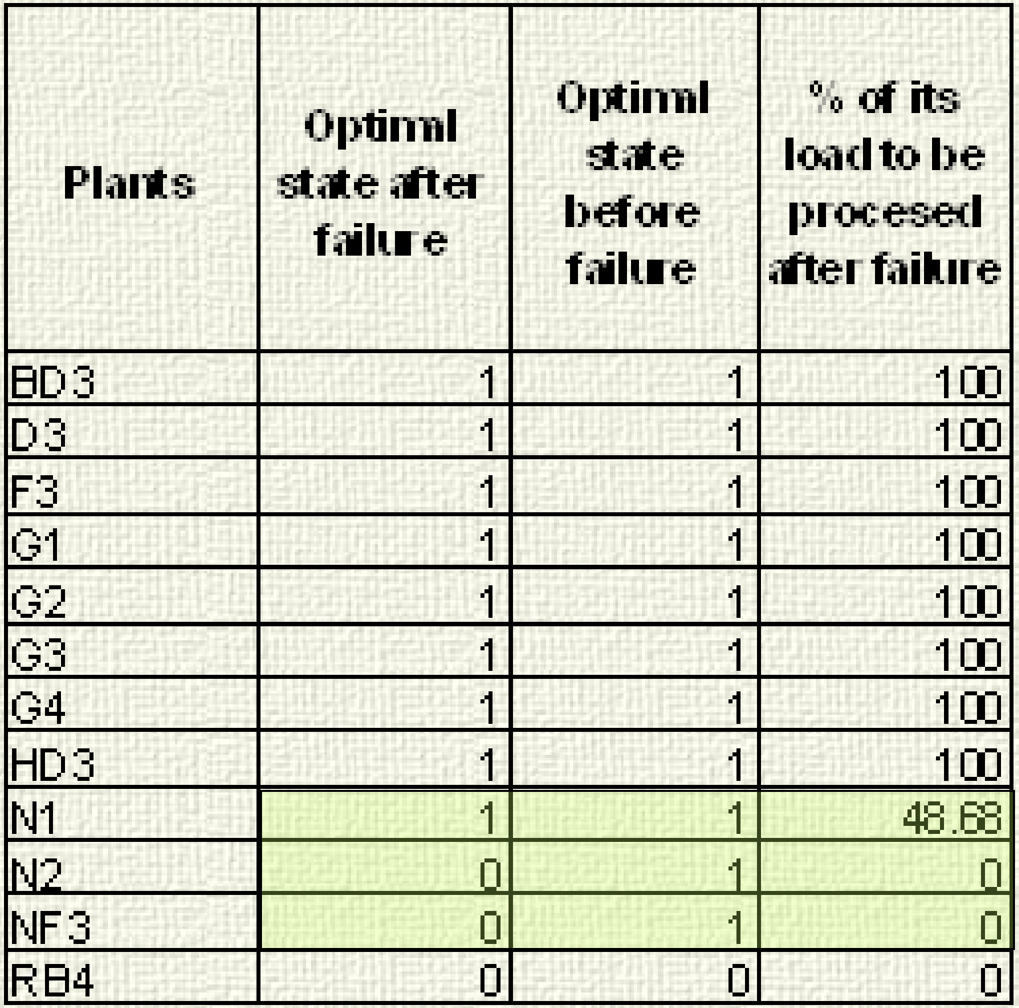
# Optimal redistribution after a drop in P1 production of 55.6%.

H3 reached its upper limit but H4 decreased production due to the network structure numbers in %



| | Nm3h Optimal distribution | N m3h reconciliation |
|---|---|---|
| H3 | 20.26 | 14.37 |
| H4 | 31.01 | 39.15 |
| P1 | 7.46 | 16.83 |
| P2 | 29.65 | 29.65 |
| Total | 88.38 | 100.00 |
| FG | 27.25 | 30.98 |

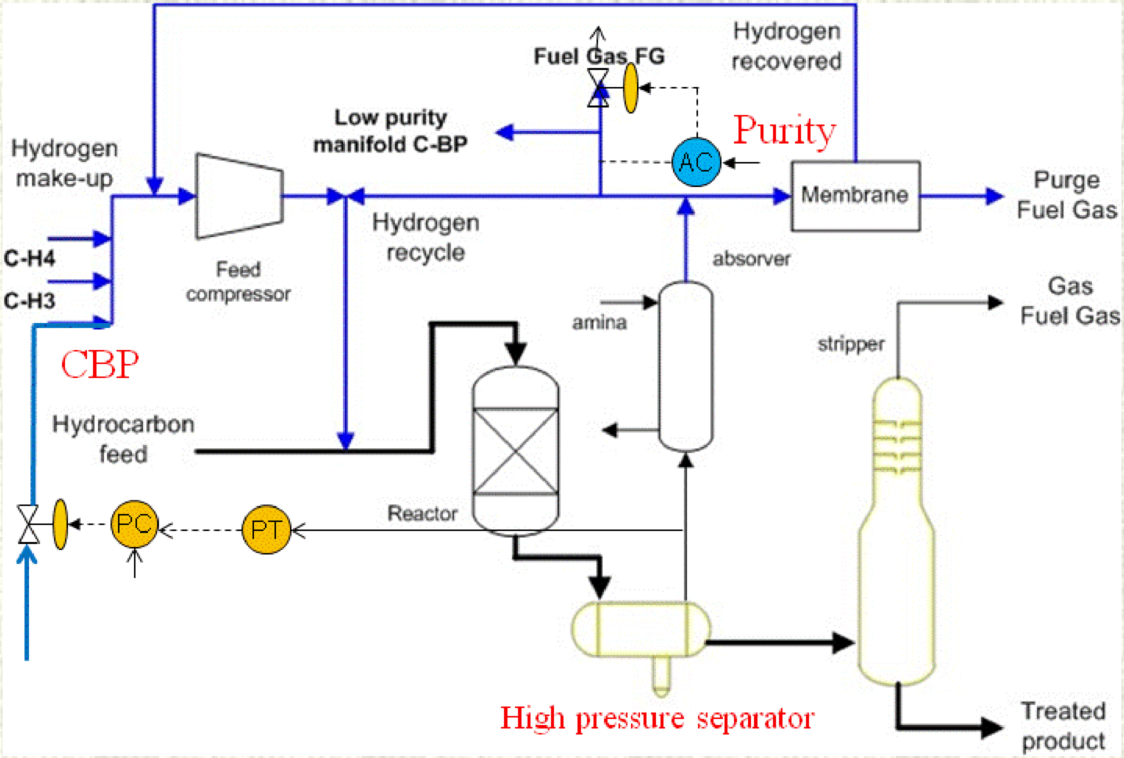
HC load reduction and state of the plants before/after failure
1 running, 0 stopped



| Plants | Optimal state after failure | Optimal state before failure | % of its load to be procesed after failure |
|---|---|---|---|
| BD3 | 1 | 1 | 100 |
| D3 | 1 | 1 | 100 |
| F3 | 1 | 1 | 100 |
| G1 | 1 | 1 | 100 |
| G2 | 1 | 1 | 100 |
| G3 | 1 | 1 | 100 |
| G4 | 1 | 1 | 100 |
| HD3 | 1 | 1 | 100 |
| N1 | 1 | 1 | 48.68 |
| N2 | 0 | 1 | 0 |
| NF3 | 0 | 1 | 0 |
| RB4 | 0 | 0 | 0 |

# Implementation

- ✓ Basic control helps matching model hypothesis and the actual process: steady state / mismatch

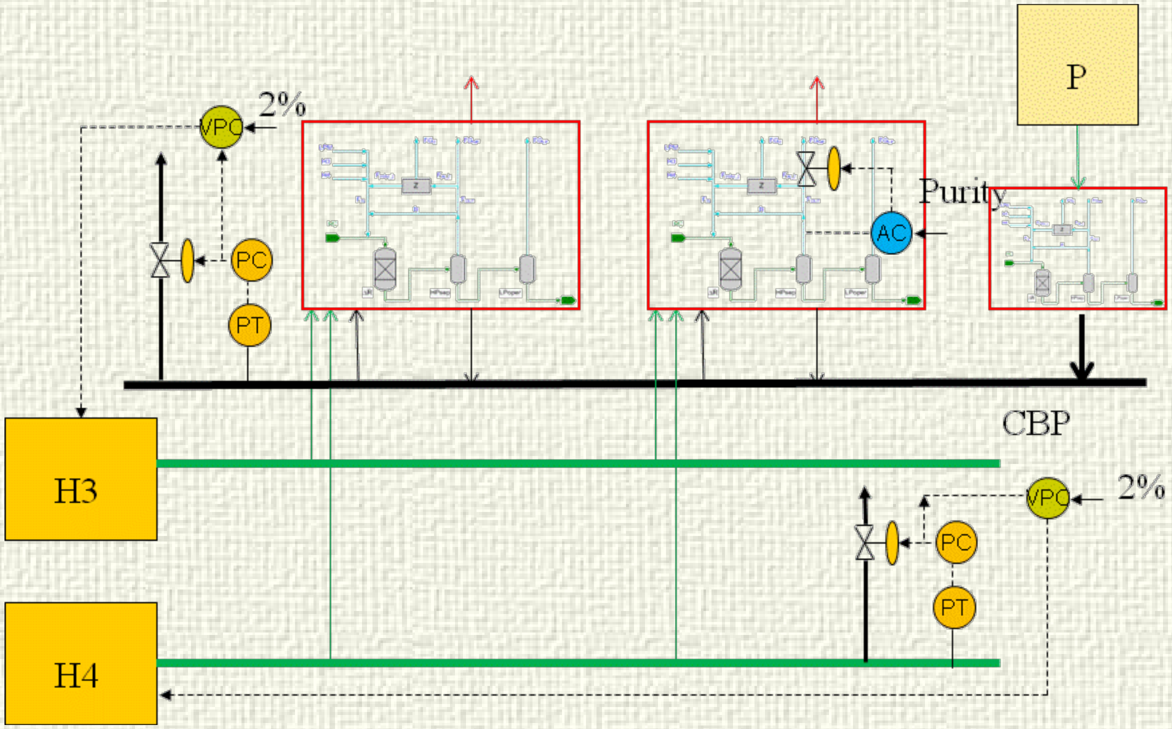


Maintaining steady state balances with pressure control loops

Unbalances are moved to the CBP collector

$H_2$ purity control loops maintain the impurities balance

# Implementation



Collectors pressure control maintain global balances

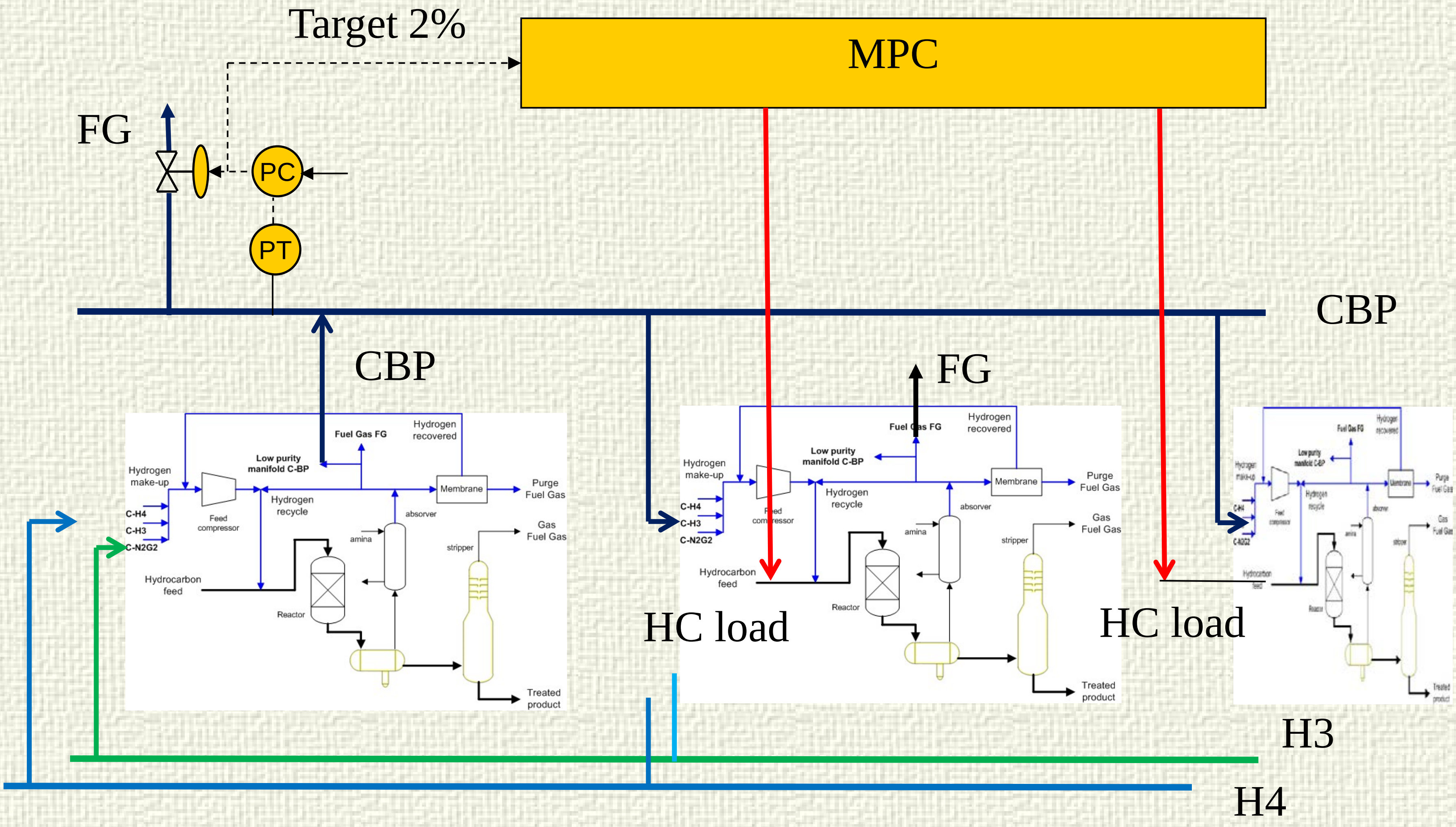
Mismatch process-model is corrected with VPCs that minimize global losses to FG

The optimizer fixes the best distribution

This will affect all plants

Different from self-optimizing control: RTO is applied on line, basic control helps reducing mismatches

# Dynamic plant operation



# Conclusions

- ✓ An approach has been presented to optimally manage the hydrogen network of a petrol refinery
- ✓ Data reconciliation and optimal hydrogen distribution problems are now under evaluation in the plant.
- ✓ The system is able to reduce utility cost by increasing hydrogen recovery in consumer units and reducing the overall production of H2 in the hydrogen suppliers
- ✓ Implementation plays an important role