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

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# Outline

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- ✓ 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

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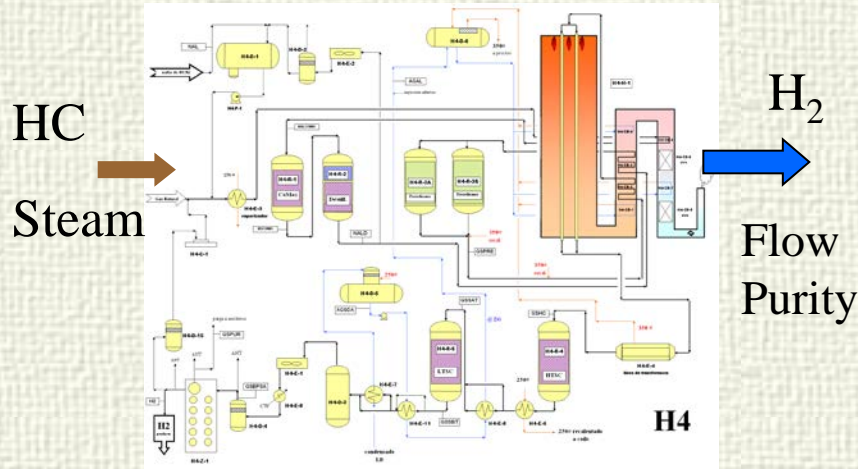


Hydrogen is used in modern refineries in processes that have two main purposes:

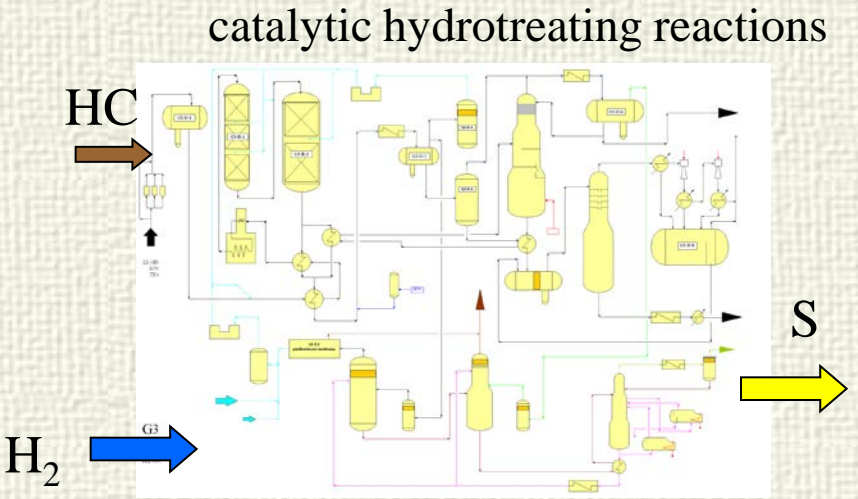
- ✓ Increase the value of the hydrocarbons (platformers, hydrocracking, etc.)
- ✓ Reduce the sulphur content of the products, (HDS),...



# Hydrogen plants (producers / consumers)

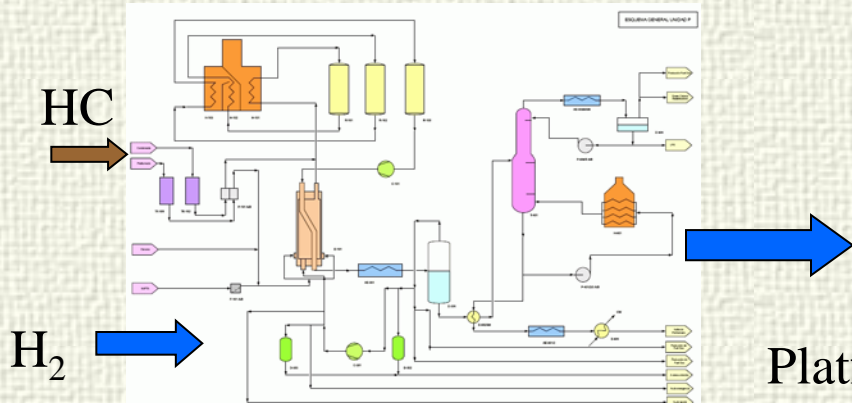


Hydrogen producer plant



Hydrodesulphurization plant HDS

Hydrocrackers

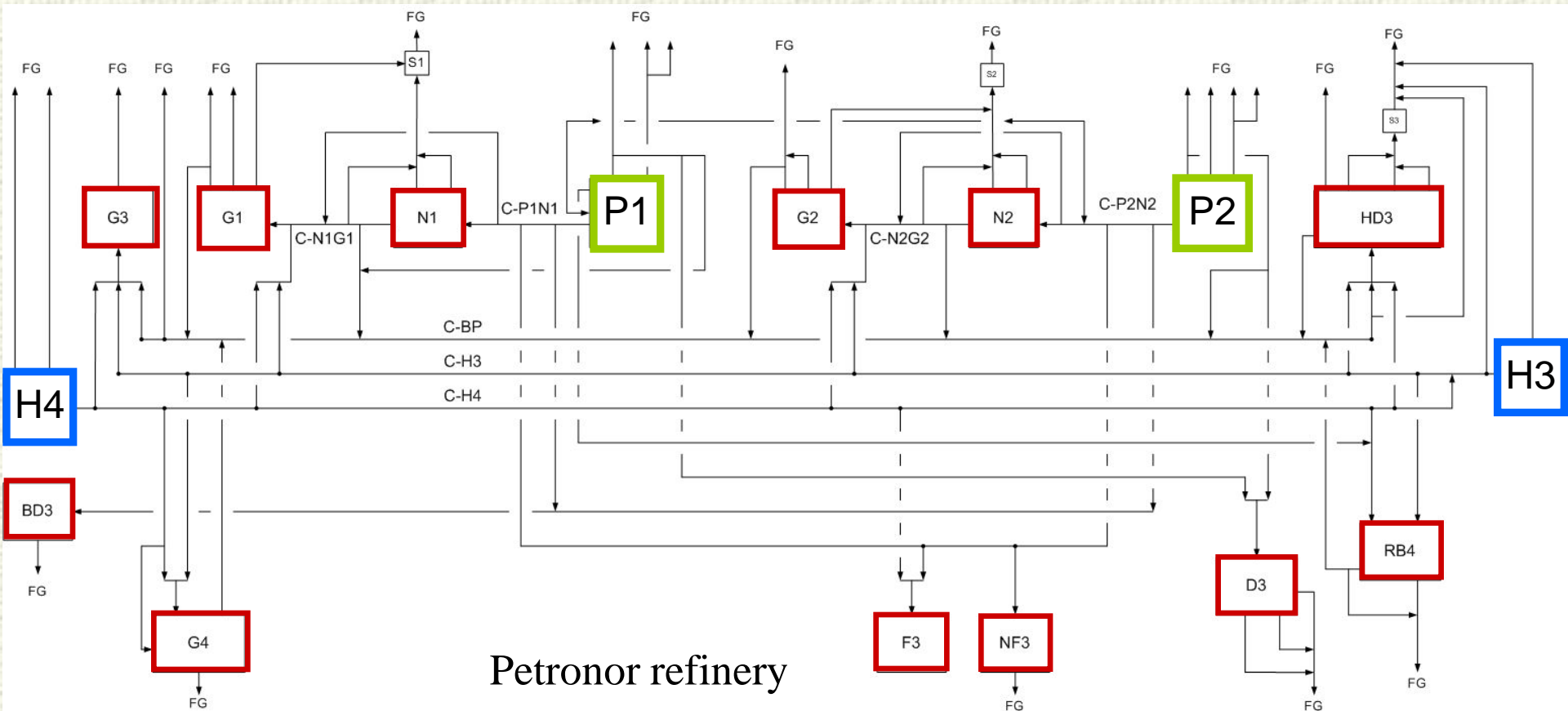


Low purity H<sub>2</sub>  
obtained as a by-product


Platformer



# Distribution network



 H<sub>2</sub> production units (2)

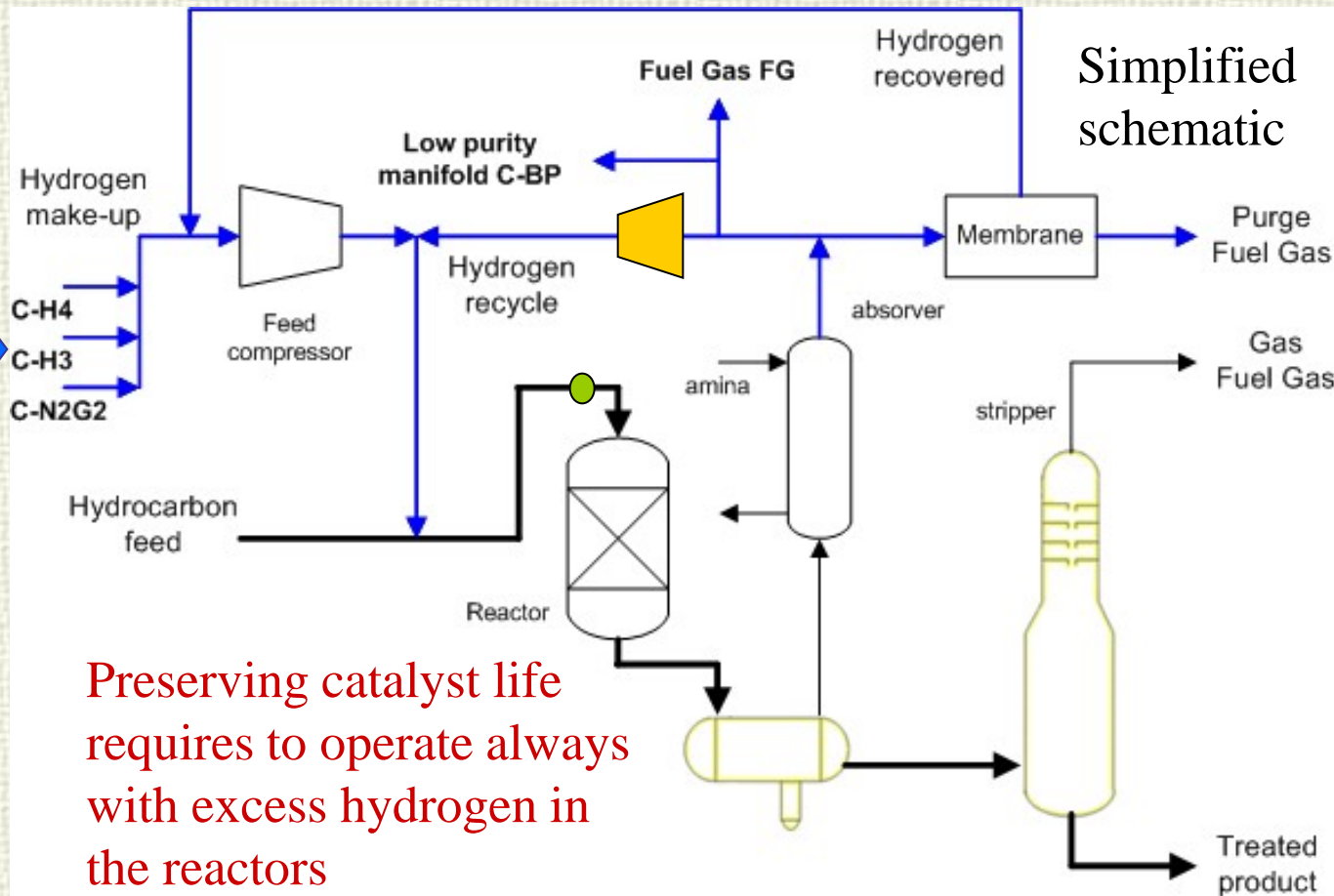
 H<sub>2</sub> production units as by product (2)

 H<sub>2</sub> consuming units (12)

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



# HDS



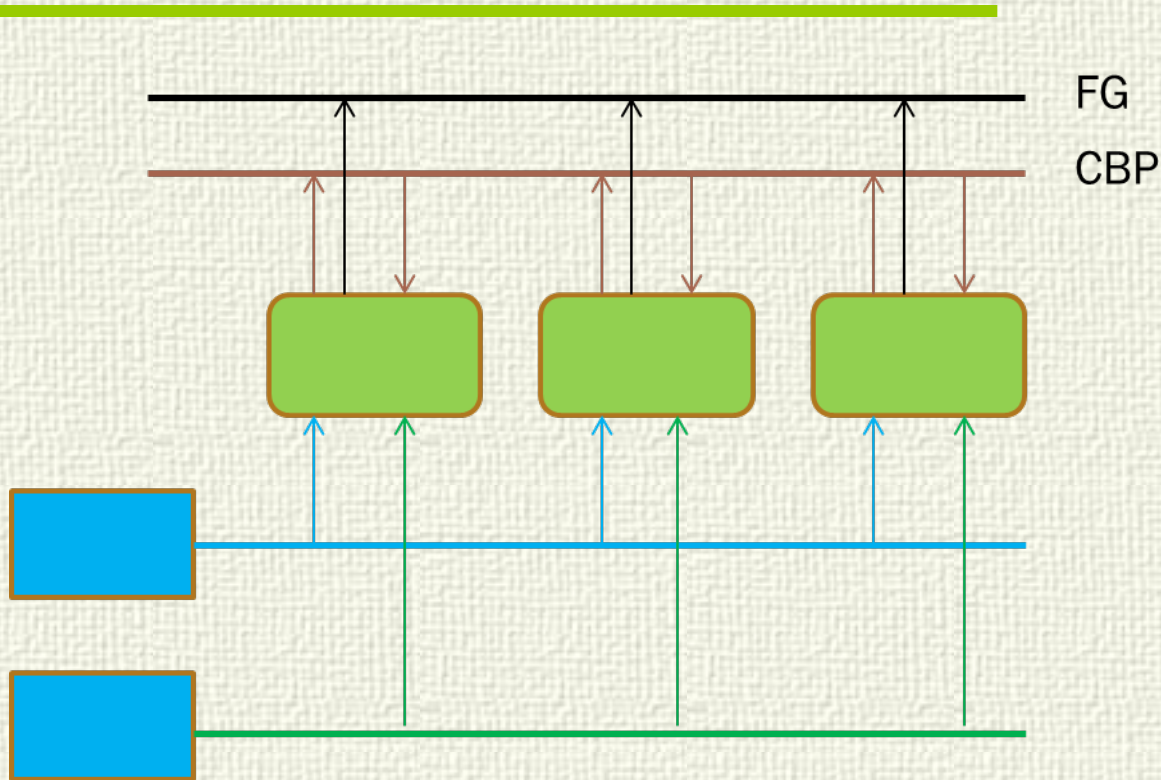
Preserving catalyst life requires to operate always with excess hydrogen in the reactors

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



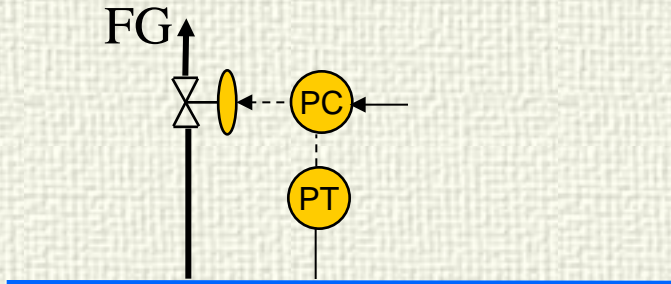
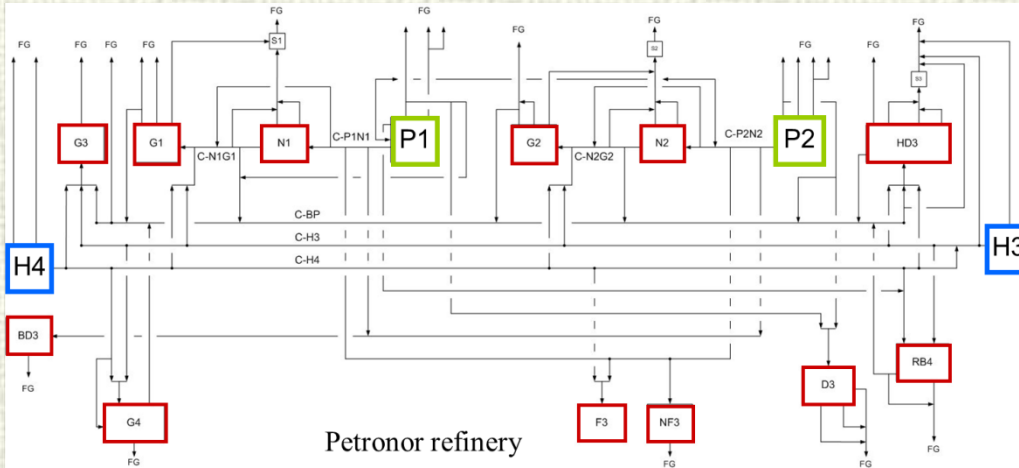
Burnt  
Recycled

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



Hydrogen is an expensive product

Variable hydrogen demands

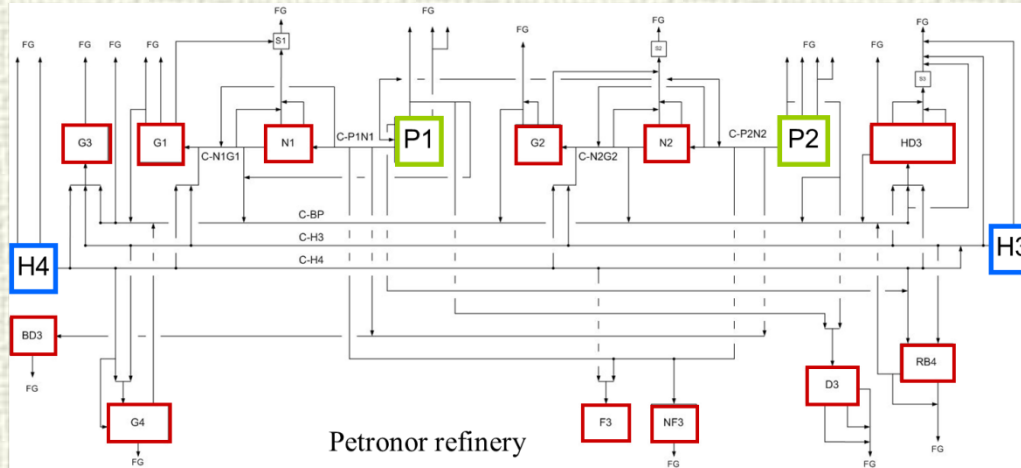
No significant H<sub>2</sub> accumulation in the network

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



- ✓ 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

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## ✓ Many possible economic targets:

- Minimizing the production of fresh H<sub>2</sub>, maximizing the profits, minimizing the flow of H<sub>2</sub> to the fuel gas network, maximizing the use of low purity H<sub>2</sub>, 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

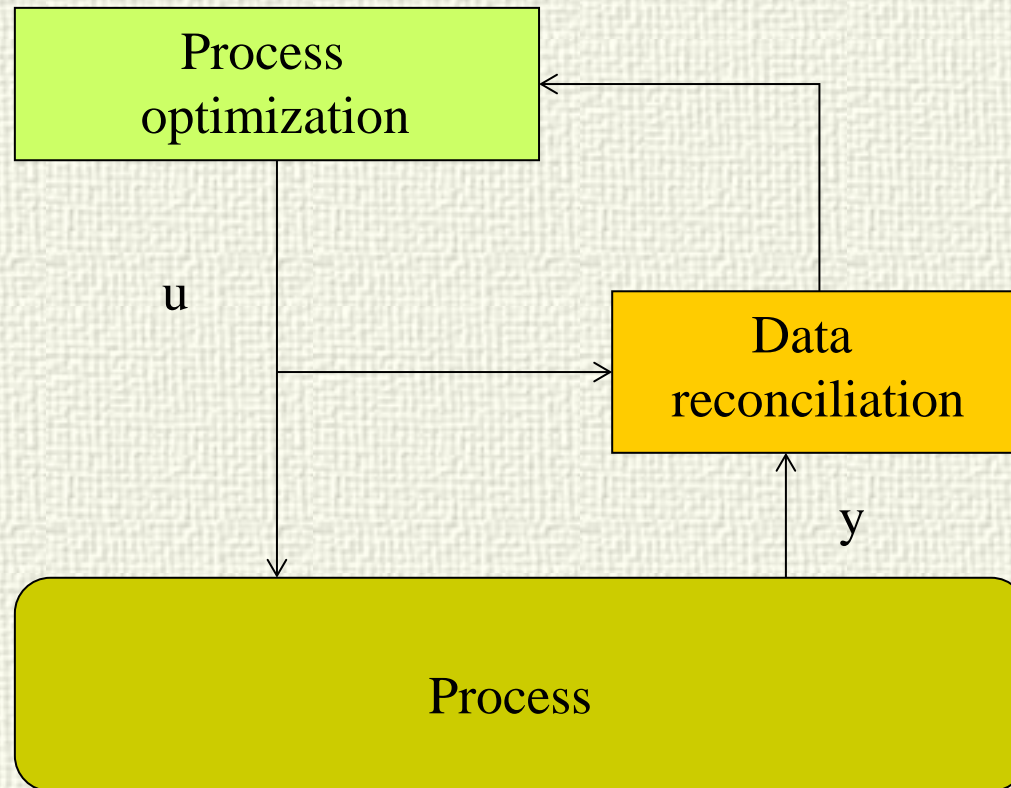
- ✓ Variable hydrogen demands from the consumer units
- ✓ Volumetric flow measurements that must be compensated to obtain massflows. Pressure, temperature **and molecular weight** are required
- ✓ Hydrogen **purity** is not always available. Moreover, the gas stream contains impurities of unknown and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



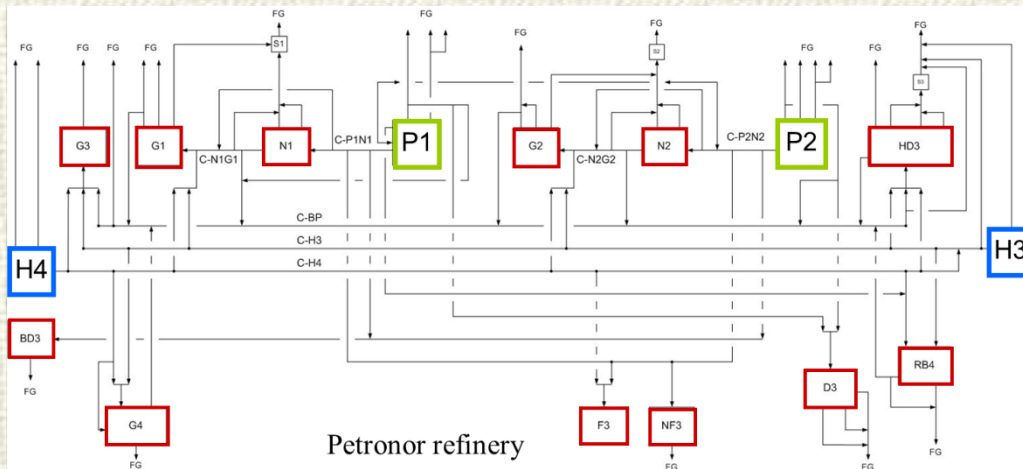
# RTO



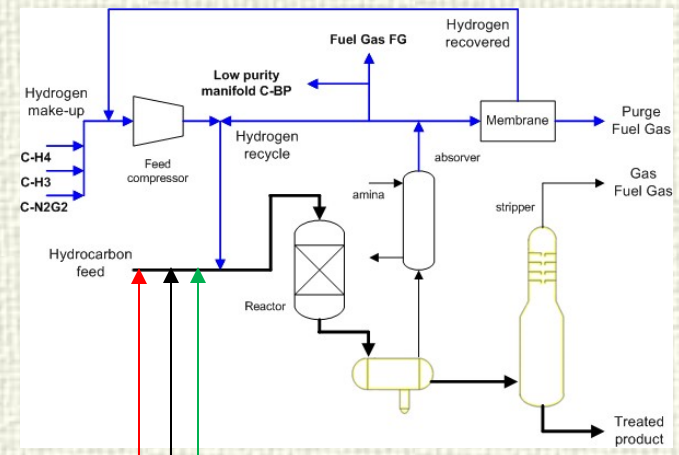


# Approach

- ✓ 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

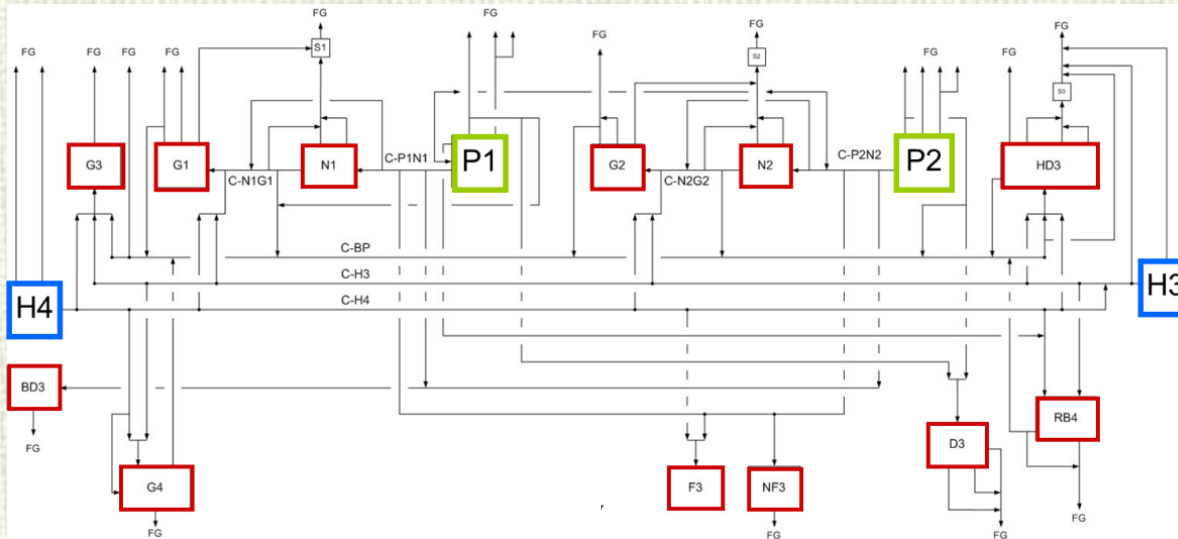


HC from different sources and compositions



# 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

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

$F_j$  [Nm<sup>3</sup>/h]

Normalized volumetric flows

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

$X_j^{H2}$  [% vol.]

Purity of hydrogen in each stream

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

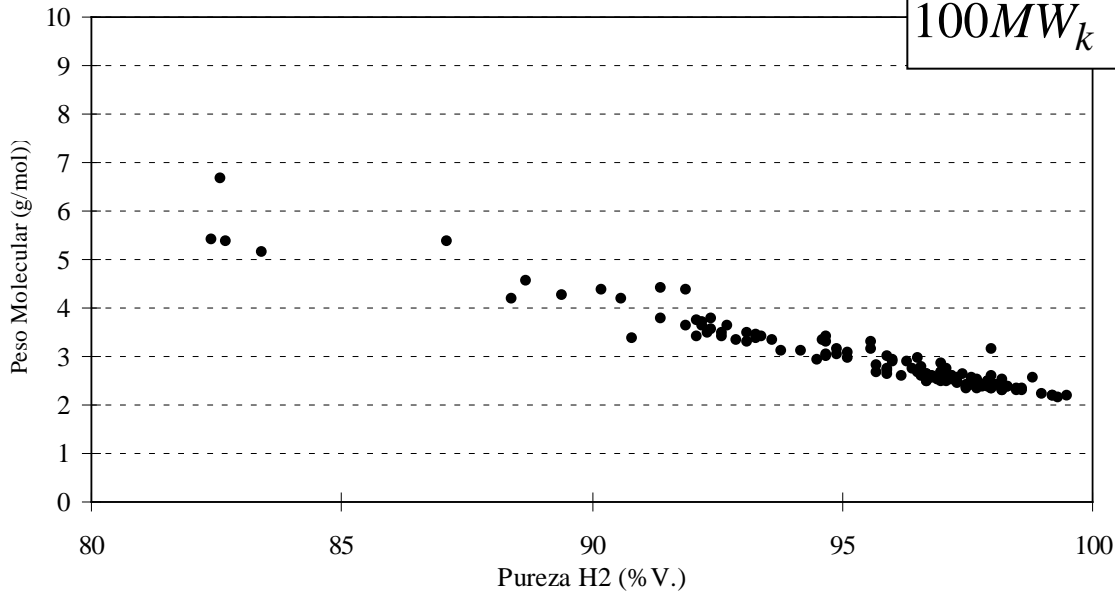
$MW_j$  [g/mol]

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<sub>2</sub> purity



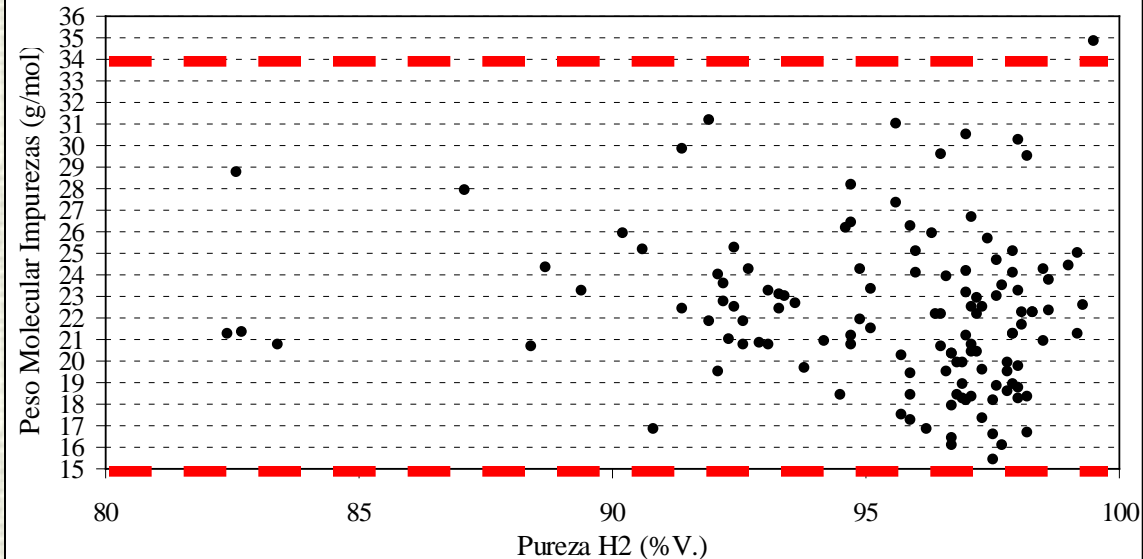
$$100MW_k = MW^{H2} X_k^{H2} + (100 - X_k^{H2}) MW_k^I$$

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 ( $MW_k^I$ )







# 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 ( $\beta$ ) depending on:

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

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

➡ **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

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

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

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

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

$$\sum_{i,sale} F_{N,i} = \sum_{j,entra} F_{N,j} \quad \text{At each node } j$$

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

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

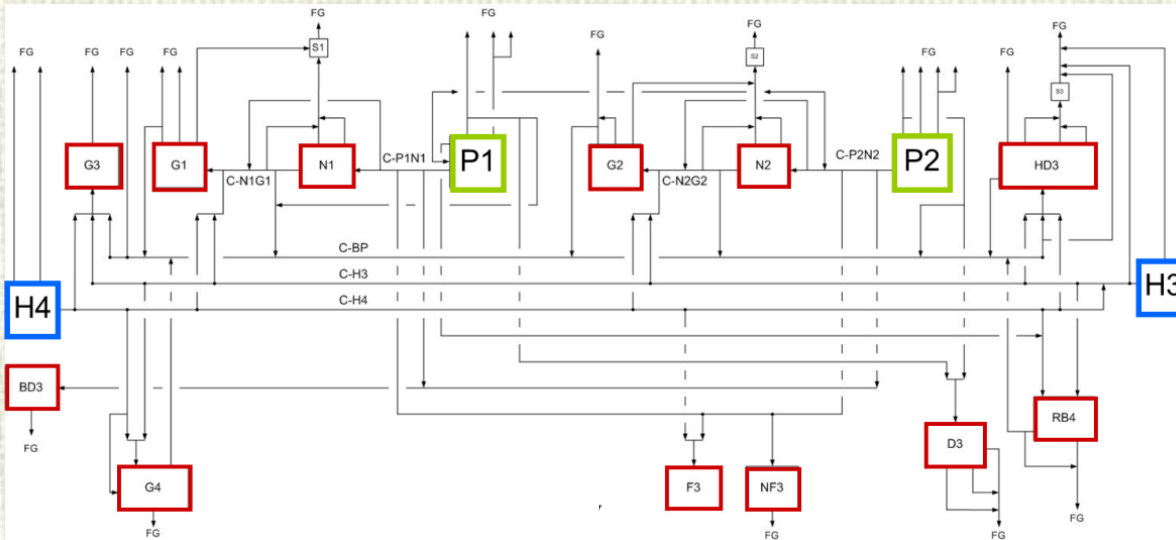
$$PM \sum_{i,sale} F_{N,i} = \sum_{j,entra} PM_j F_{N,j}$$

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

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

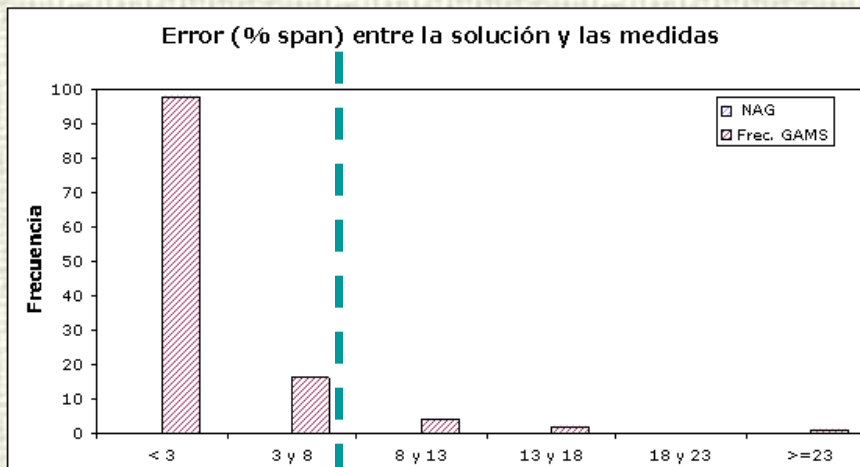


The model can be reconfigured prior to the optimization according to the operational state of the plant: Plants in operation, use of collectors, ....



# Experimental results

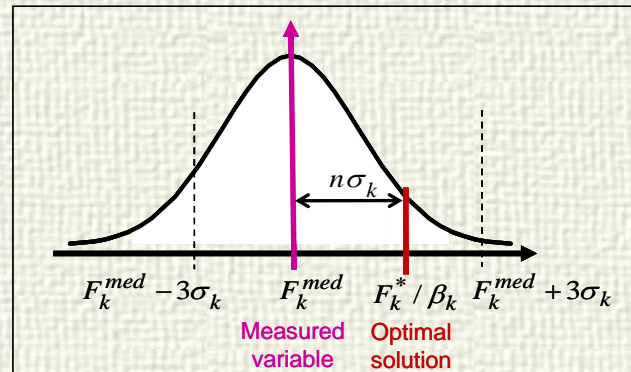
## Number of sigma ( $\sigma$ ) between reconciled data (optimal solution) and measures



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

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

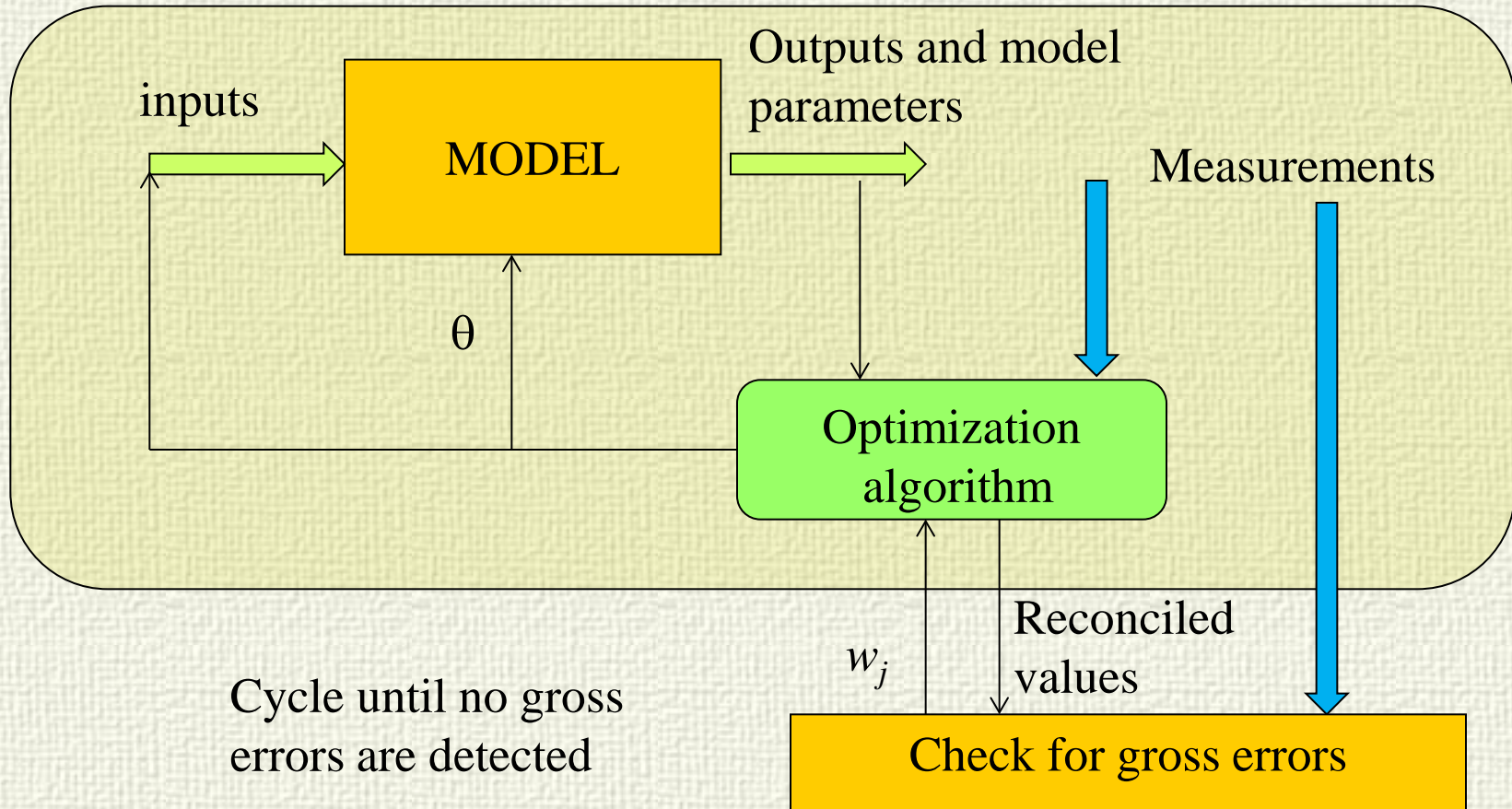
166 measured data



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



# Data reconciliation





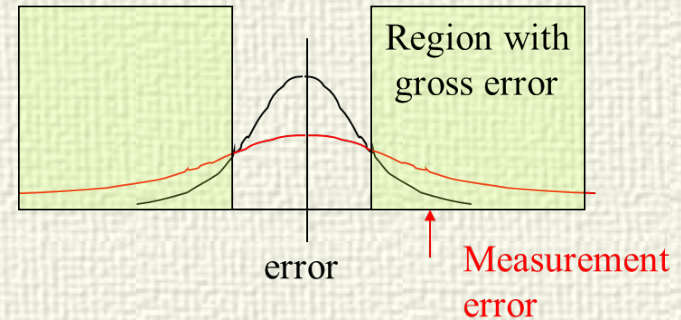
# Gross error detection



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

- ✓ Bivariate error distribution

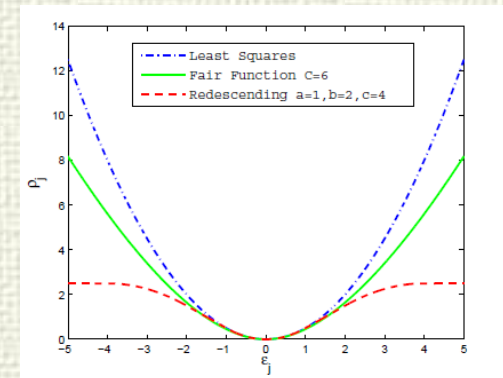
$$\min_{x,p,b} [-\log L] = \min_{x,p,b,\sigma,\theta} \sum_i \left[ (1-p) \frac{\exp\left[-\frac{(x_i - x_{mi})^2}{2\sigma^2}\right]}{\sqrt{2\pi}} + p \frac{\exp\left[-\frac{(x_i - x_{mi})^2}{2(\sigma b)^2}\right]}{b\sqrt{2\pi}} \right] + \sum_i \log \sigma$$



- ✓ Robust estimators

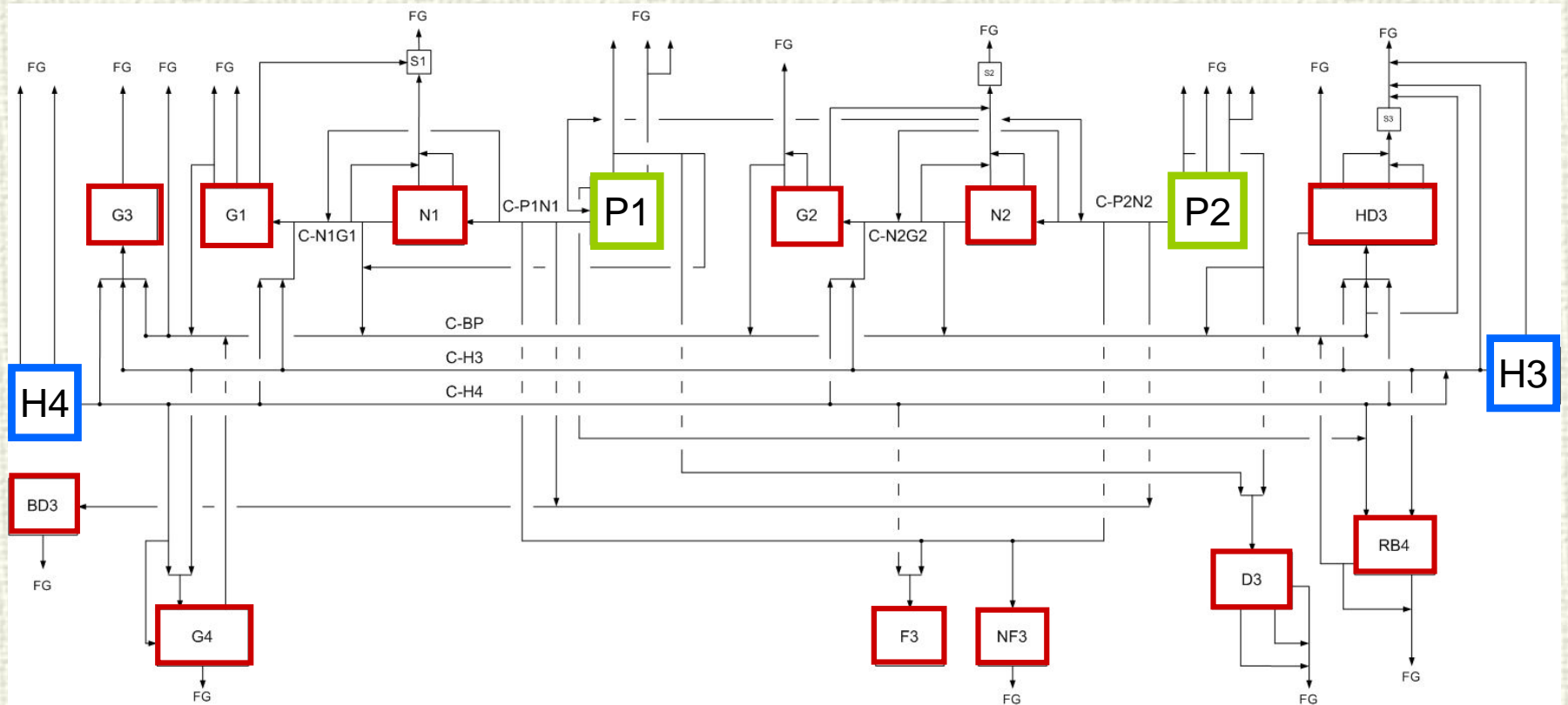
$$F_j = c^2 \left[ \frac{|\varepsilon_j|}{c} - \log \left( 1 + \frac{|\varepsilon_j|}{c} \right) \right]$$

Fair function, Redescending, tuning





# Optimal hydrogen management



 H<sub>2</sub> production units (2)

Hydrogen distribution



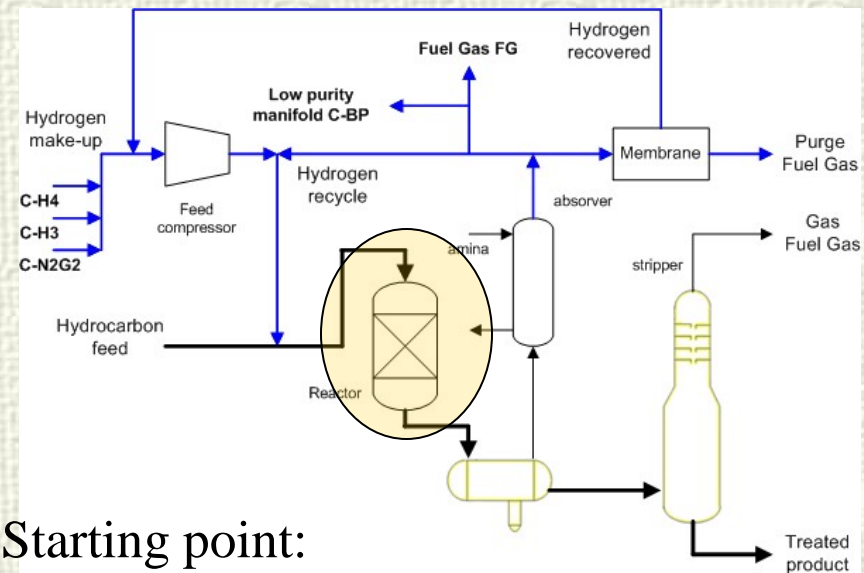
# Optimal hydrogen management

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<sub>2</sub>/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



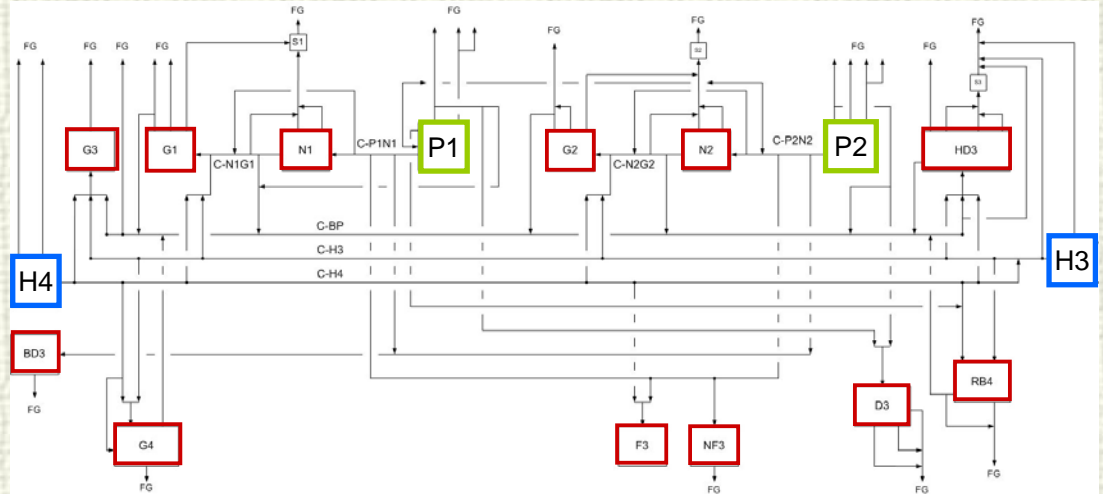
Starting point:  
reconciled values





# Hydrogen shortages

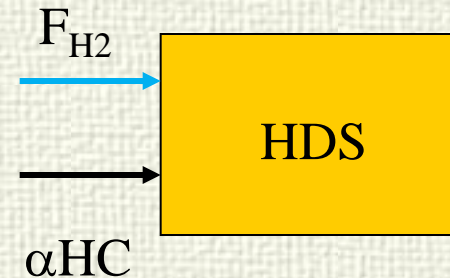
The problem has been enlarged to include reaction to hydrogen shortages that can take place due to several reasons (breakdown of equipment, failures in the platformer plants, etc.)



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:

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

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

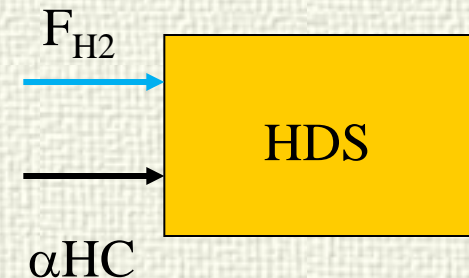
$$HC_{min} y_j \leq HC_j \alpha_j \leq HC_{max} y_j$$

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

Mix integer problem MINLP

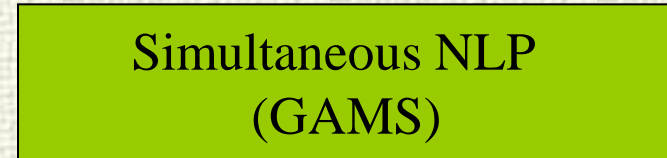
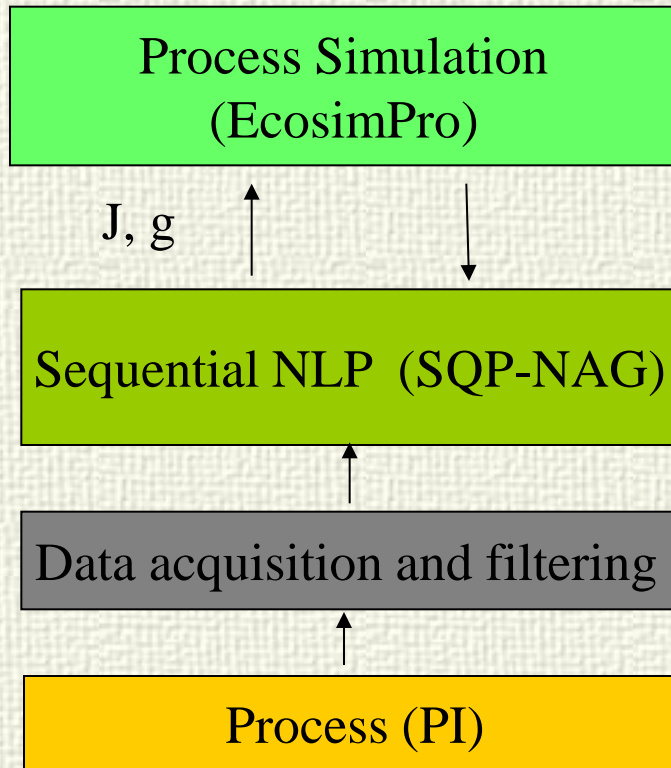
$w_l$  weights reflecting priorities

Range of operation between a minimum and a maximum capacity





# Two solutions



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

The screenshot displays the EcosimPro 4.8.0 software interface. The main window shows a schematic diagram of a process flow, labeled 'G2'. The diagram includes various components such as tanks, mixers, and separators, connected by lines representing flow streams. The interface includes a menu bar (File, Edit, View, Tools, Window, Help), a toolbar, and a workspace area. A library of components is visible on the left, with a table listing the components and their paths.

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

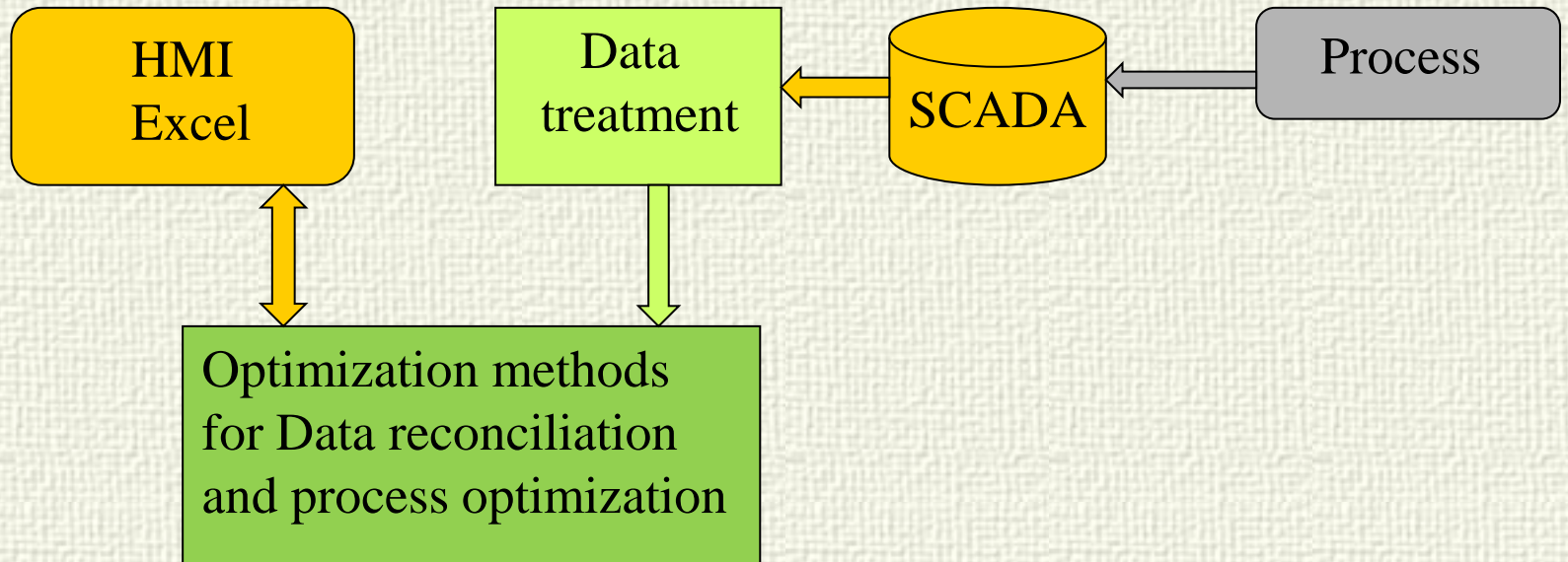
The schematic diagram shows a complex network of flow streams and components. Key components include tanks (e.g., FC\_315, FC\_311, FC\_306, FC\_303, FC\_302, FC\_301, FC\_300, FC\_299, FC\_298, FC\_297, FC\_296, FC\_295, FC\_294, FC\_293, FC\_292, FC\_291, FC\_290, FC\_289, FC\_288, FC\_287, FC\_286, FC\_285, FC\_284, FC\_283, FC\_282, FC\_281, FC\_280, FC\_279, FC\_278, FC\_277, FC\_276, FC\_275, FC\_274, FC\_273, FC\_272, FC\_271, FC\_270, FC\_269, FC\_268, FC\_267, FC\_266, FC\_265, FC\_264, FC\_263, FC\_262, FC\_261, FC\_260, FC\_259, FC\_258, FC\_257, FC\_256, FC\_255, FC\_254, FC\_253, FC\_252, FC\_251, FC\_250, FC\_249, FC\_248, FC\_247, FC\_246, FC\_245, FC\_244, FC\_243, FC\_242, FC\_241, FC\_240, FC\_239, FC\_238, FC\_237, FC\_236, FC\_235, FC\_234, FC\_233, FC\_232, FC\_231, FC\_230, FC\_229, FC\_228, FC\_227, FC\_226, FC\_225, FC\_224, FC\_223, FC\_222, FC\_221, FC\_220, FC\_219, FC\_218, FC\_217, FC\_216, FC\_215, FC\_214, FC\_213, FC\_212, FC\_211, FC\_210, FC\_209, FC\_208, FC\_207, FC\_206, FC\_205, FC\_204, FC\_203, FC\_202, FC\_201, FC\_200, FC\_199, FC\_198, FC\_197, FC\_196, FC\_195, FC\_194, FC\_193, FC\_192, FC\_191, FC\_190, FC\_189, FC\_188, FC\_187, FC\_186, FC\_185, FC\_184, FC\_183, FC\_182, FC\_181, FC\_180, FC\_179, FC\_178, FC\_177, FC\_176, FC\_175, FC\_174, FC\_173, FC\_172, FC\_171, FC\_170, FC\_169, FC\_168, FC\_167, FC\_166, FC\_165, FC\_164, FC\_163, FC\_162, FC\_161, FC\_160, FC\_159, FC\_158, FC\_157, FC\_156, FC\_155, FC\_154, FC\_153, FC\_152, FC\_151, FC\_150, FC\_149, FC\_148, FC\_147, FC\_146, FC\_145, FC\_144, FC\_143, FC\_142, FC\_141, FC\_140, FC\_139, FC\_138, FC\_137, FC\_136, FC\_135, FC\_134, FC\_133, FC\_132, FC\_131, FC\_130, FC\_129, FC\_128, FC\_127, FC\_126, FC\_125, FC\_124, FC\_123, FC\_122, FC\_121, FC\_120, FC\_119, FC\_118, FC\_117, FC\_116, FC\_115, FC\_114, FC\_113, FC\_112, FC\_111, FC\_110, FC\_109, FC\_108, FC\_107, FC\_106, FC\_105, FC\_104, FC\_103, FC\_102, FC\_101, FC\_100, FC\_99, FC\_98, FC\_97, FC\_96, FC\_95, FC\_94, FC\_93, FC\_92, FC\_91, FC\_90, FC\_89, FC\_88, FC\_87, FC\_86, FC\_85, FC\_84, FC\_83, FC\_82, FC\_81, FC\_80, FC\_79, FC\_78, FC\_77, FC\_76, FC\_75, FC\_74, FC\_73, FC\_72, FC\_71, FC\_70, FC\_69, FC\_68, FC\_67, FC\_66, FC\_65, FC\_64, FC\_63, FC\_62, FC\_61, FC\_60, FC\_59, FC\_58, FC\_57, FC\_56, FC\_55, FC\_54, FC\_53, FC\_52, FC\_51, FC\_50, FC\_49, FC\_48, FC\_47, FC\_46, FC\_45, FC\_44, FC\_43, FC\_42, FC\_41, FC\_40, FC\_39, FC\_38, FC\_37, FC\_36, FC\_35, FC\_34, FC\_33, FC\_32, FC\_31, FC\_30, FC\_29, FC\_28, FC\_27, FC\_26, FC\_25, FC\_24, FC\_23, FC\_22, FC\_21, FC\_20, FC\_19, FC\_18, FC\_17, FC\_16, FC\_15, FC\_14, FC\_13, FC\_12, FC\_11, FC\_10, FC\_9, FC\_8, FC\_7, FC\_6, FC\_5, FC\_4, FC\_3, FC\_2, FC\_1, FC\_0). The diagram also shows flow streams (e.g., F1\_29, F1\_30, F1\_31, F1\_32, F1\_33, F1\_34, F1\_35, F1\_36, F1\_37, F1\_38, F1\_39, F1\_40, F1\_41, F1\_42, F1\_43, F1\_44, F1\_45, F1\_46, F1\_47, F1\_48, F1\_49, F1\_50, F1\_51, F1\_52, F1\_53, F1\_54, F1\_55, F1\_56, F1\_57, F1\_58, F1\_59, F1\_60, F1\_61, F1\_62, F1\_63, F1\_64, F1\_65, F1\_66, F1\_67, F1\_68, F1\_69, F1\_70, F1\_71, F1\_72, F1\_73, F1\_74, F1\_75, F1\_76, F1\_77, F1\_78, F1\_79, F1\_80, F1\_81, F1\_82, F1\_83, F1\_84, F1\_85, F1\_86, F1\_87, F1\_88, F1\_89, F1\_90, F1\_91, F1\_92, F1\_93, F1\_94, F1\_95, F1\_96, F1\_97, F1\_98, F1\_99, F1\_100). The interface also includes a toolbar with various icons for editing and simulation, and a status bar at the bottom showing the current zoom level (63%) and the date (22/11/2011).

Graphical building of the network and plant structure  
Instrumentation is included  
Automatic partition generation



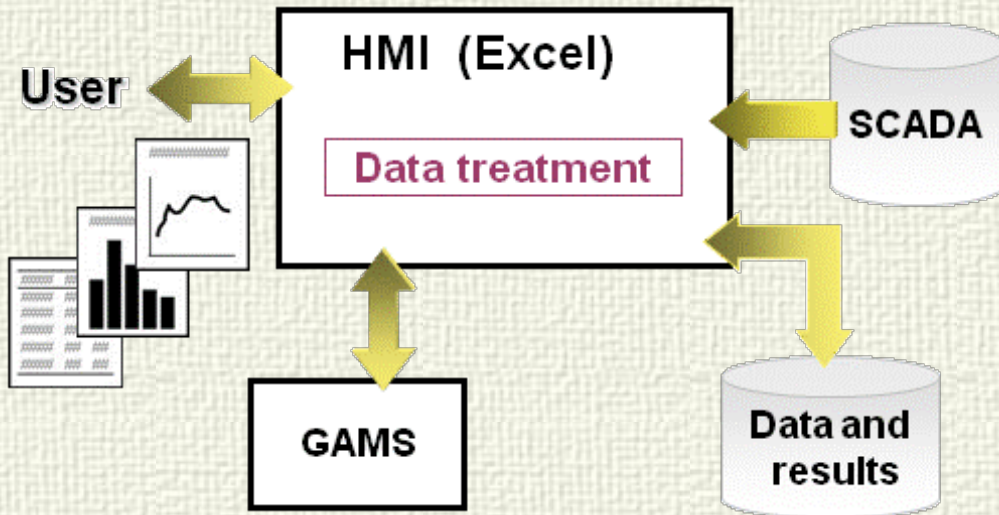
# DSS

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# Decision Support System



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.

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 inconsistencies in the raw data and decides which options are the most adequate ones



# Decision Support System

## Ejecución Simple

Fecha Inicial (dd/mm/aaaa h:mm:ss):

Periodo solución (h:mm):

Periodo muestreo (h:mm):

Horas visualización tendencias (h:mm):

### 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

Actualizar resultados

Cancelar

Grabar datos y soluciones

Cargar datos y soluciones

### 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

Ejecutar

Importar sol GAMS

### Distribución de H2

- NAG
- GAMS

Ejecutar

Importar sol GAMS

Interfaz

Estadísticas

Unidades

Medidas

Errores

Límites

Compensación

Gráficas

Plano Red

Unidades distr.

Resumen distr.

## Ejecución Consecutiva

Fecha Inicial (dd/mm/aaaa h:mm:ss):

Fecha Final (dd/mm/aaaa h:mm:ss):

Periodo solución (h:mm):

Periodo muestreo gráficas (h:mm):

Periodo ejecución aplicación (h:mm):

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

Ejecutar

### Seleccione una unidad:

B03  
P1  
P2  
N1  
N2  
G1  
G2  
HD3  
RB4  
CBP  
H3  
D3  
F1

Ir a plano

Generar gráficas

Actualizar gráficas

Borrar gráficas

Borrar estadísticas

Borrar errores

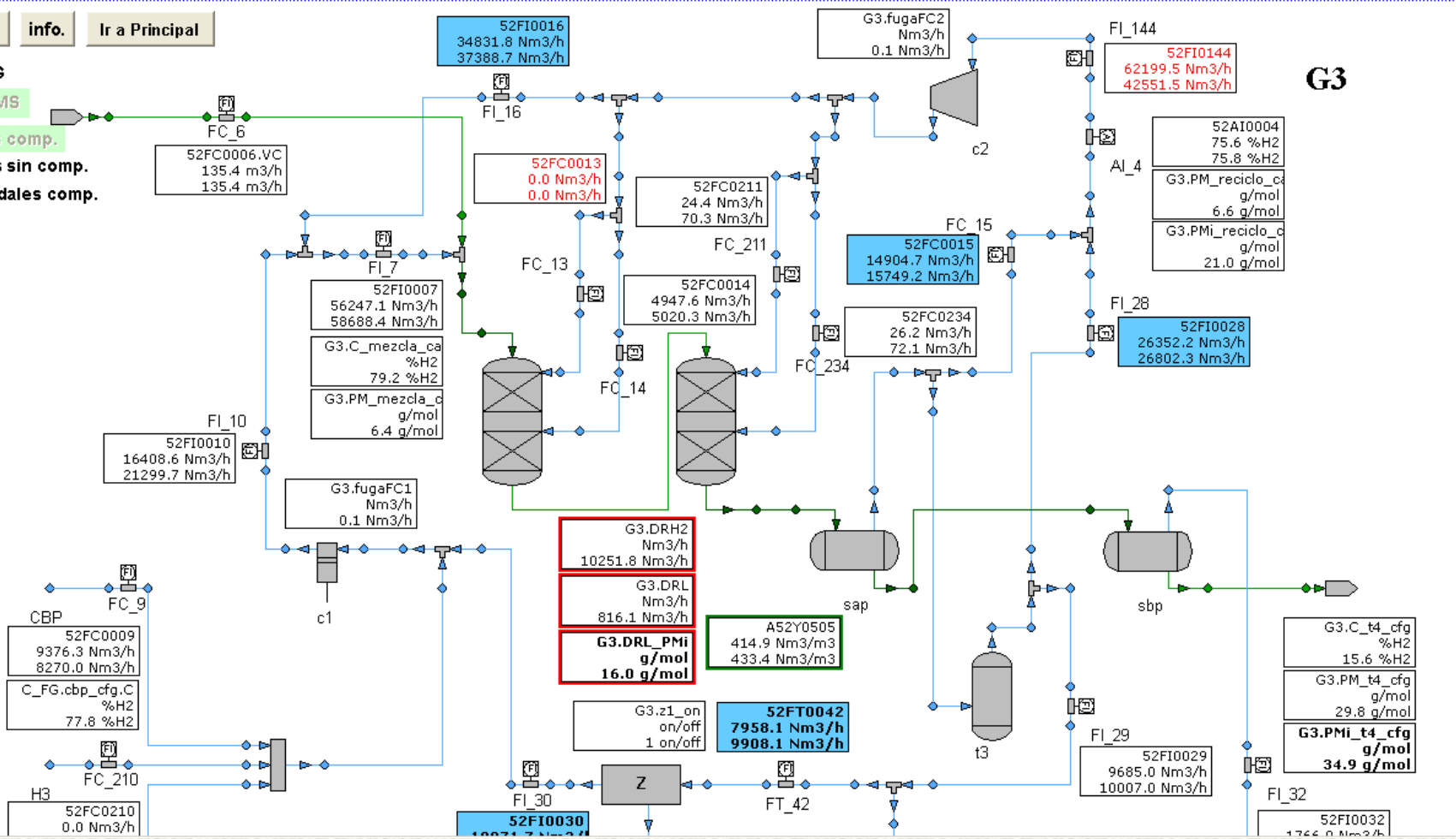
Borrar Notas



# DSS

Actualizar info. Ir a Principal

- Solución NAG
- Solución GAMS
- Sol. caudales comp.
- Sol. caudales sin comp.
- Medidas caudales comp.







# Typical results

15 out of 16 plants were in operation  
numbers in % H4 cheaper than H3

	N m3h Optimal distribution	N m3h 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	Nm3h reconciliation
H3	20.26	14.37
H4	31.01	39.15
F1	7.46	16.83
F2	29.65	29.65
Total	88.38	100.00
FG	27.25	30.98

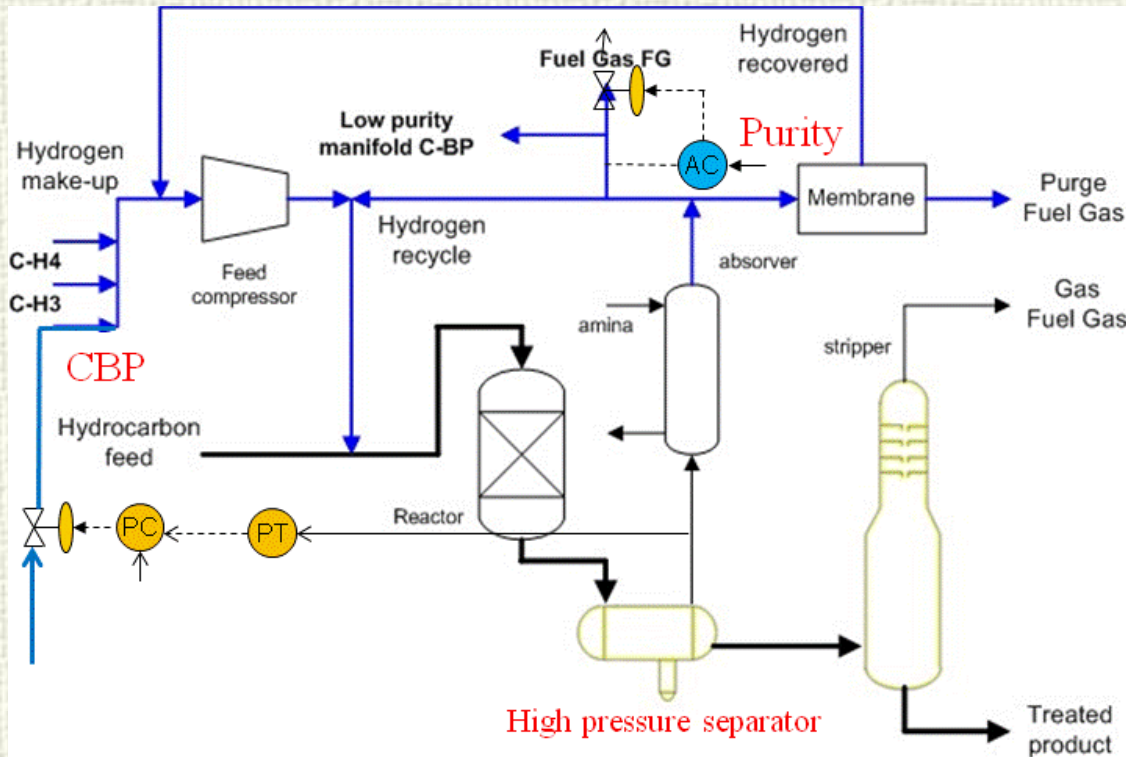
HC load reduction and state of the plants before/after failure  
1 running, 0 stopped

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



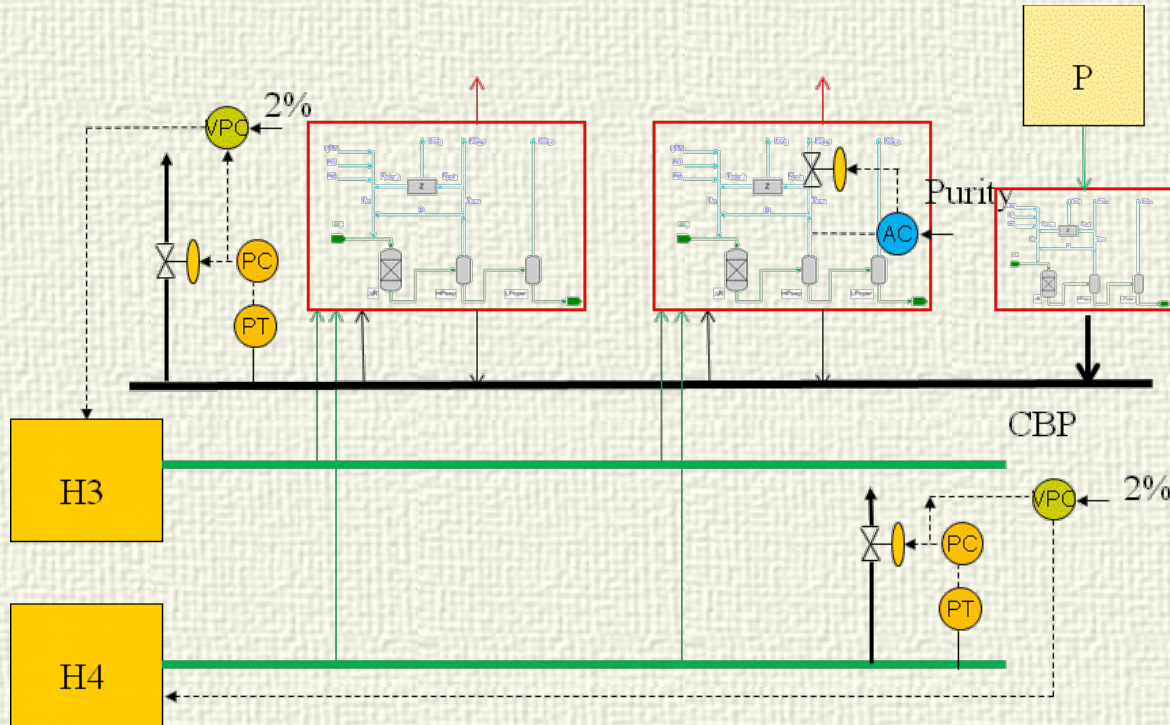
Maintaining steady state balances with pressure control loops

Unbalances are moved to the CBP collector

H<sub>2</sub> purity control loops maintain the impurities balance



# Implementation



This will affect all plants

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

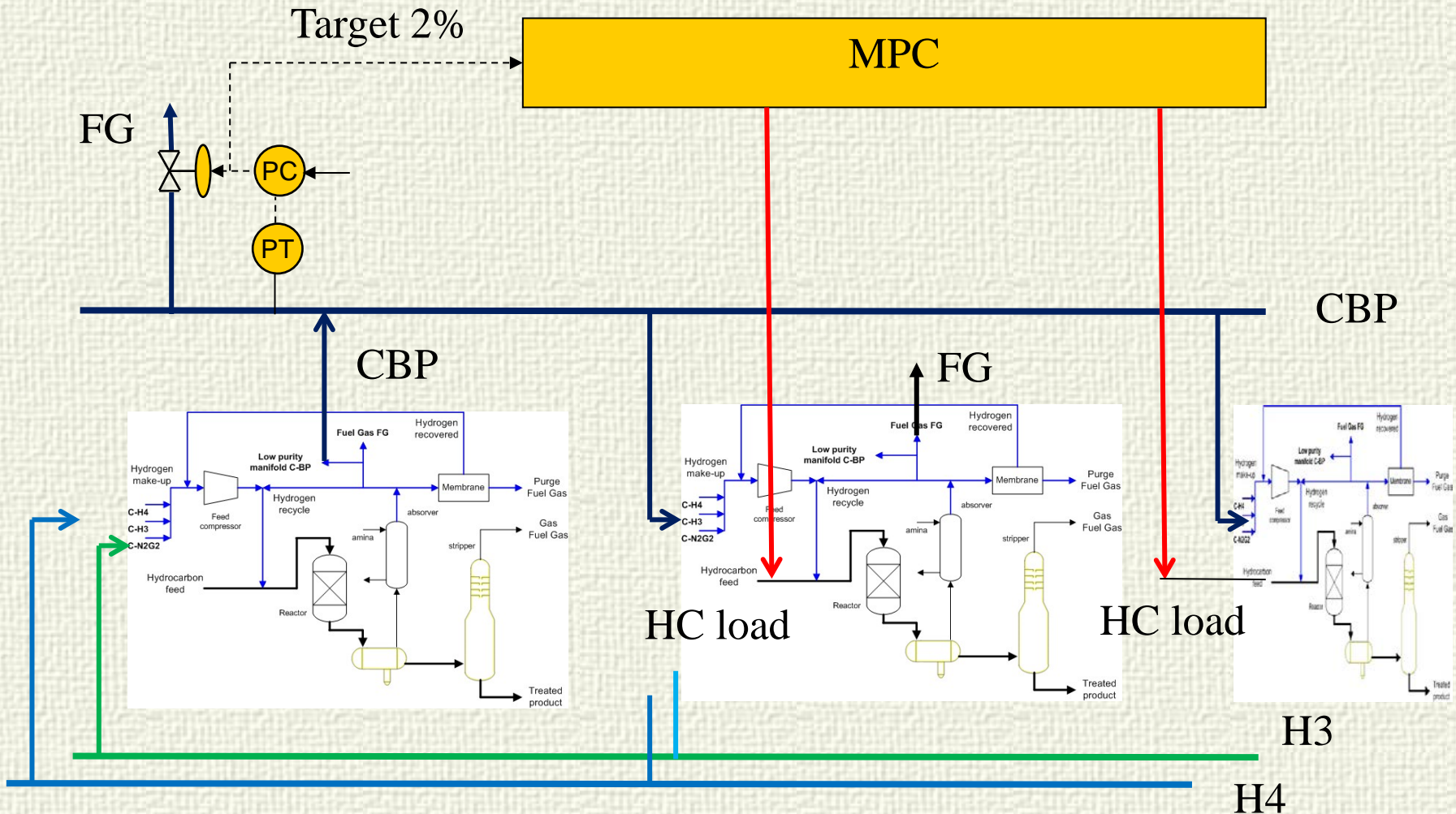
Collectors  
pressure control  
maintain global  
balances

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

The optimizer  
fixes the best  
distribution



# Dynamic plant operation





# Conclusions

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- ✓ 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 H<sub>2</sub> in the hydrogen suppliers
- ✓ Implementation plays an important role