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
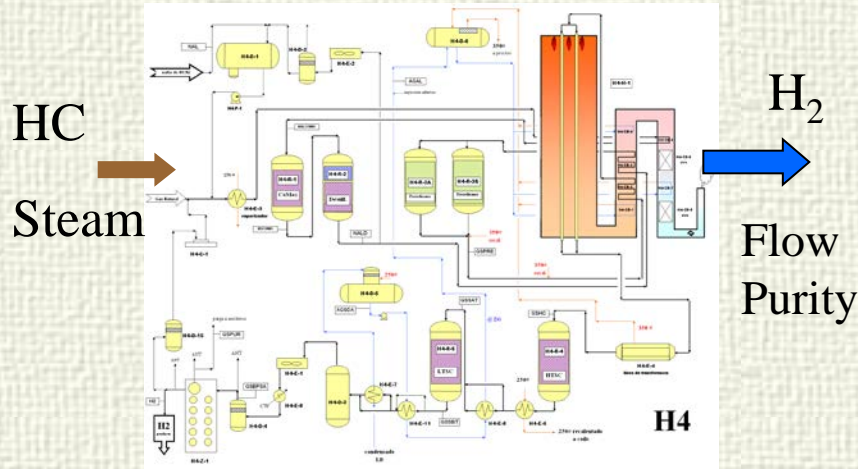- ✓ Results
- ✓ Conclusions

Hydrogen in petrol refineries

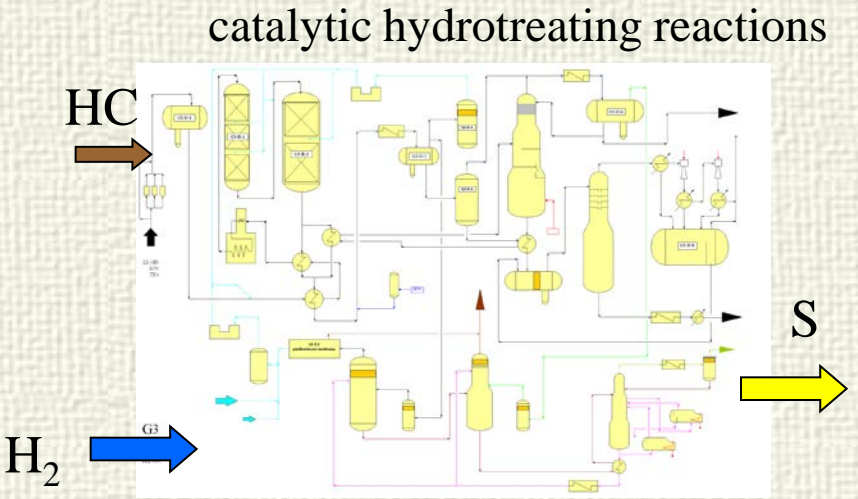Hydrogen is used in modern refineries in processes that have two main purposes:
✓ Increase the value of the hydrocarbons (platformers, hydrocraking, etc.)
✓ Reduce the sulphur content of the products, (HDS),..

Hydrogen plants (producers / consumers)

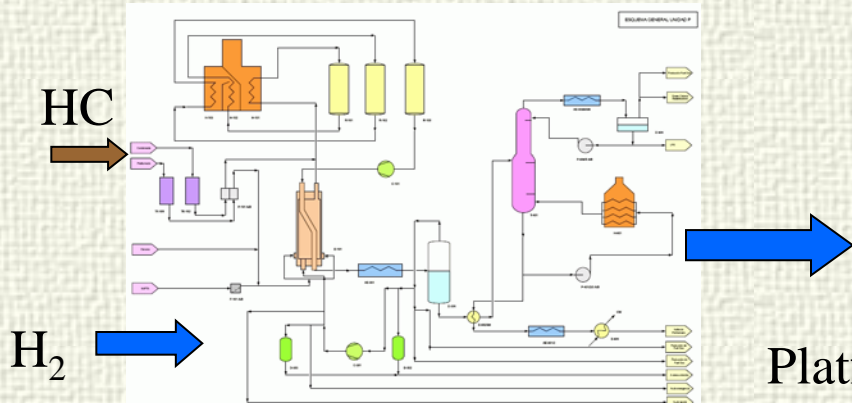catalytic hydrotreating reactions

HC

Steam

H_2

Flow
Purity

Hydrogen producer plant

HC

H_2

Platformer

HC

H_2

S

Hydrodesulphurization plant HDS

Hydrocrakers

Low purity H_2 obtained as a by-product

Distribution network

Petronor refinery

Sub-networks with different pressures and purities / several supply sources
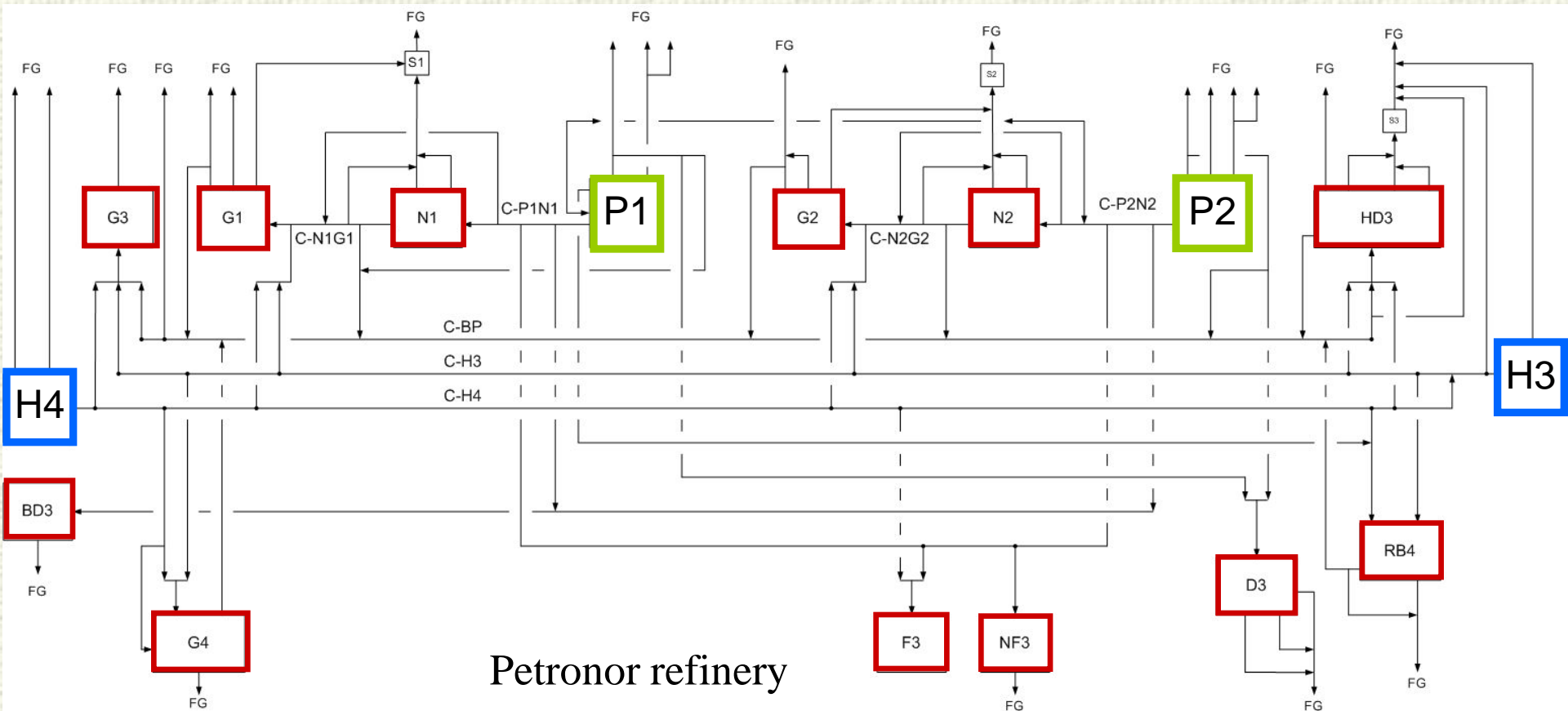
- H_2 production units (2)
- H_2 production units as by product (2)
- H_2 consuming units (12)
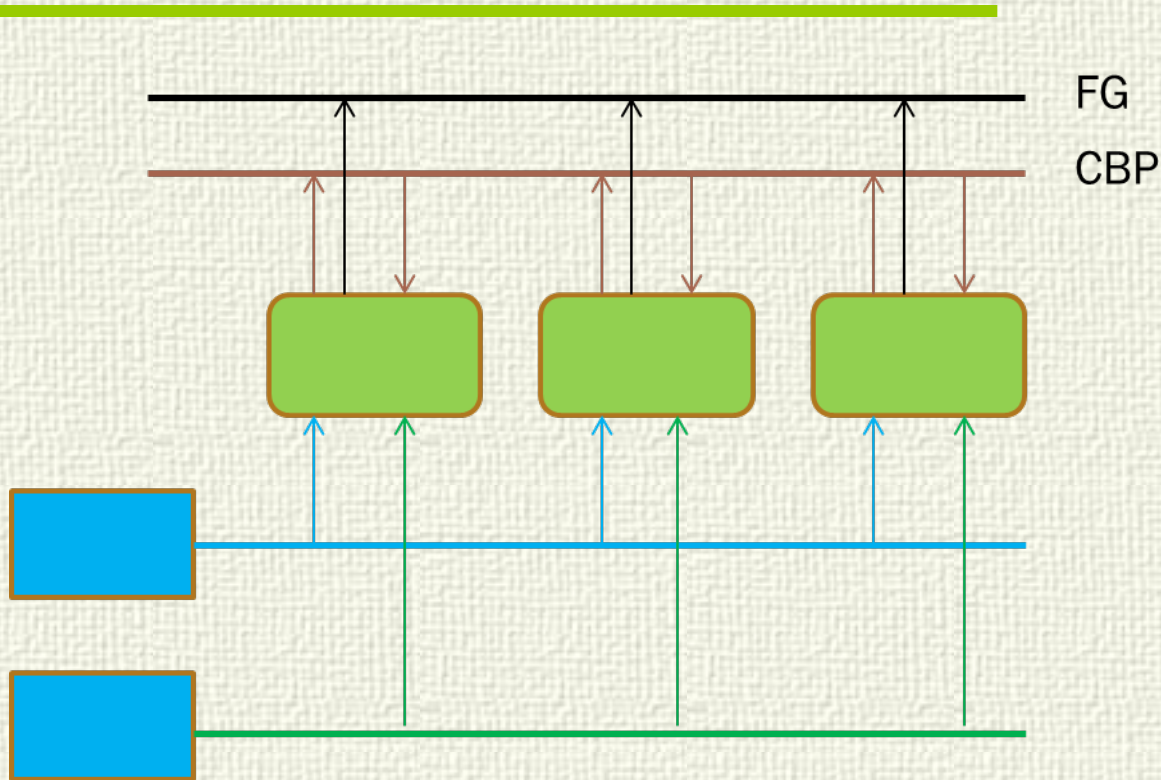
HDS

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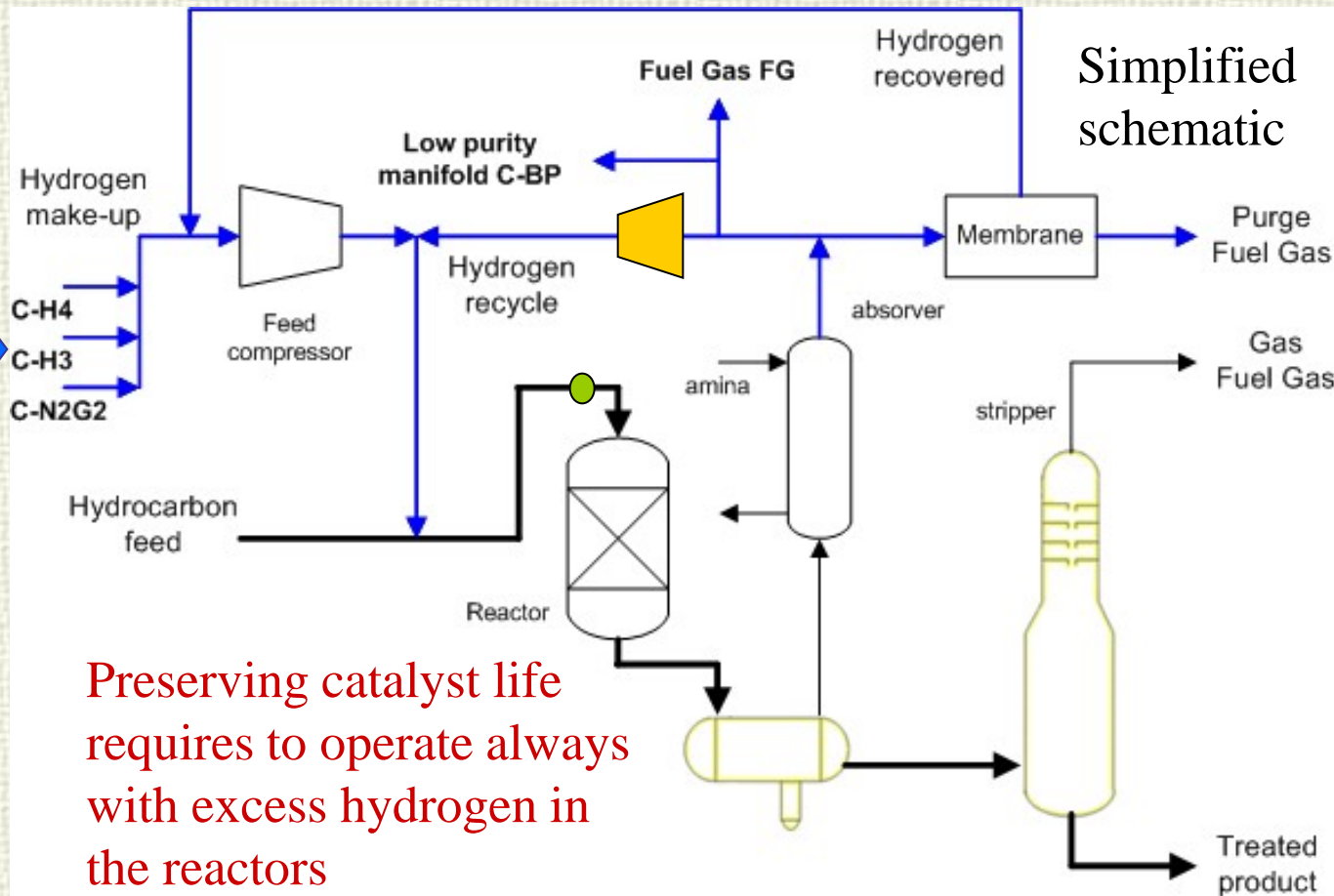
Preserving catalyst life requires to operate always with excess hydrogen in the reactors

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
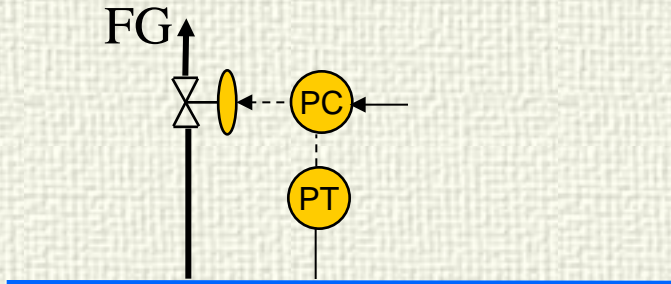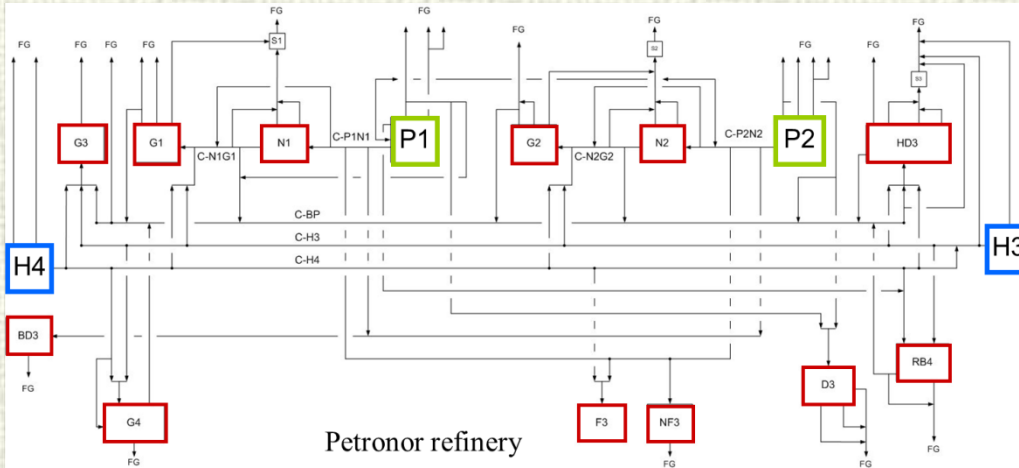
Networks

FG

CBP

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

FG

Hydrogen is an expensive product
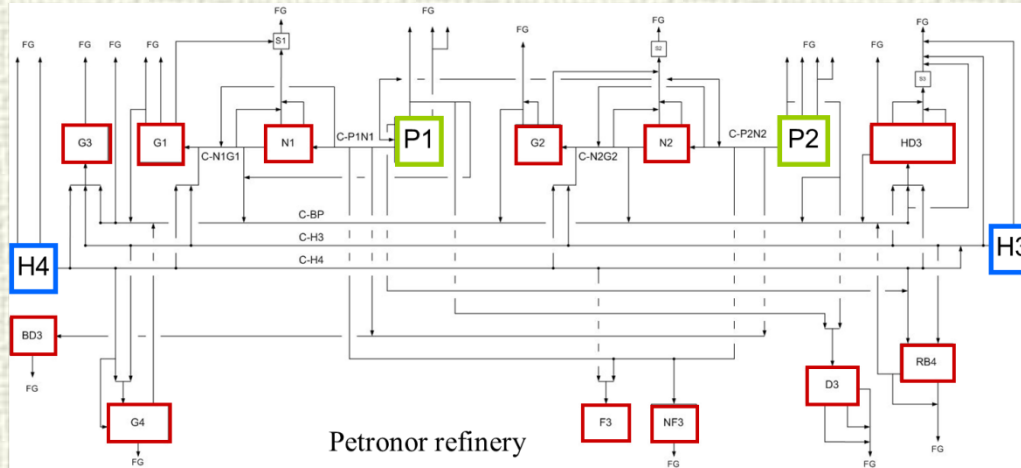
Variable hydrogen demands

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

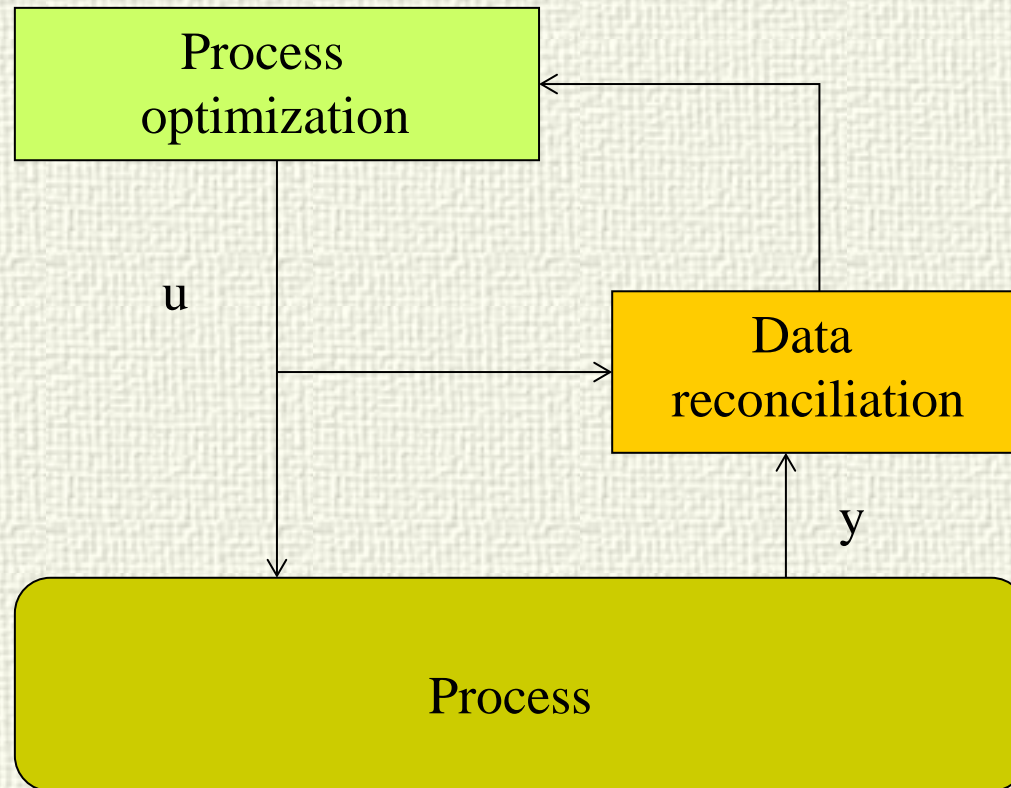– The large scale of the system / size and time scales

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%.
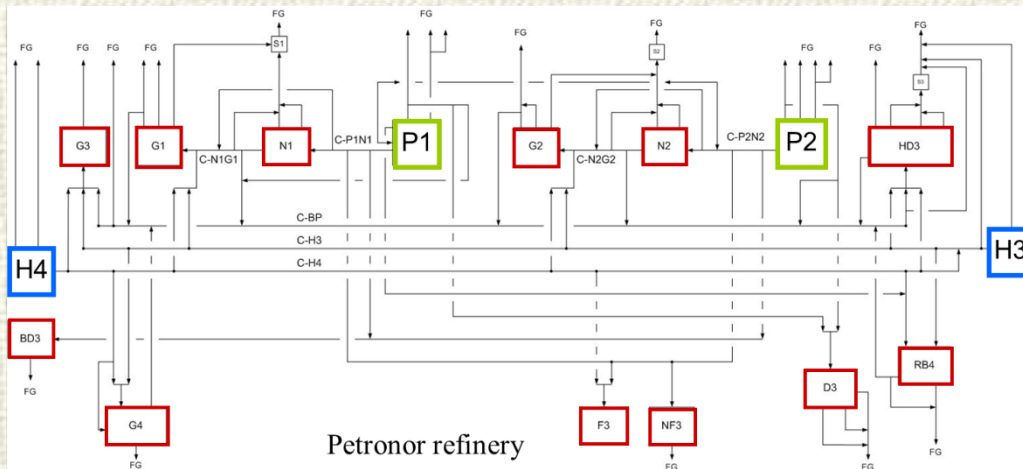- ✓ Compensated flows and purities are not always reliable.

RTO

Process optimization
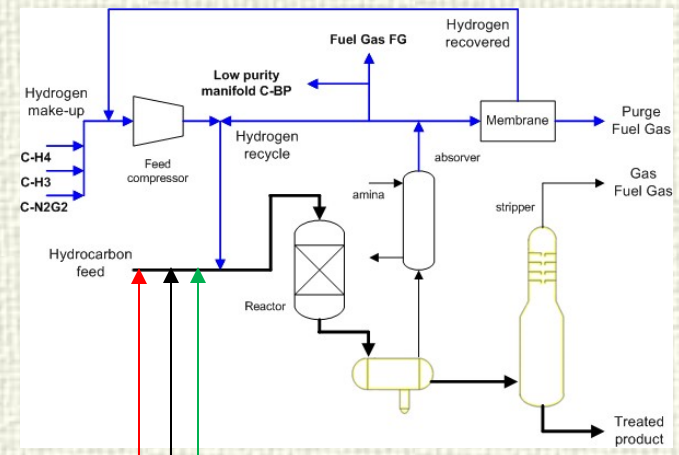
u

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

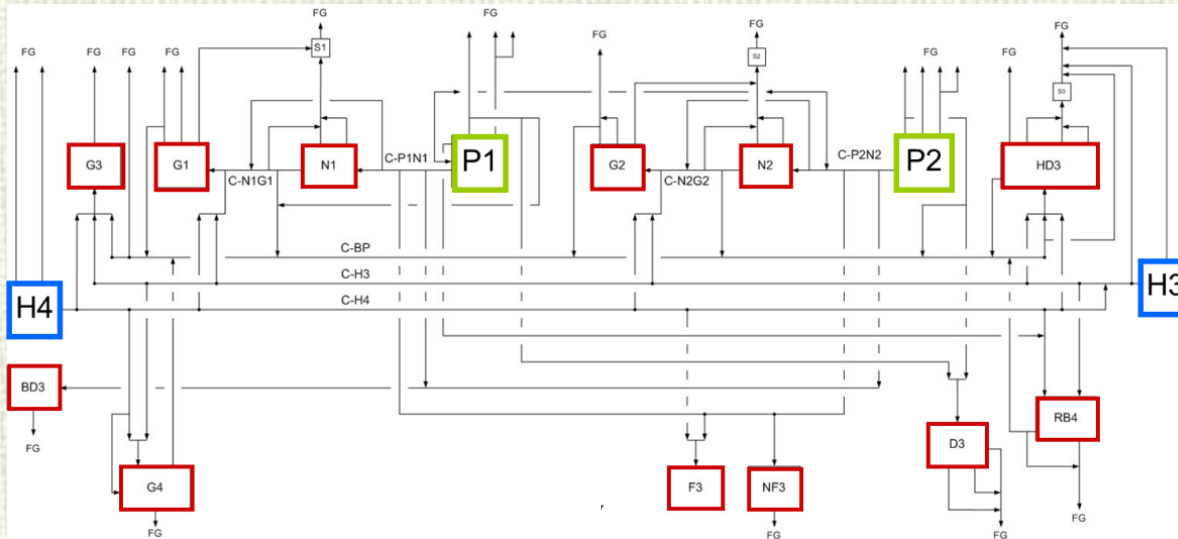Separate the period when a HC change takes place from the rest

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

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

F_j [Nm3/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**

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

Molecular weight vs H$_2$ purity
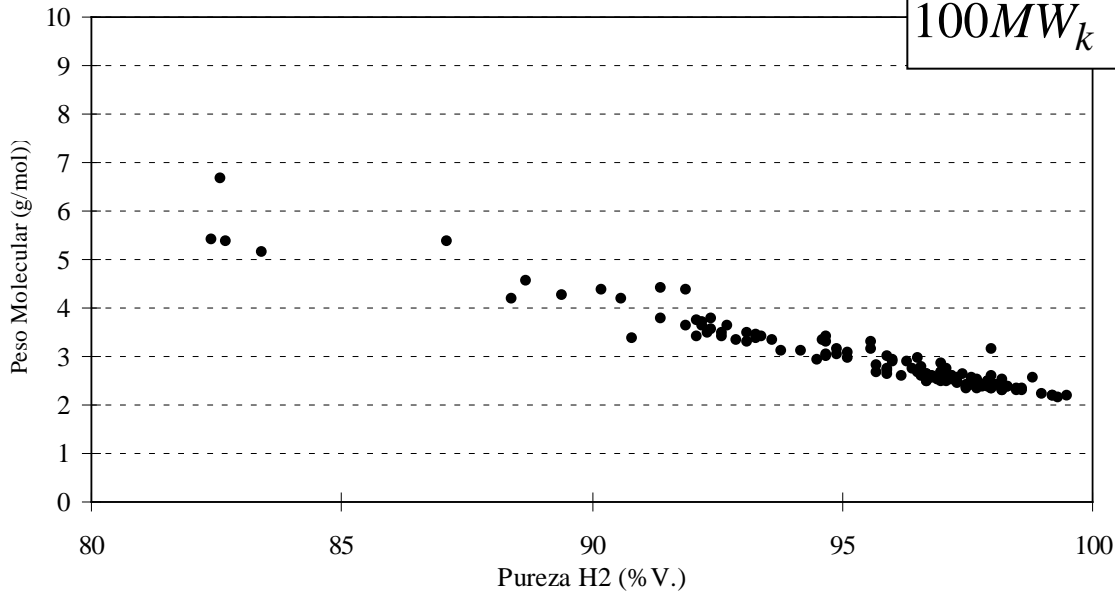
$$100MW_k = MW^{H2}X_k^{H2} + (100 - X_k^{H2})MW_k^I$$

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)
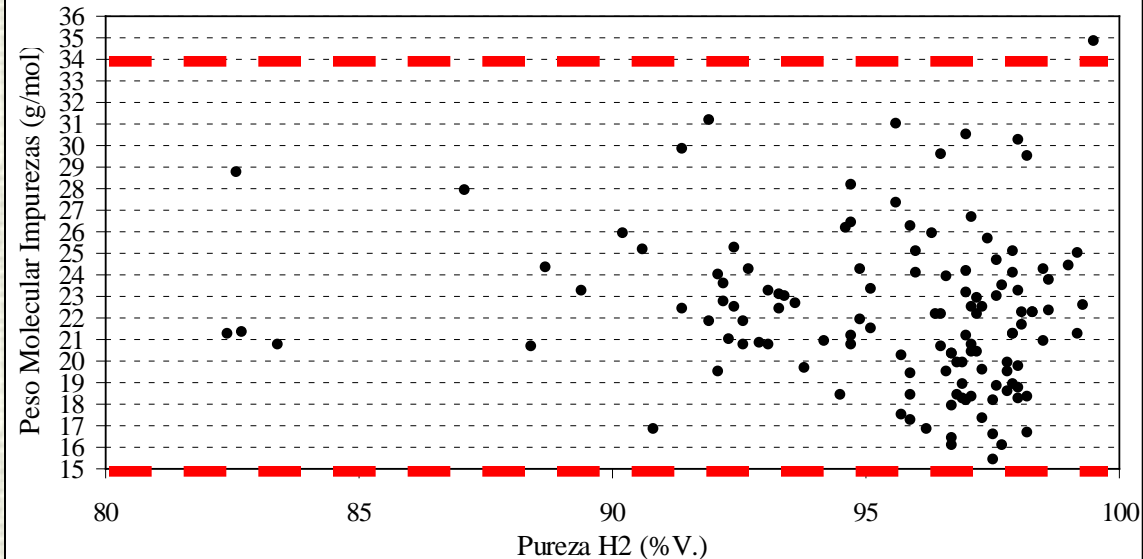
Compensated flow measurements

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

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

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

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

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

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

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

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

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

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.

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

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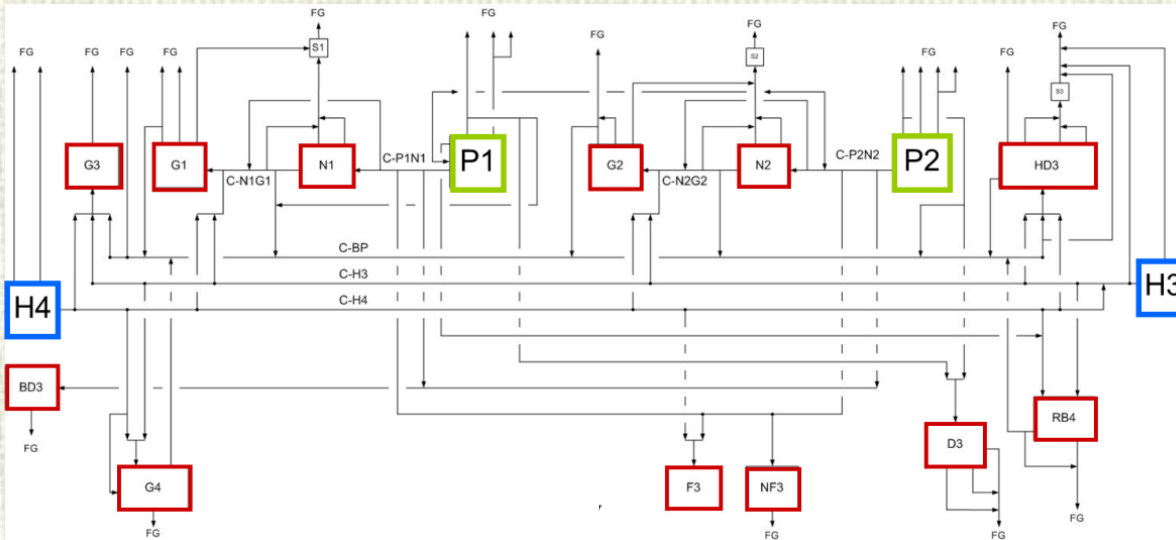
The model can be reconfigured prior to the optimization according to the operational state of the plant: Plants in operation, use of collectors, ….

Experimental results

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

Error (% span) entre la solución y las medidas
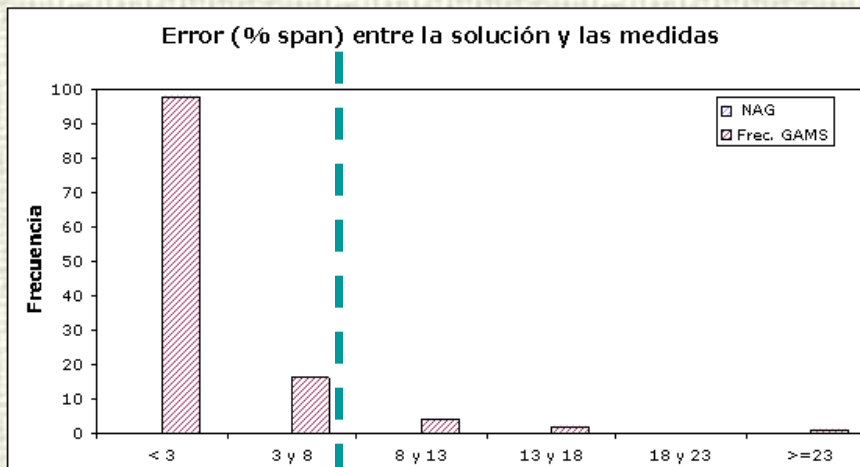
Flows:
$$n\sigma_k = \frac{(F_k^* / \beta_k - F_k^{med})}{\sigma_k}$$

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

166 measured data

$n\sigma_k$

$F_k^{med} - 3\sigma_k$ $\quad$ F_k^{med} $\quad$ F_k^* / β_k $\quad$ $F_k^{med} + 3\sigma_k$

Measured variable $\quad$ Optimal solution
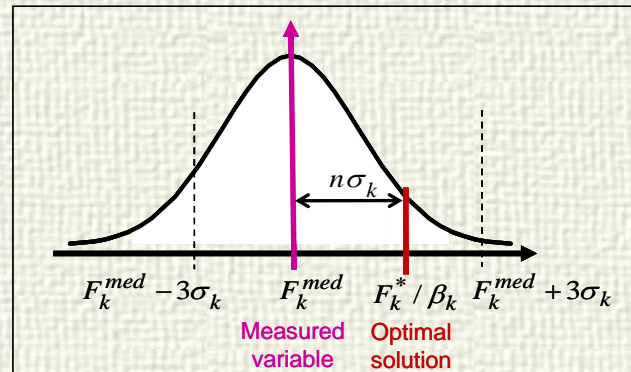
Eliminate the wrong data from the cost function and repeat the DR

Data reconciliation

inputs

MODEL

Outputs and model parameters

Measurements

θ

Optimization algorithm

w_j

Reconciled values

Cycle until no gross errors are detected

Check for gross errors
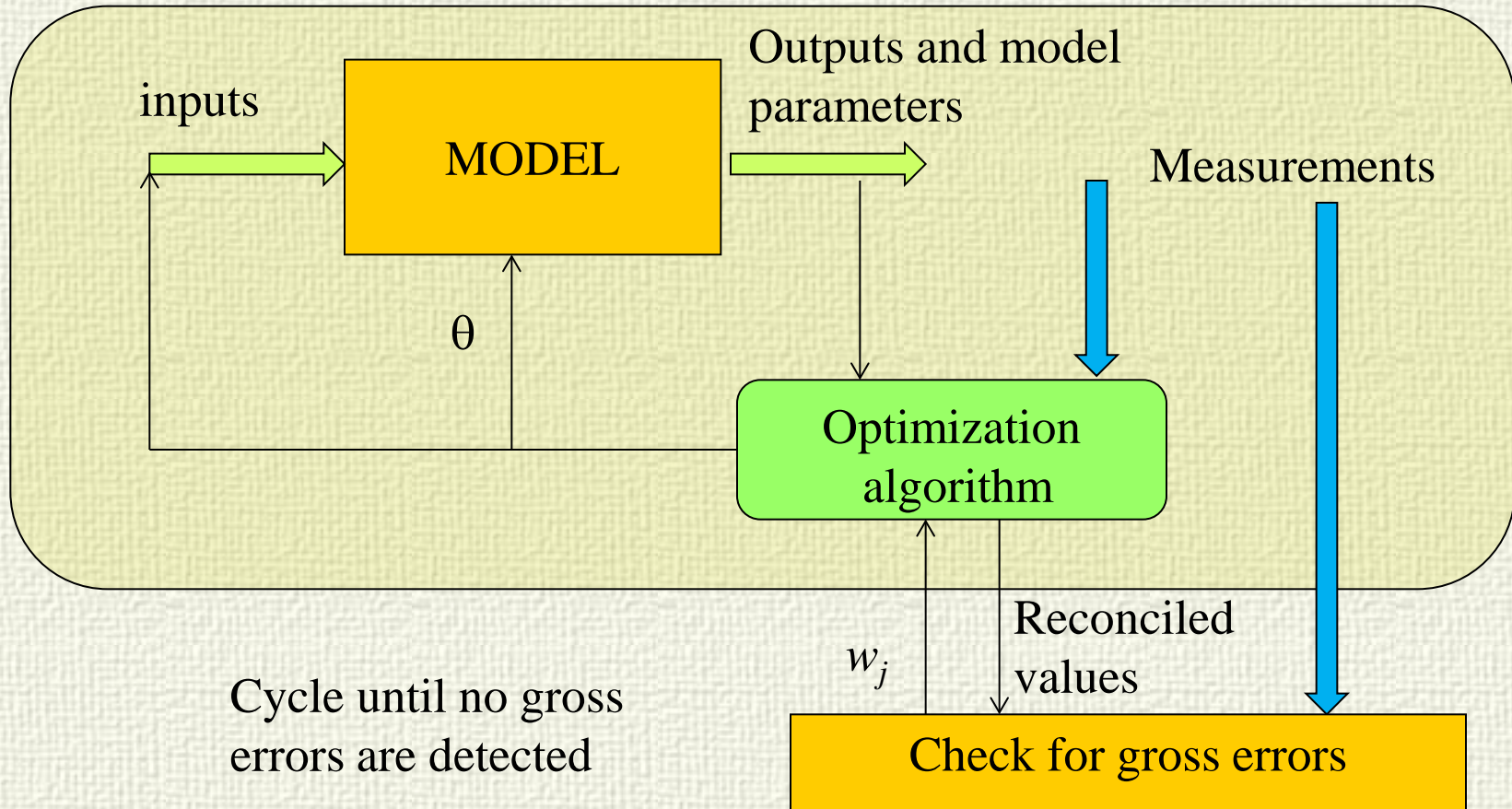
Gross error detection

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

- ✓ Bivariate error distribution

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

Region with gross error

error

Measurement error
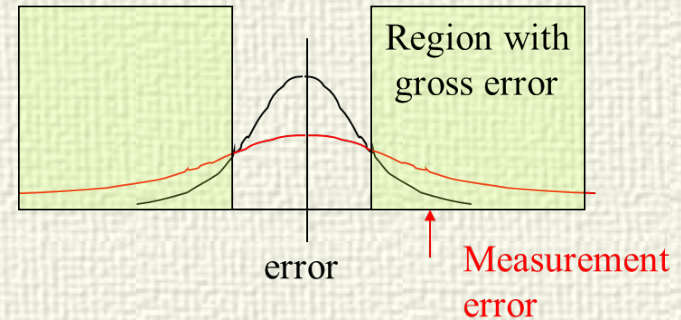
- ✓ Robust estimators

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

Fair function, Redescending, tuning
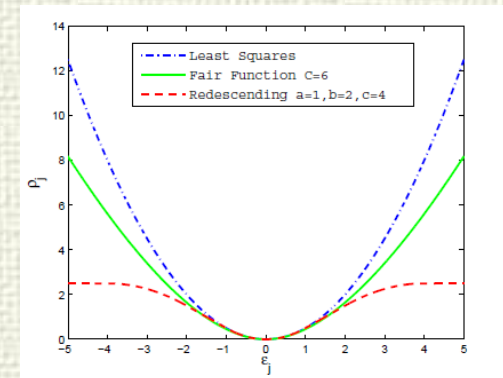
Optimal hydrogen management
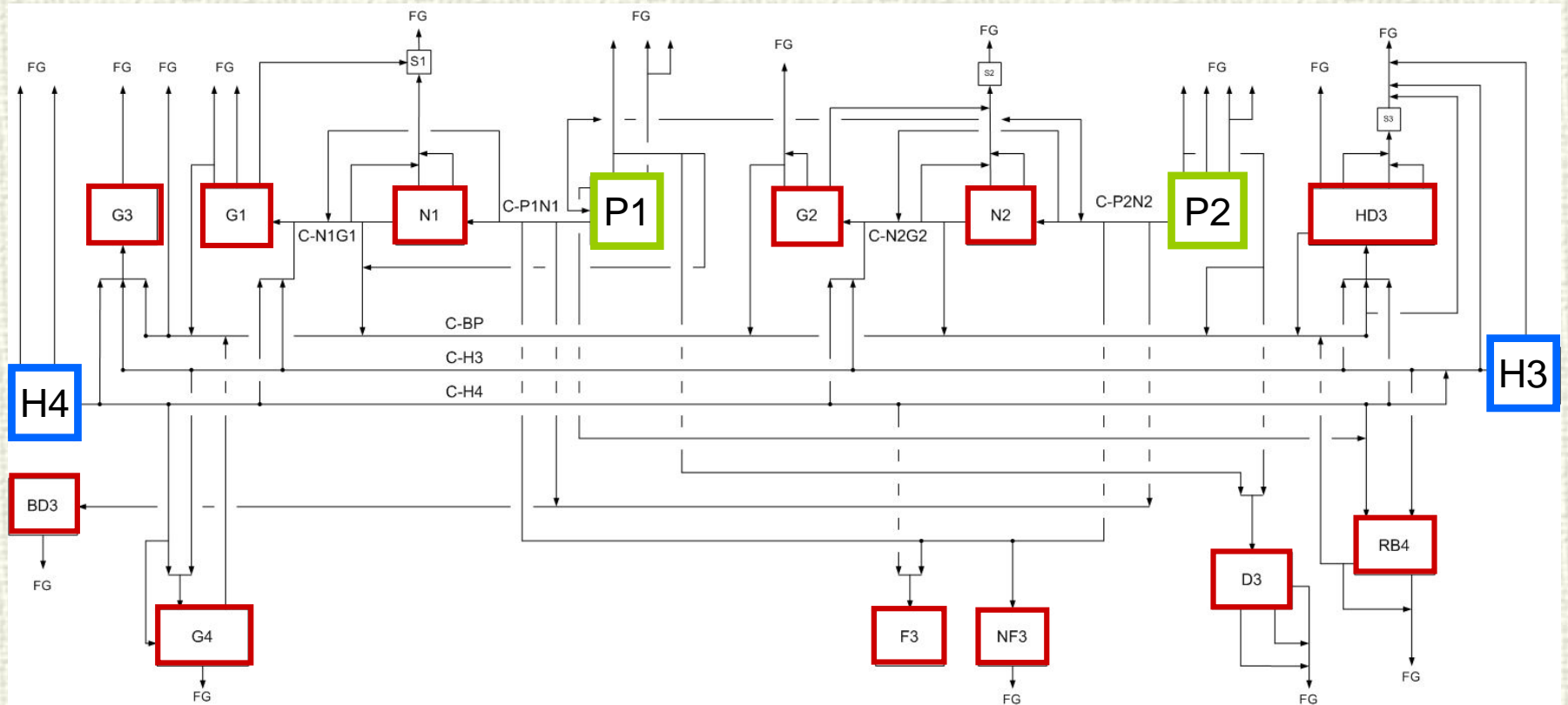
H$_2$ production units (2)

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
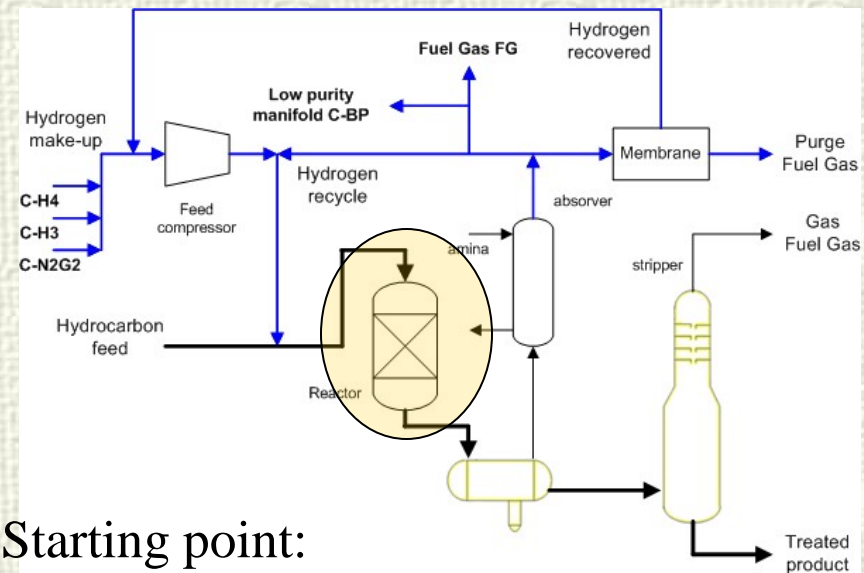
Starting point: reconciled values

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.)
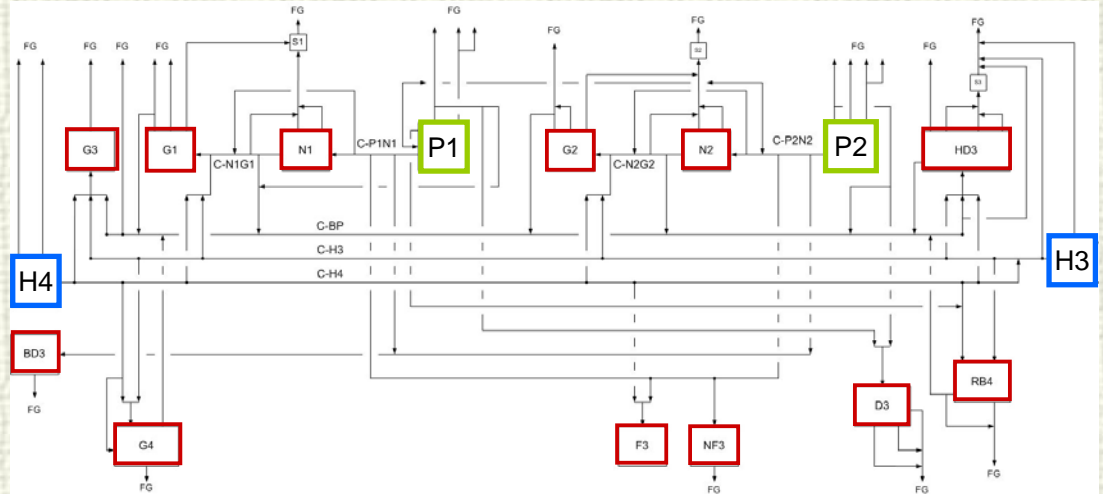
Two new variables are added by consumer plant:

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

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

F_{H2}

αHC

HDS
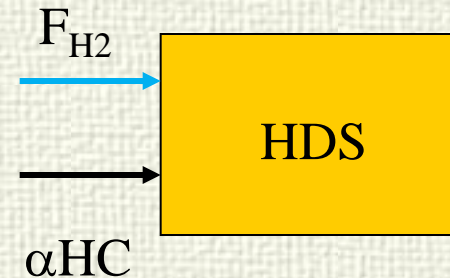
Some plants must reduce their hydrocarbon load or be stopped

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

Two solutions

Process Simulation
(EcosimPro)

J, g

Sequential NLP (SQP-NAG)

Data acquisition and filtering
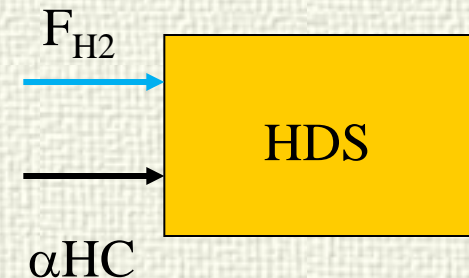
Process (PI)

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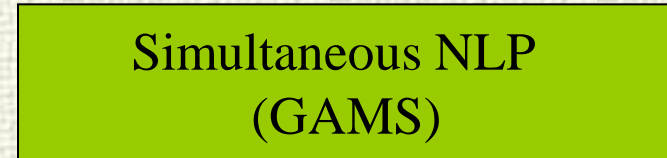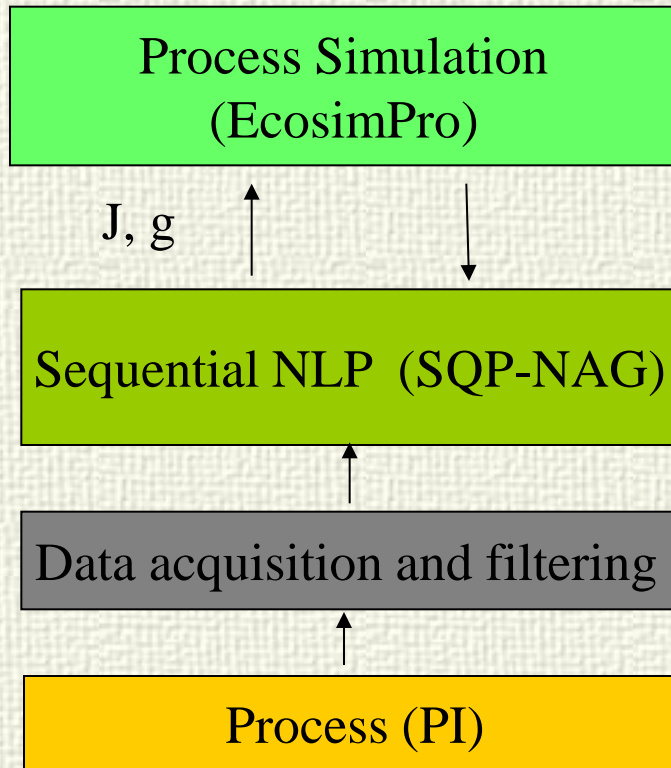
922 variables from 220 streams, 14 reactors, membranes, separators,.. Slack variables included to obtain feasible solutions totalling 1667 variables in 1631 equality and inequality equations

166 process measurements

Modelling tools

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

DSS

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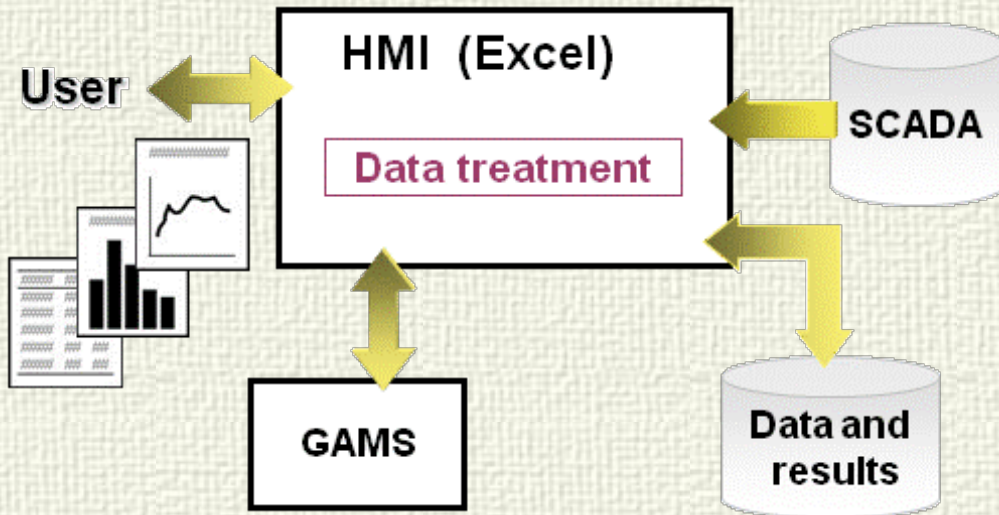
To deal with big changes, the network is formulated as a superstructure that allows to remove groups of equations depending on the value of binary variables that represent the state of the plants.

Decision Support System

DSS

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	Nm3h 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

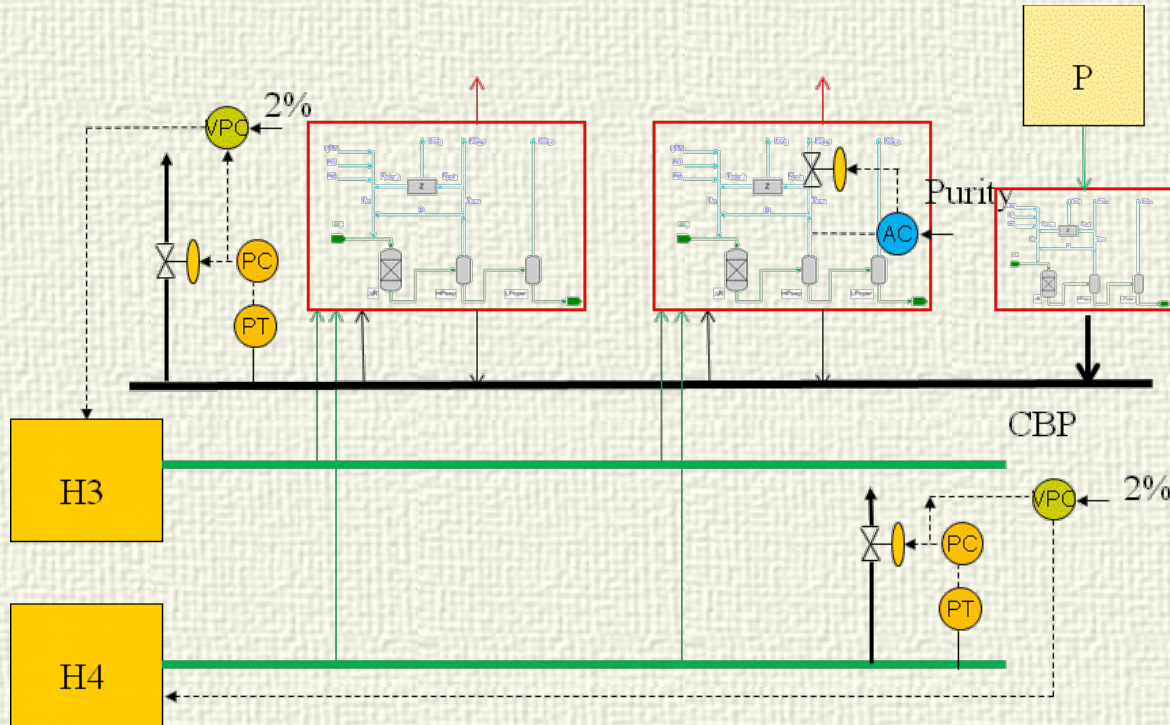✓ Basic control helps matching model hypothesis and the actual process: steady state / mismatch
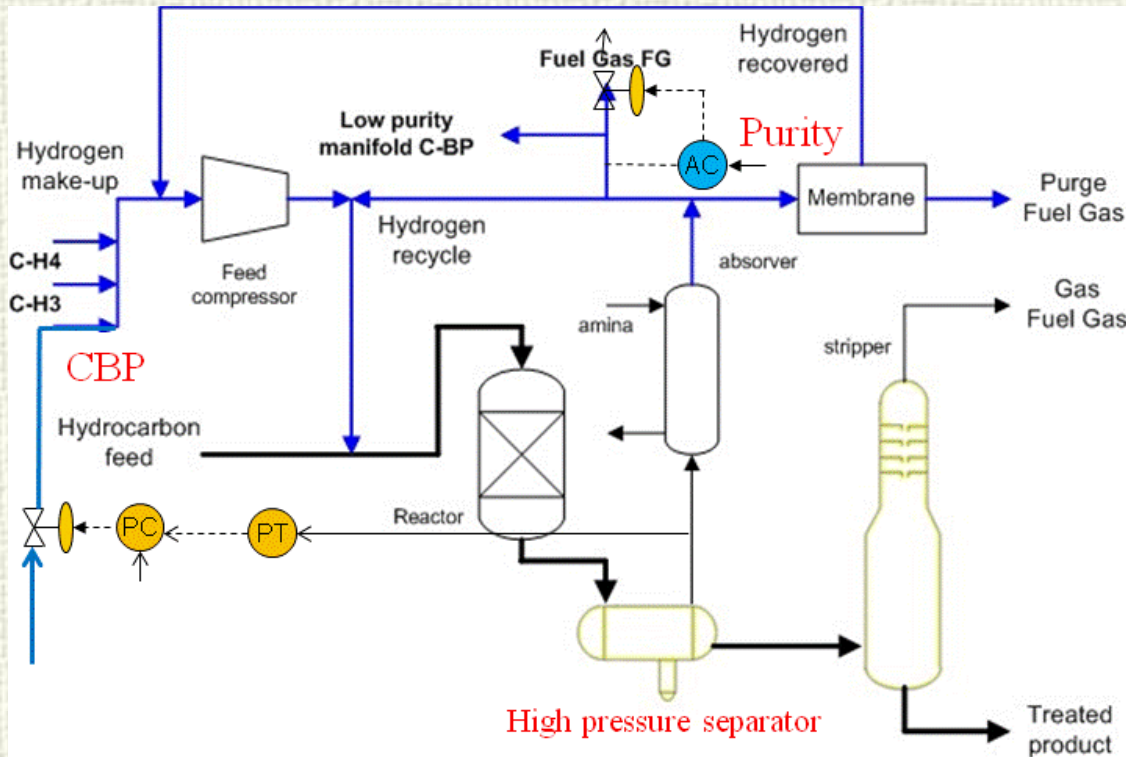
Maintaining steady state balances with pressure control loops

Unbalances are moved to the CBP collector

H_2 purity control loops maintain the impurities balance

Implementation

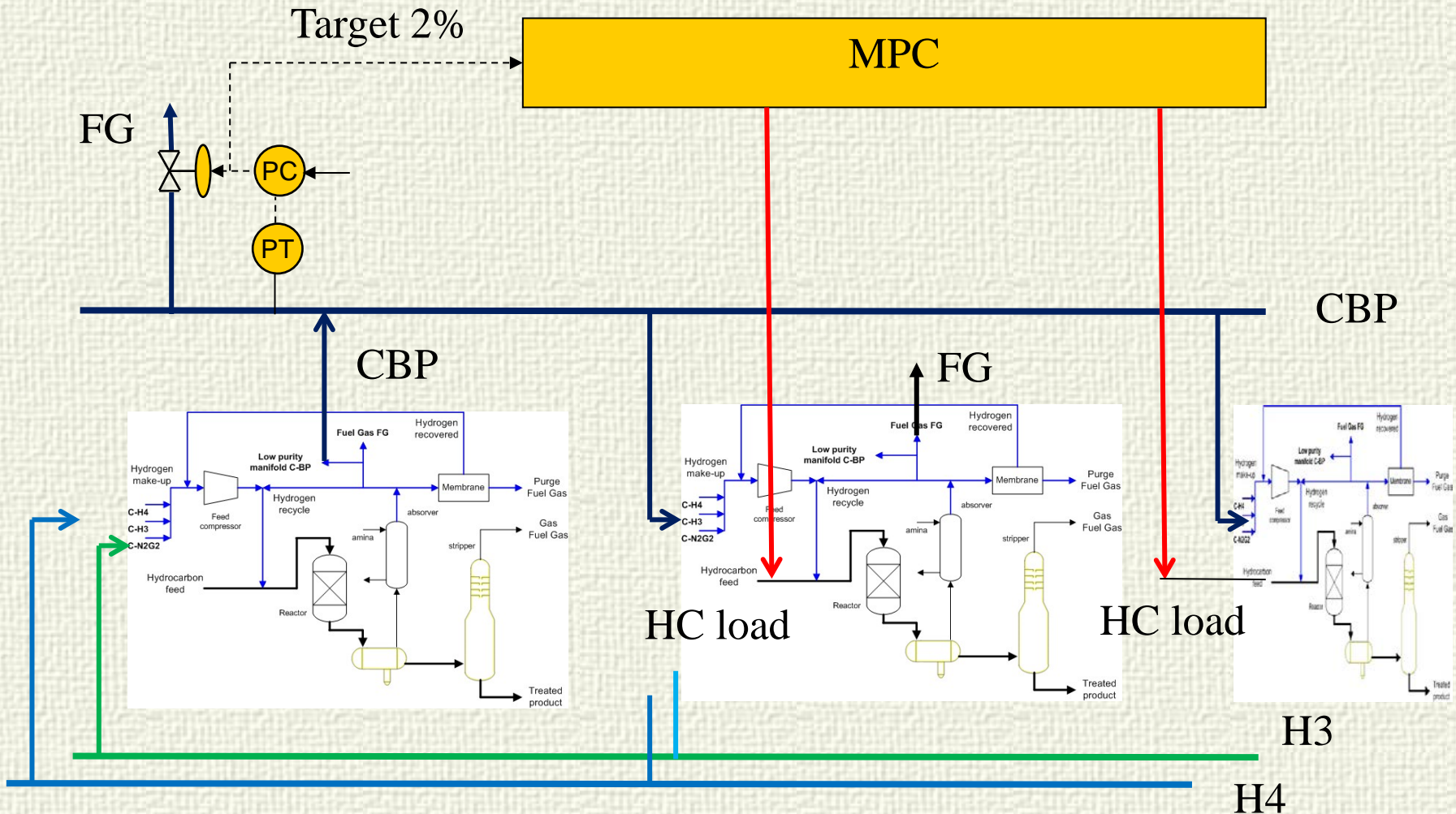Collectors pressure control maintain global balances

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