



**Universidad  
de Valladolid**



Integrated plant-wide control and  
optimization for industry4.0

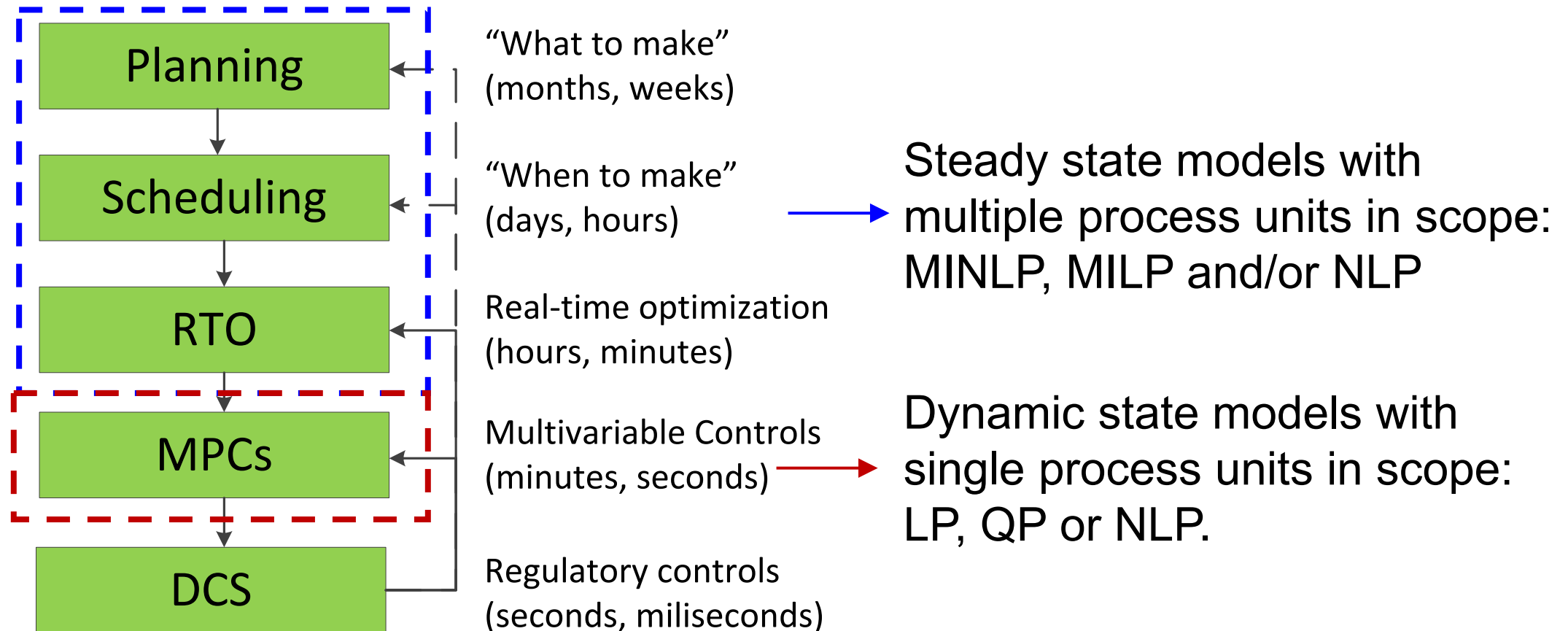


# Simulación Predictiva de la red de H<sub>2</sub> de una Refinería de Petróleo

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**Workshop final  
20-21 junio, 2022**

## DECISION-MAKING PROCESS IN MANUFACTURING OPERATIONS

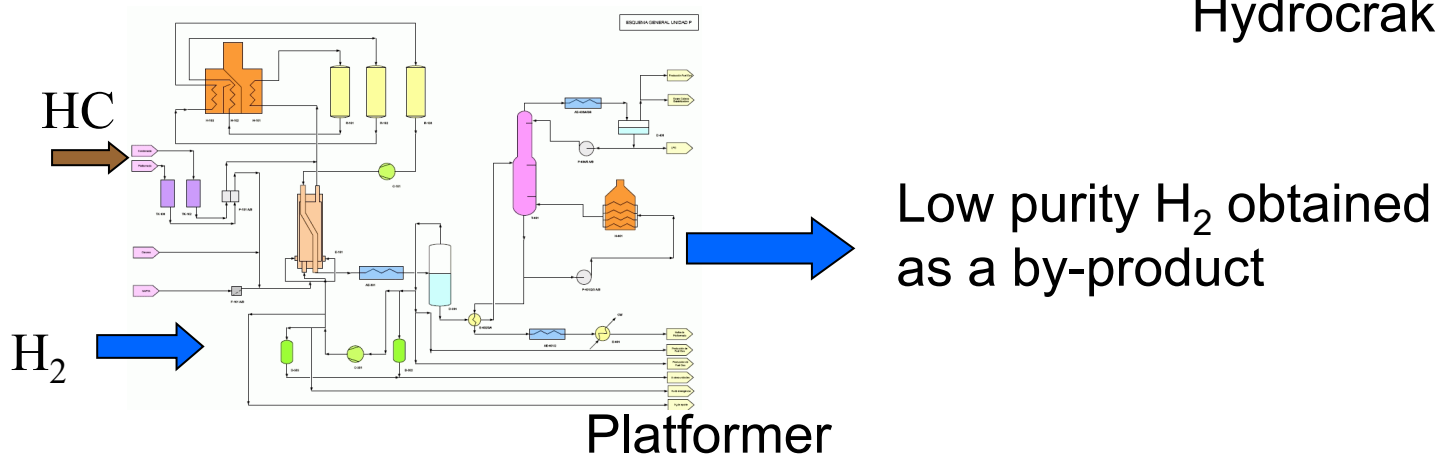
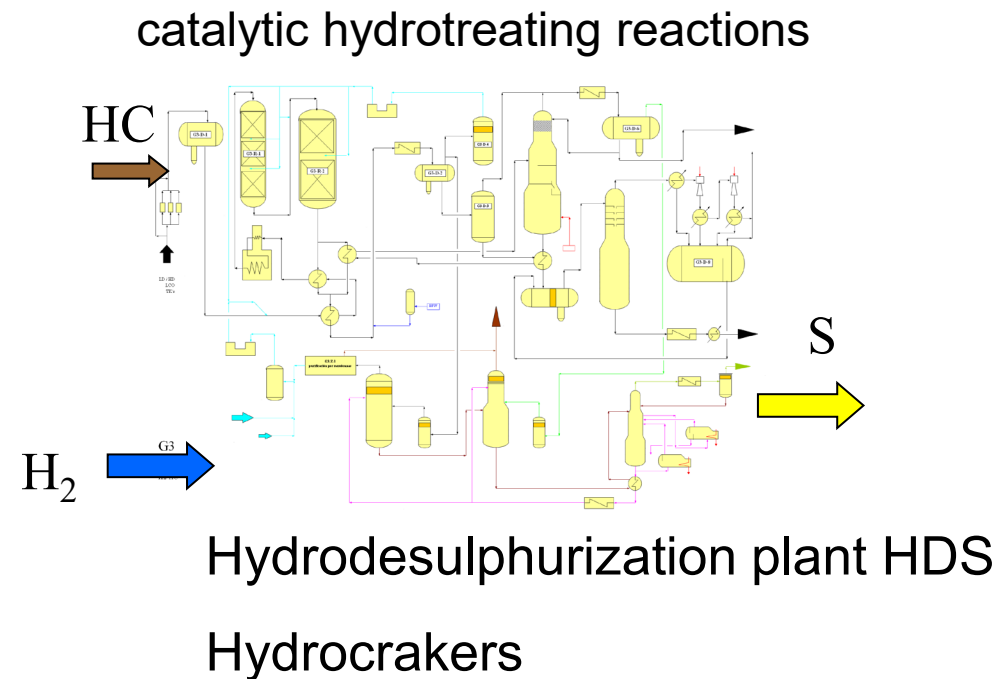
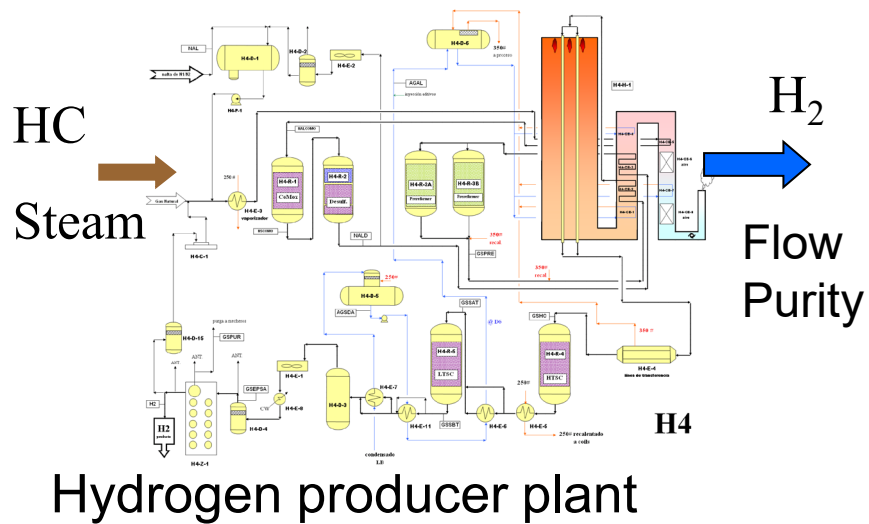




Hydrogen is used in modern refineries in processes that have two main purposes:

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

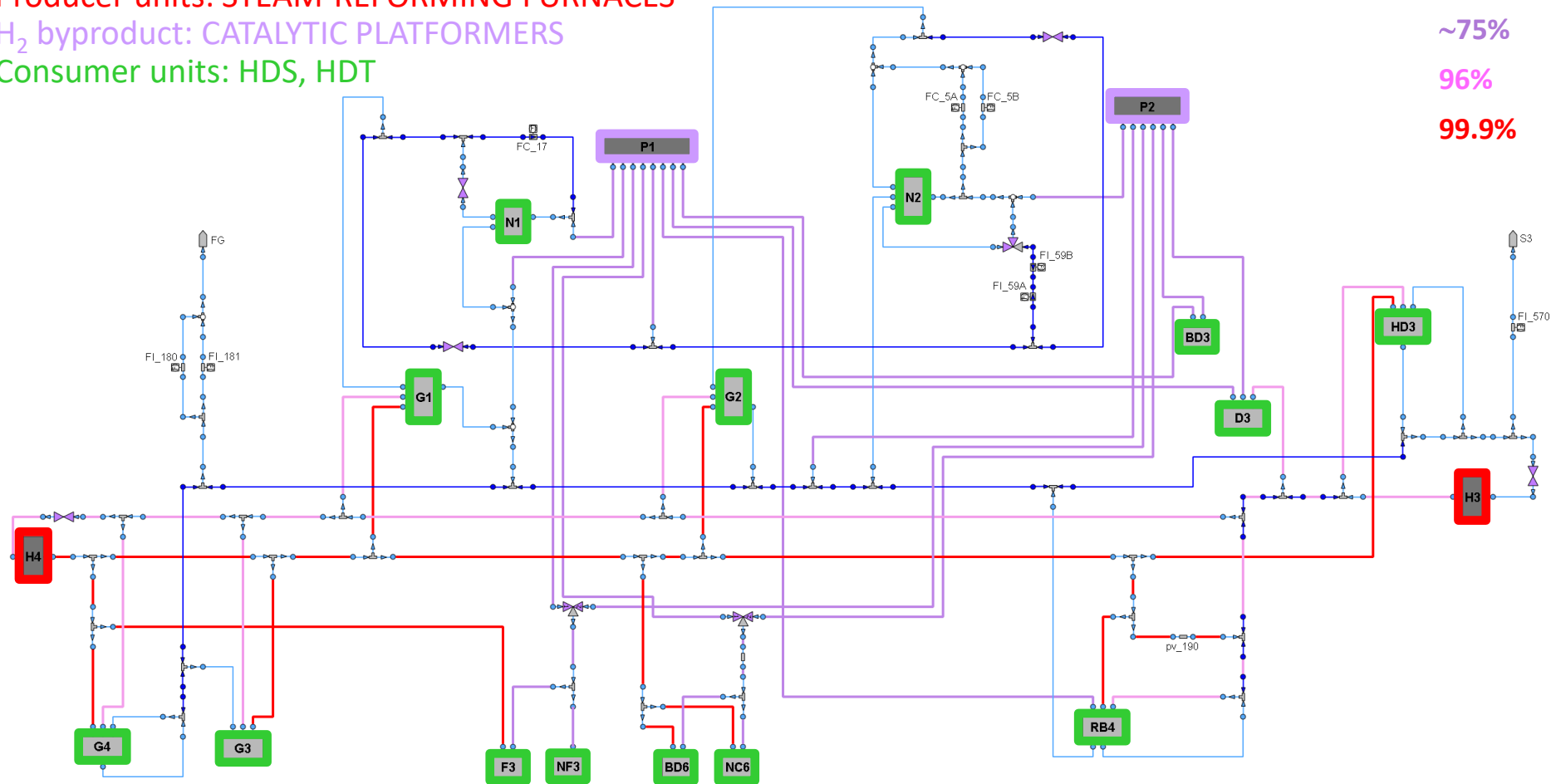
# Hydrogen plants (producers/consumers)



Producer units: STEAM-REFORMING FURNACES

H<sub>2</sub> byproduct: CATALYTIC PLATFORMERS

Consumer units: HDS, HDT



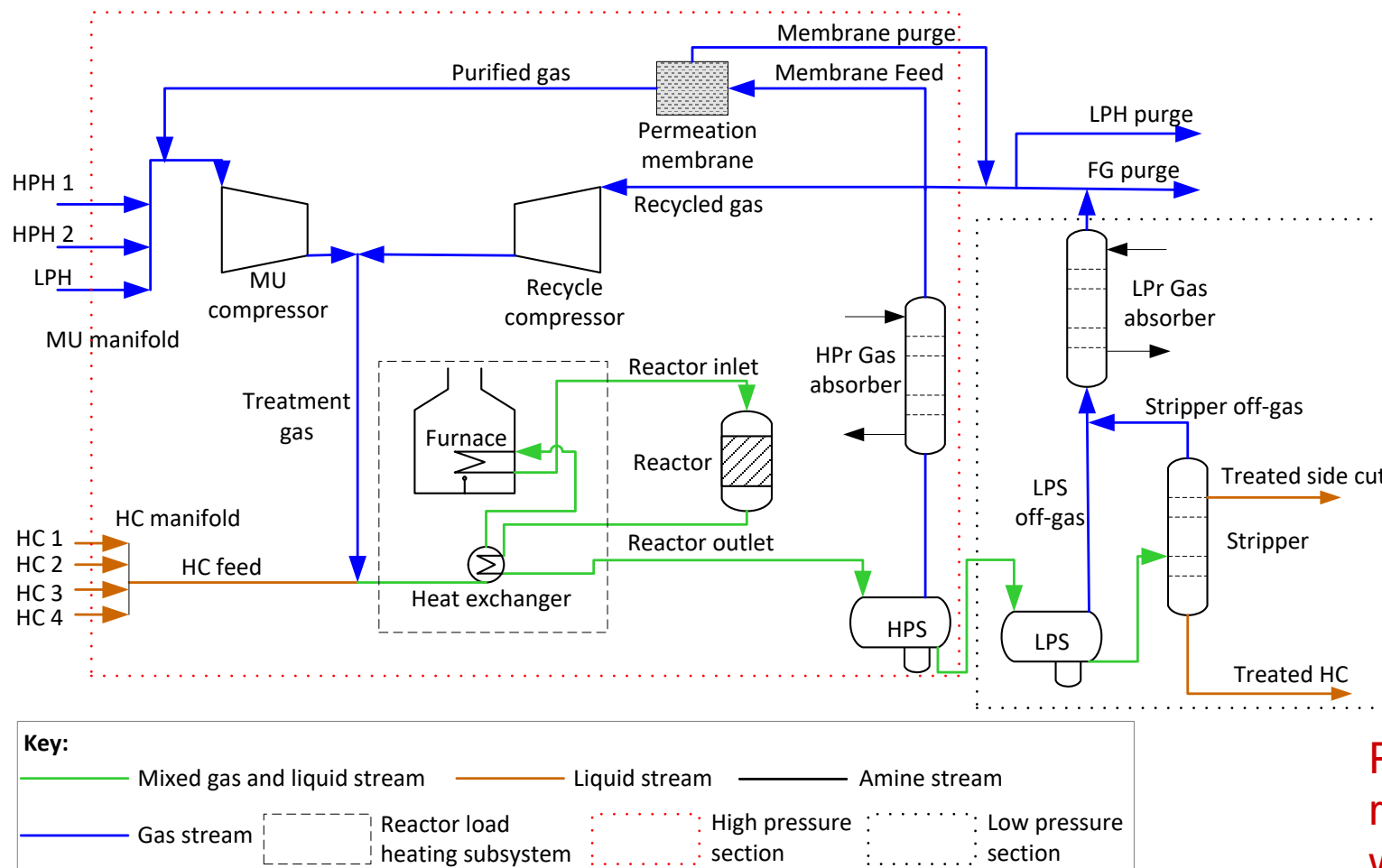
~75%

96%

99.9%

# Hydrodesulfurization Process Units (HDS)

## Simplified schematic

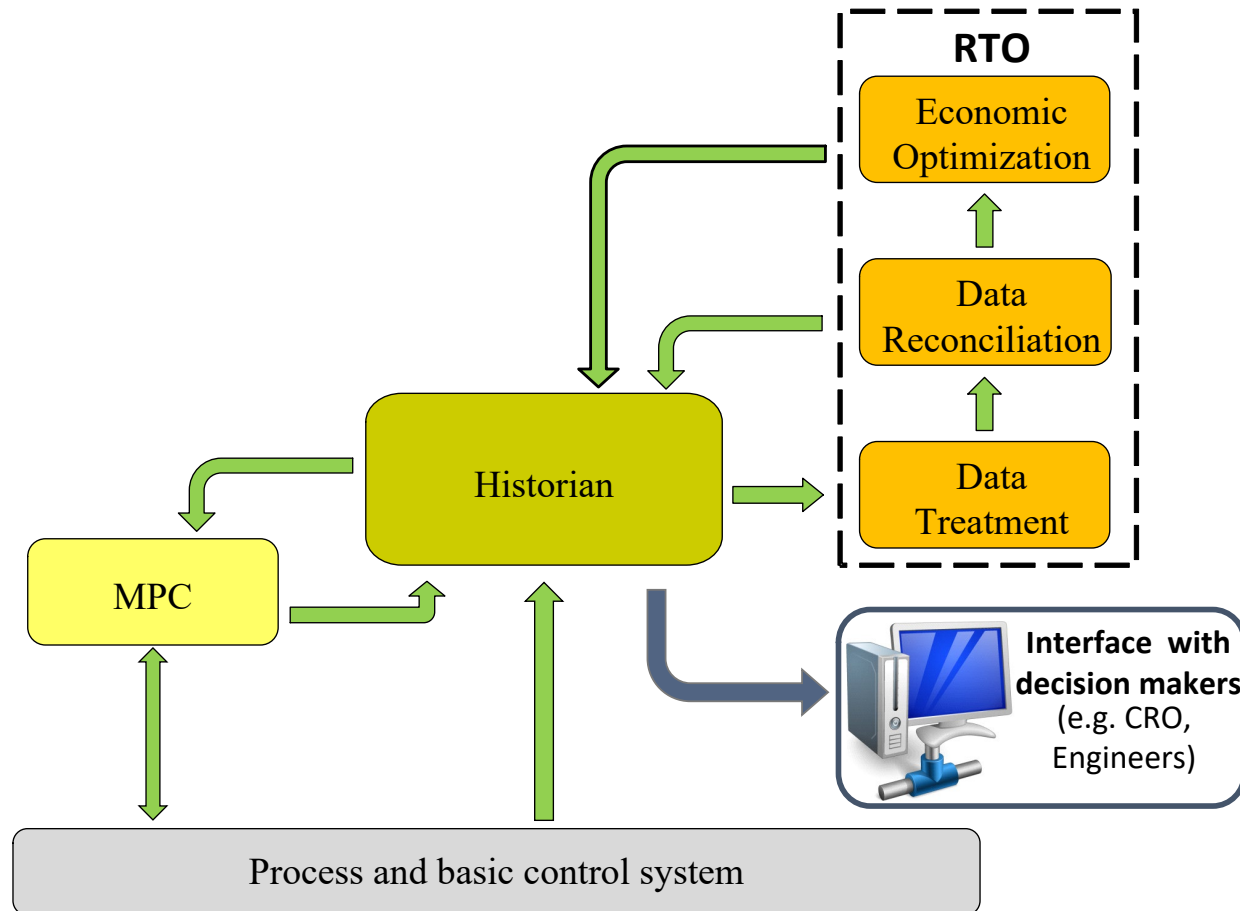


Variable hydrogen demand according to the type and flow of the hydrocarbon being treated

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

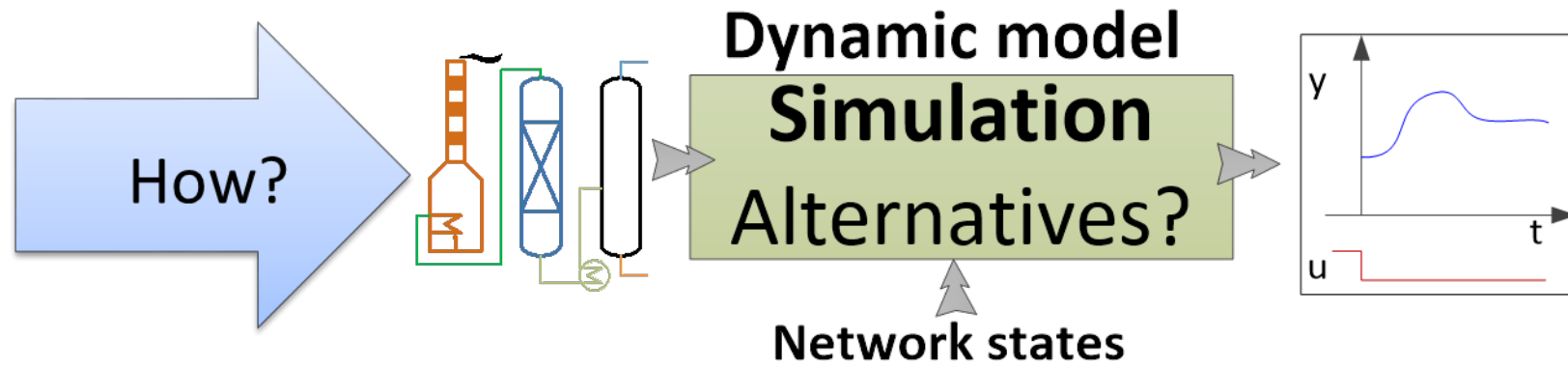
Preserving catalyst life requires to operate always with excess hydrogen in the reactors

# Current Hydrogen Network Control Architecture

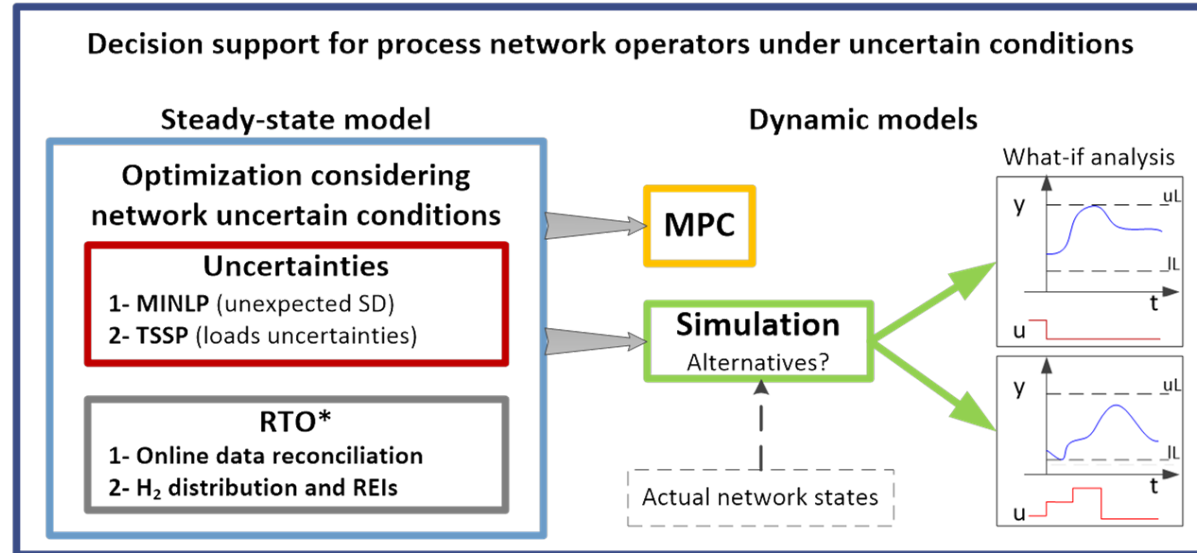


- RTO implementation led to improvements in H<sub>2</sub> network management strategies (e.g. purification units use)
- Better understanding of impacts of changes across the network

RTO: Real-time optimization.  
MHE: Moving horizon estimation.  
MPC: Model predictive control.  
CRO: Control room operators.







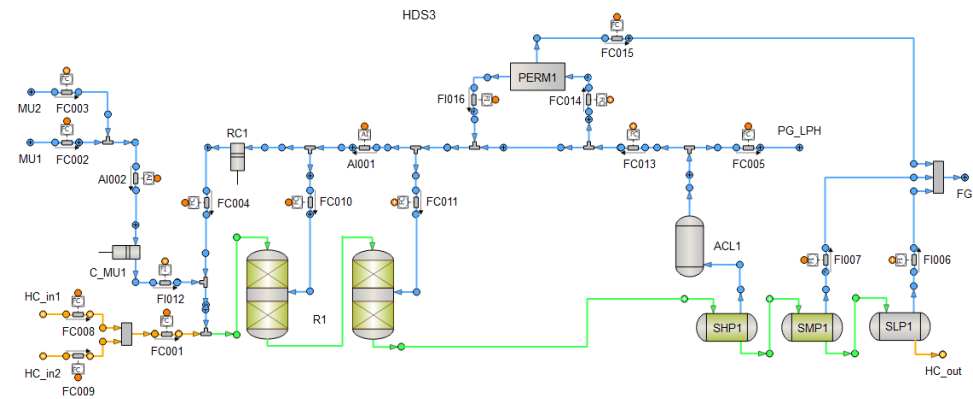
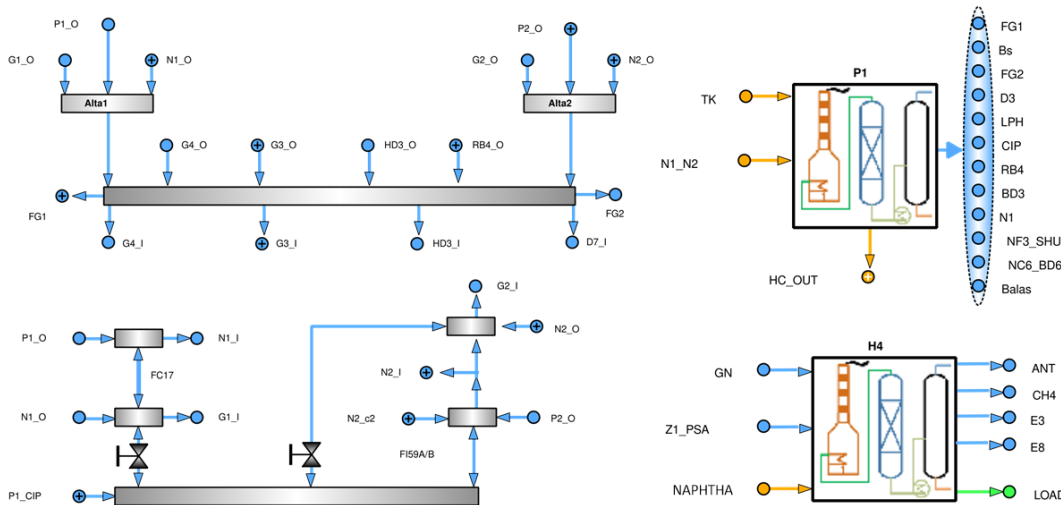
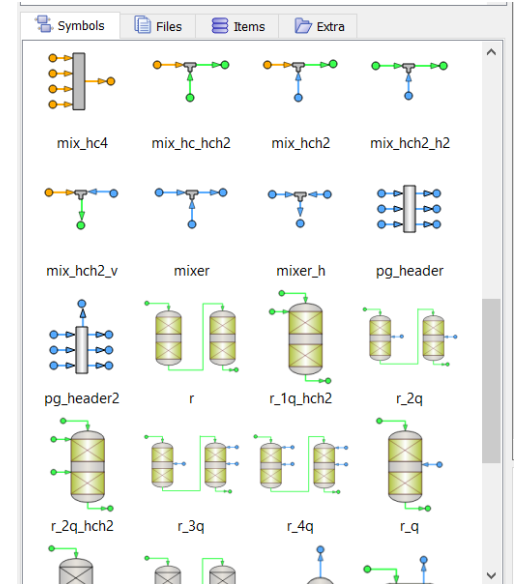
- Develop tools that fit together smoothly
- Enable decision-making at process unit and plant level
- Account for uncertainties
- Expand operator's visibility w.r.t. process change of conditions

## Objective

Develop a comprehensive first-principles based library, capable of:

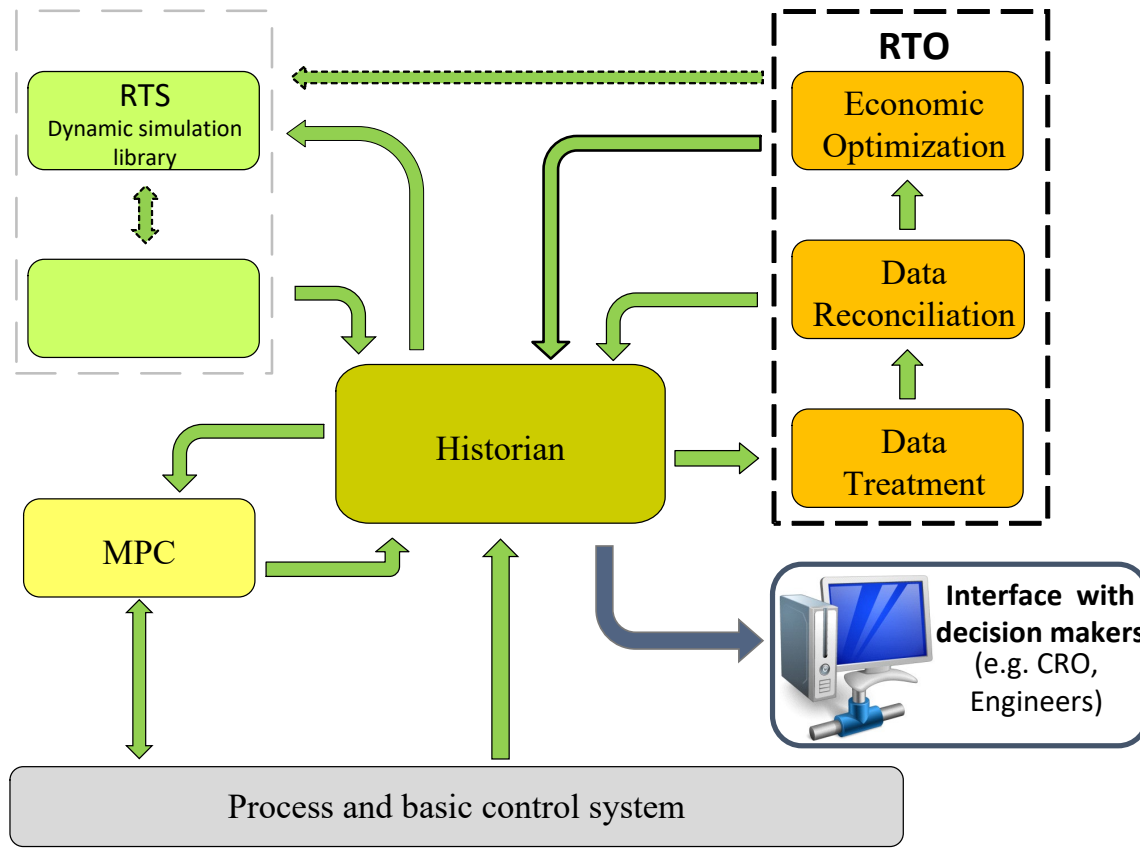
- representing an actual process network,
- its dynamics for a hydrogen network case study, and
- run with real-time data inputs and offline data.

Proosis / EcoSimPro®<sup>1</sup>



## Implementation in real-time environment

- Use in a decision support framework structure



RTS: Real-time simulation.  
RTO: Real-time optimization.  
MHE: Moving horizon estimation.  
MPC: Model predictive control.  
CRO: Control room operators.

## MHE formulation

Given:

- $H_2$  network dynamic nonlinear model (1,2)
- Plant measurements (e.g.: HC loads, gas purity / flowrates; 3)
- Previous manipulated variables values (3)
- Presence of disturbances ( $w$ , 1, 4)

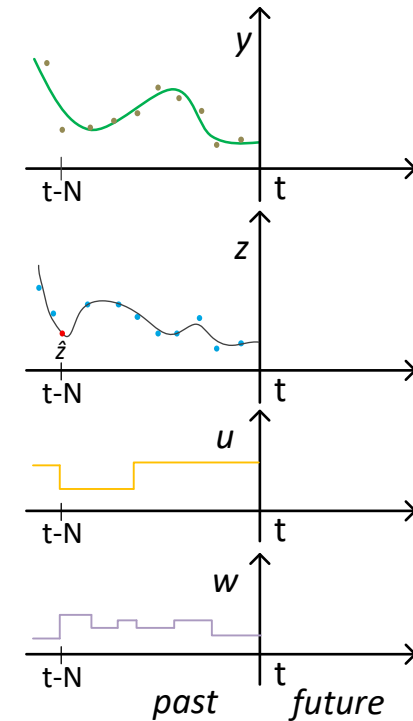
$$f(z(t), \dot{z}(t), u(t), p, w(t)) = 0, \quad z(0) = z_0, \quad (1)$$

$$y_m(t) = h(z(t), u(t), p), \quad (2)$$

$$I^{(N)}_k \triangleq \text{col}(y_{k-N}, \dots, y_k, u_{k-N}, \dots, u_{k-1}), \quad (3)$$

$$\Delta w_k = w(k) - w(k-1), \quad (4)$$

$$k = 1, 2, \dots, N$$



## MHE formulation

Solve:

$$\min_{(\hat{z}_{t-N}, w_{k-N}, \dots, w_k, \hat{p})} \left\{ \|\hat{z}_{t-N|t} - \bar{z}_{t-N}\|_P^2 + \sum_{i=k-N}^k \|\Delta w_{k-i}\|_Q^2 + \sum_{i=k-N}^k \|y_i - y_m(i)\|_R^2 \right\} \quad (5)$$

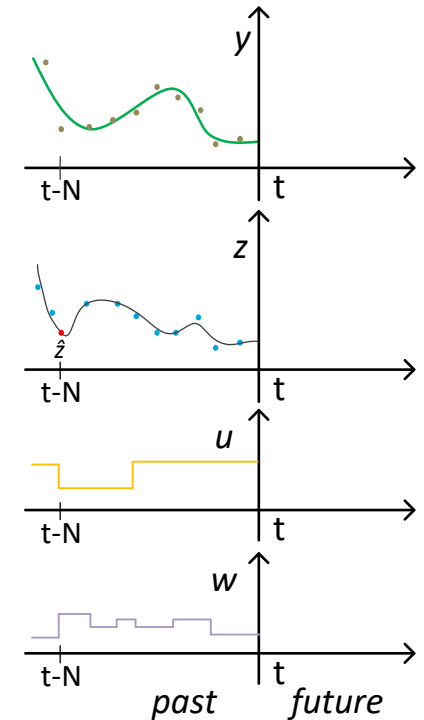
$$\begin{aligned} \text{s.t.} \quad & z_{lb} \leq \hat{z}_k \leq z_{ub} \\ & y_{lb} \leq y_m \leq y_{ub} \\ & w_{lb} \leq w_k \leq w_{ub} \end{aligned}$$

Then the DAEs for initial time  $t-N$  to current time  $t$  to find current state  $z_t$  is solved

Using:  $\hat{p}, \hat{w}_k$

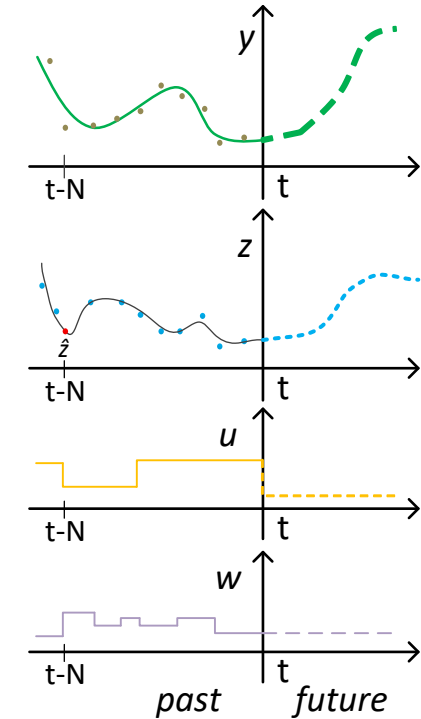
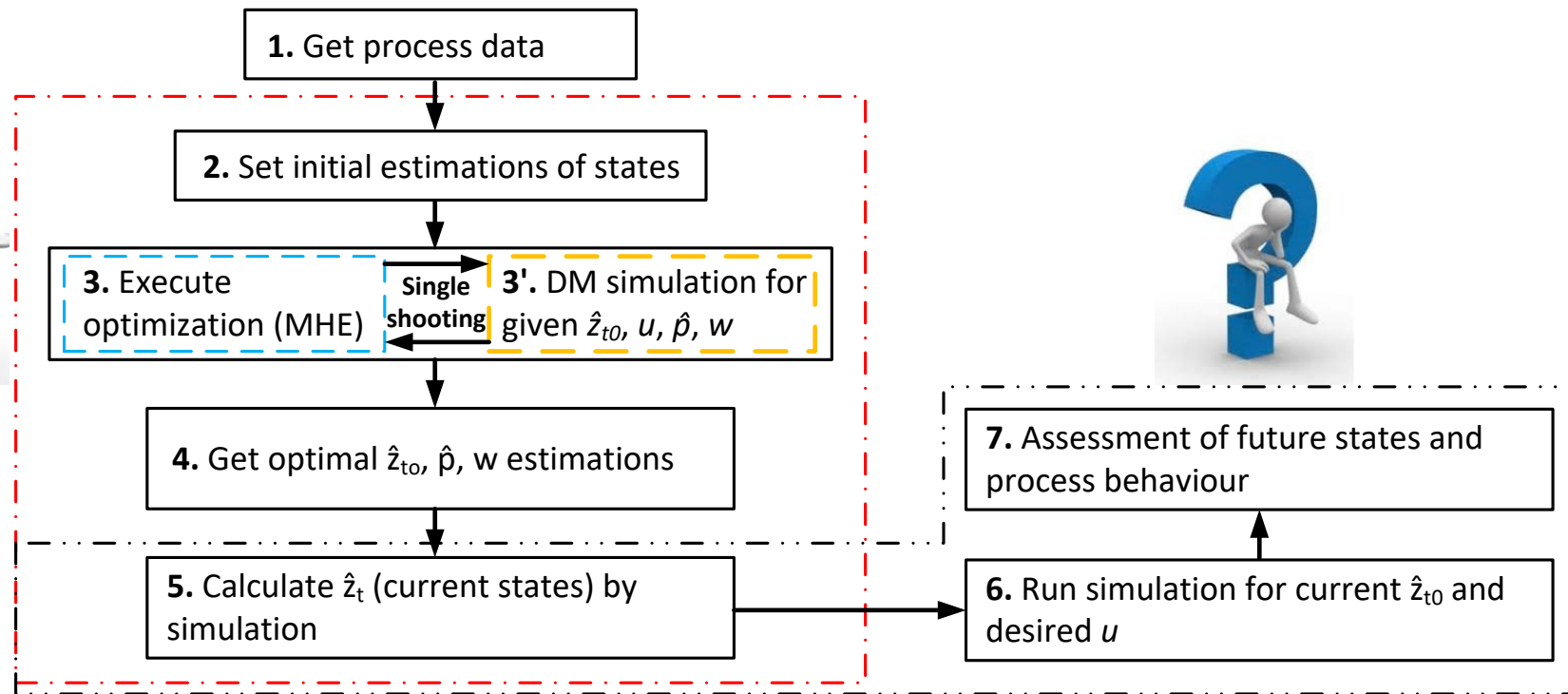
$$f(z, \dot{z}, u, p, w, t) = 0$$

$$z(t - N) = \hat{z}_{t-N}$$



## MHE and simulation integration

Roadmap implemented on Proosis / EcoSimPro®<sup>1</sup>

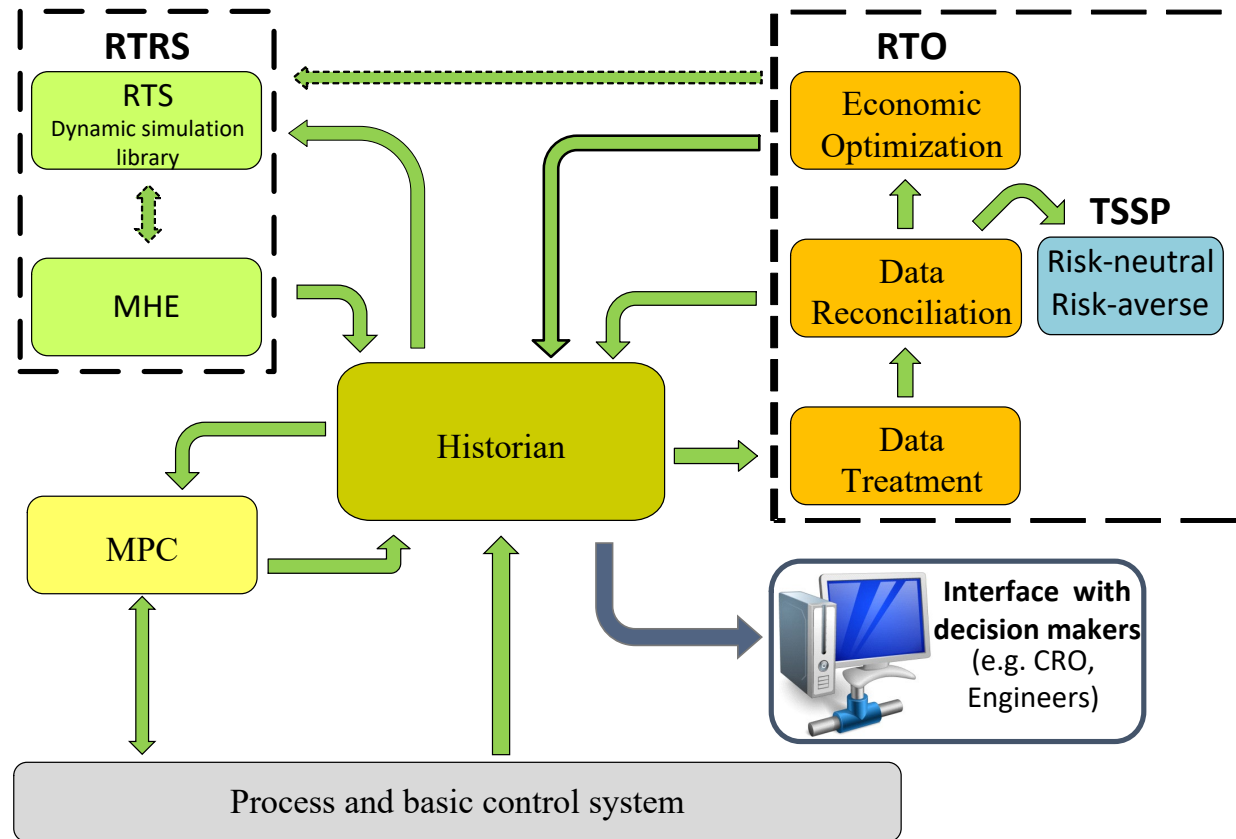


Key: State & Parameter estimation  
Process simulation



Implementation in real-time environment

Use in a decision support framework structure



TSSP: Two-stage stochastic programming.

RTRS: Real-time reconciled simulation.

RTS: Real-time simulation.

RTO: Real-time optimization.

MHE: Moving horizon estimation.

MPC: Model predictive control.

CRO: Control room operators.

## Case study

- H<sub>2</sub> network (simplified)
- 2 producers and 3 consumers
- Analyse RTRS value as decision support tool

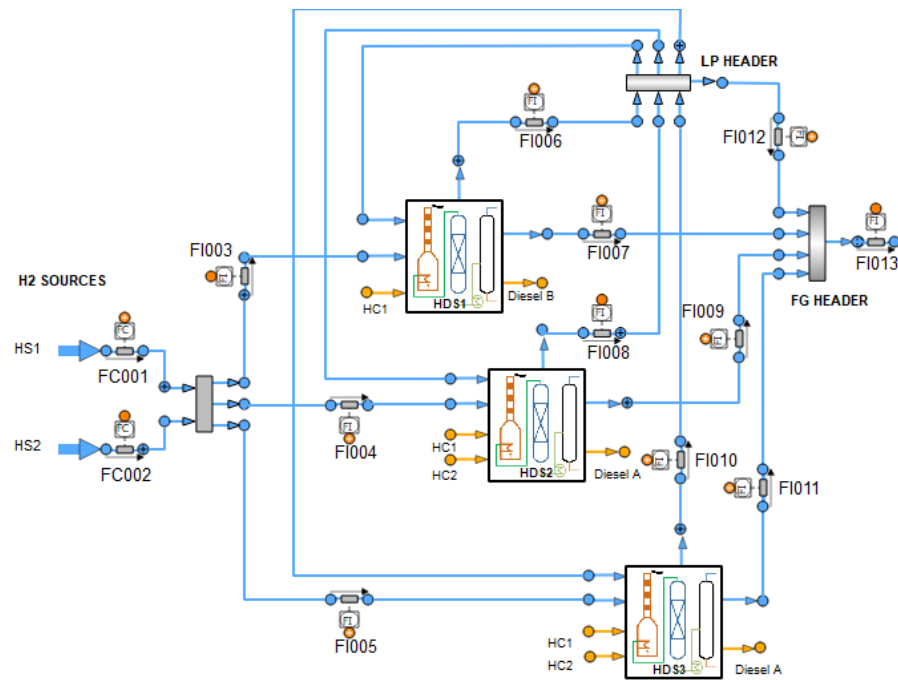


Table 2.1. Summary of characteristics of the

model	INFO	VALUE
	Number of equations	1279
	Number of boxes (coupled subsystems of equations)	5
	Number of input DATA	590
	Number of input BOUNDARIES	13
	Number of output EXPLICIT	1247
	Number of output DYNAMICS or DERIVATIVES	27
	Number of output ALGEBRAICS	5
	Size of Jacobian matrix (DYNAMIC+ALGEBRAIC).	32x32
	Default integration method	DASSL

PC Intel® Core™ i7-6500U CPU @2.50 GHz  
RAM 16 GB, and takes on average 40s per sample time.



## Case study

- 15 Manipulated variables (N = 5)
- Scenario-based analysis (What-if)

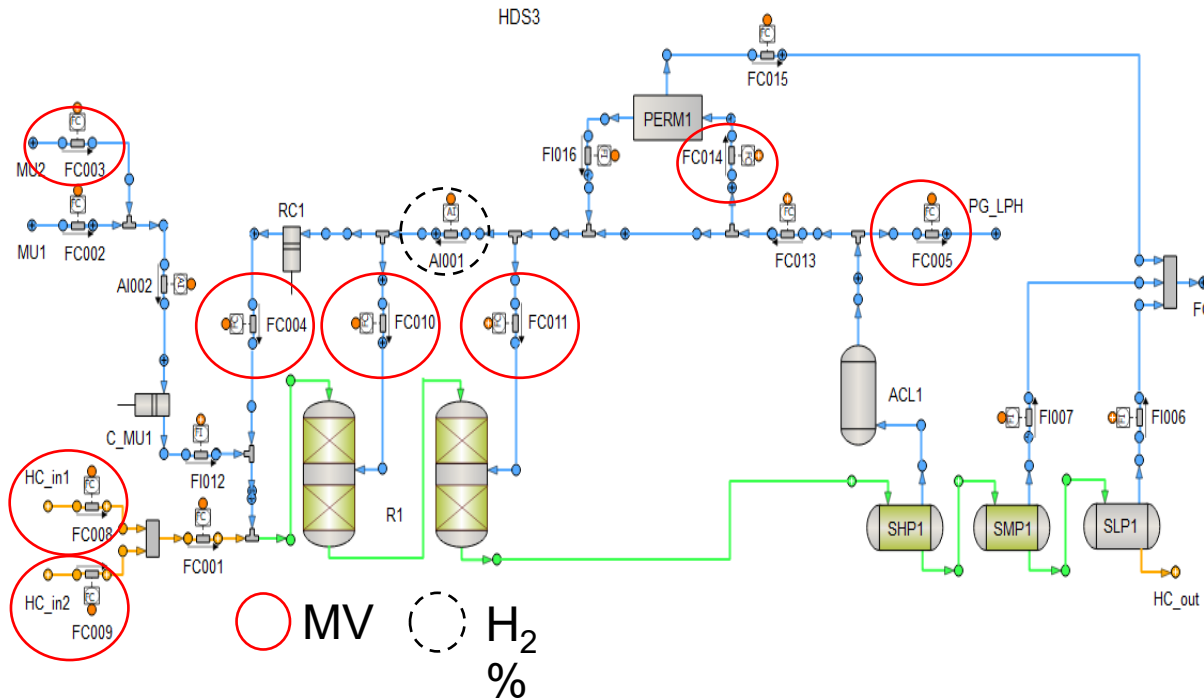
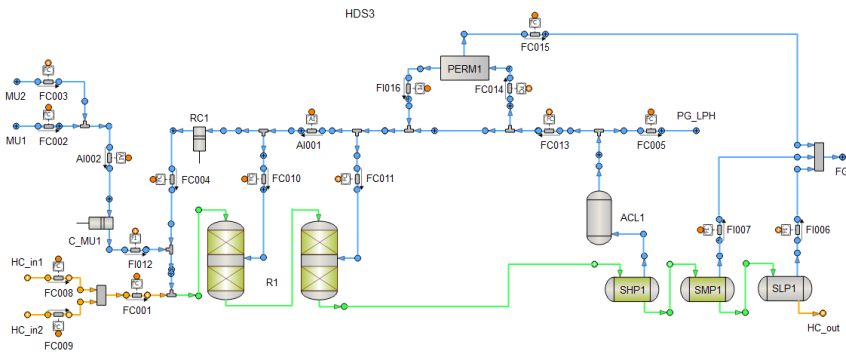
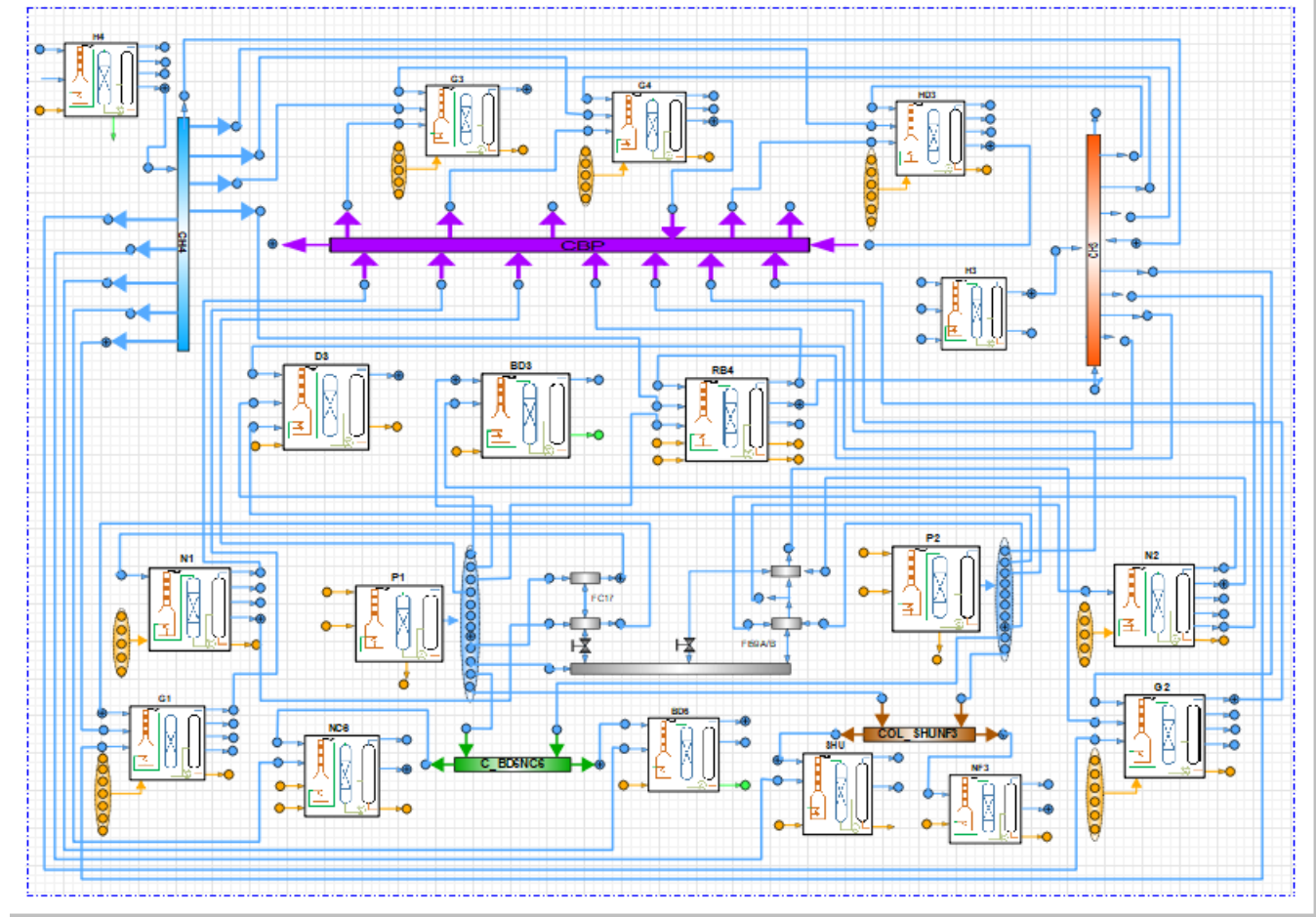
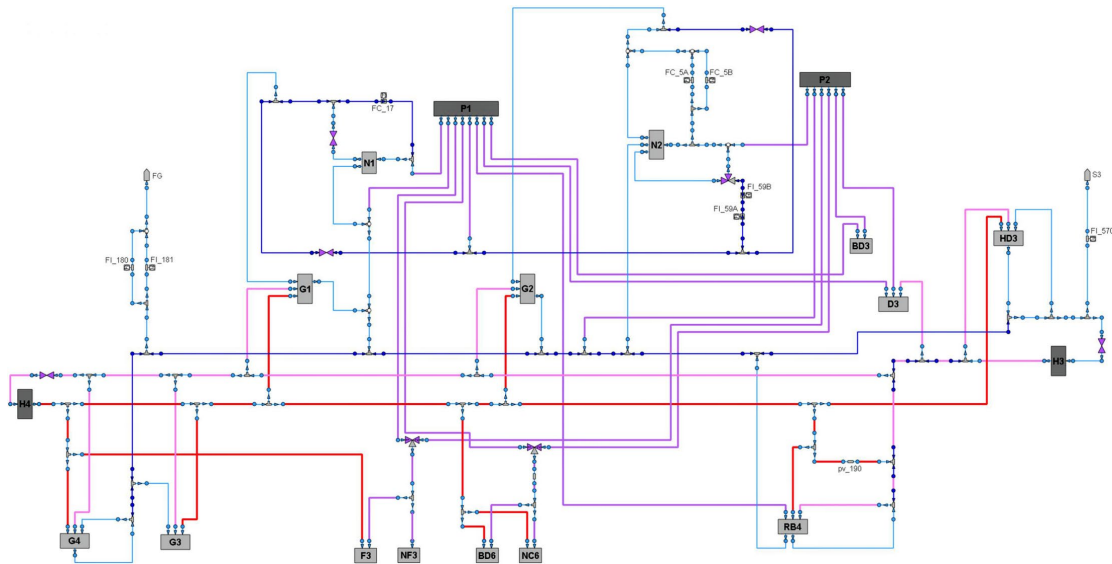
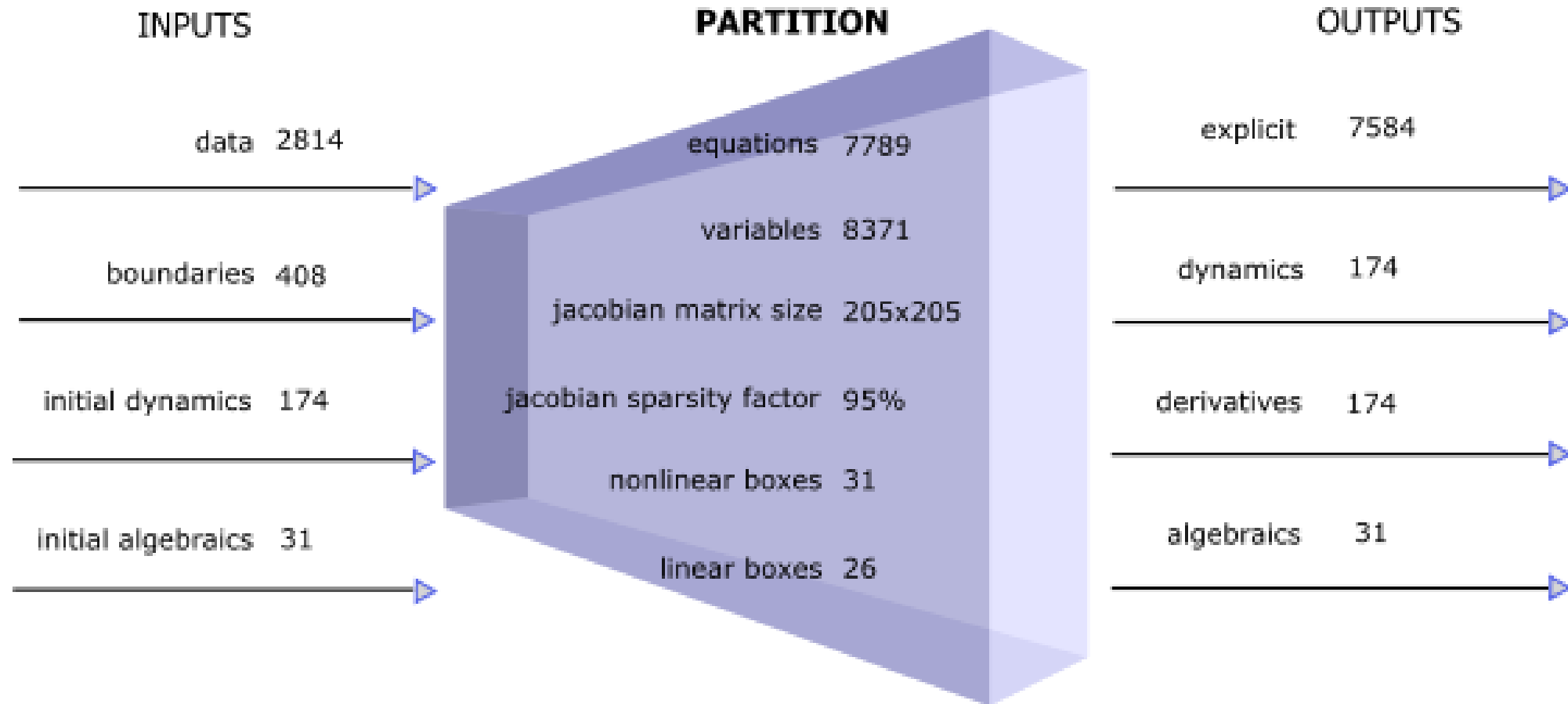
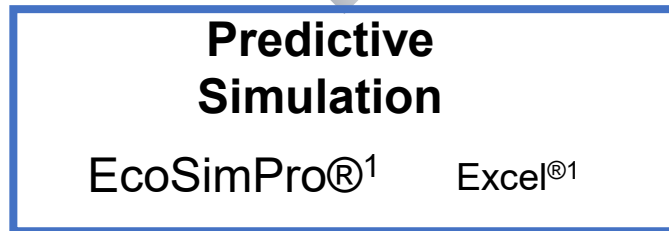
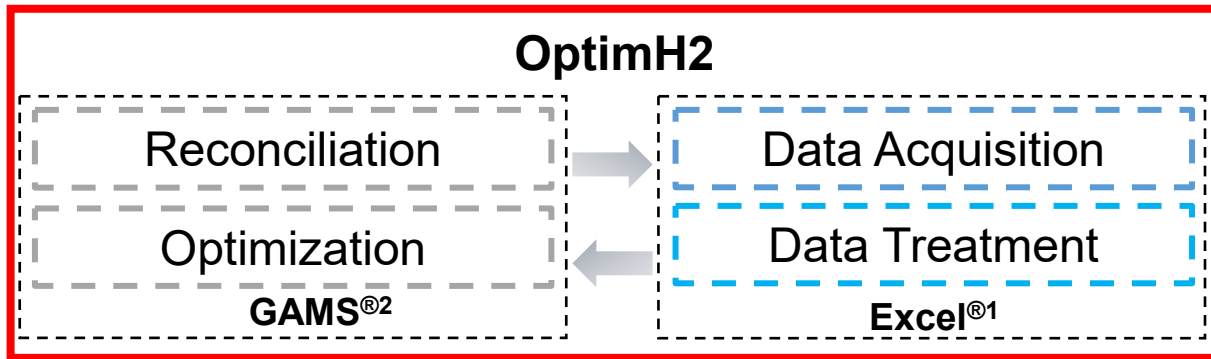


Table 2.2. Summary of manipulated variables of each HDS in the model.

	HDS1	HDS2	HDS3
FC001	MV1		
FC002	MV2		
FC003		MV1	MV1
FC004	MV3	MV2	MV2
FC005	MV4	MV3	MV3
FC008		MV4	MV4
FC009		MV5	MV5
FC014			MV6



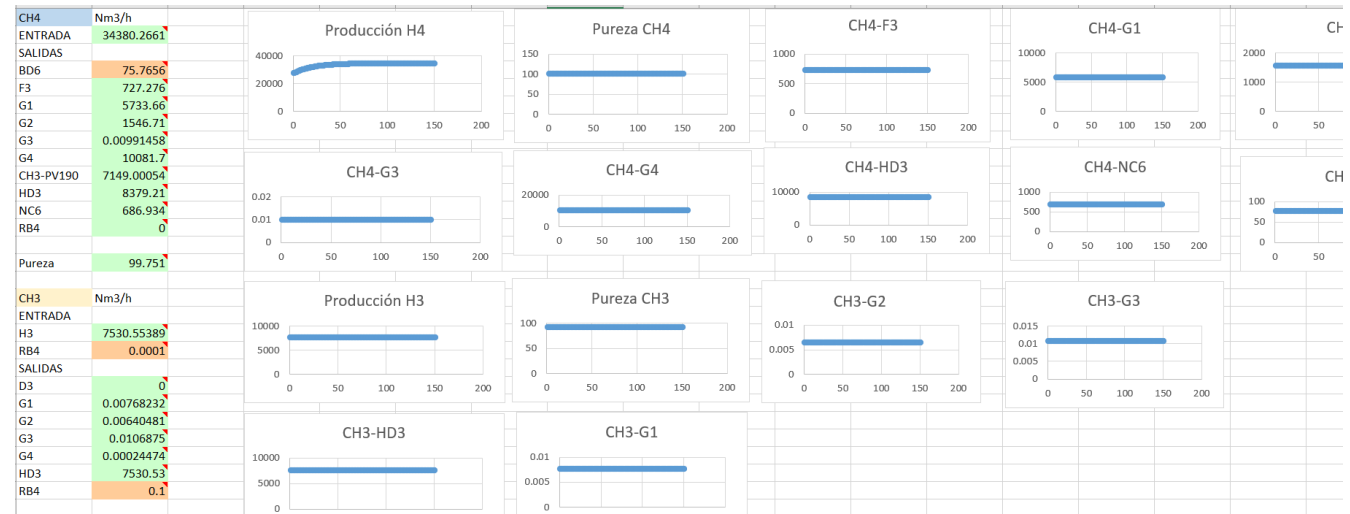




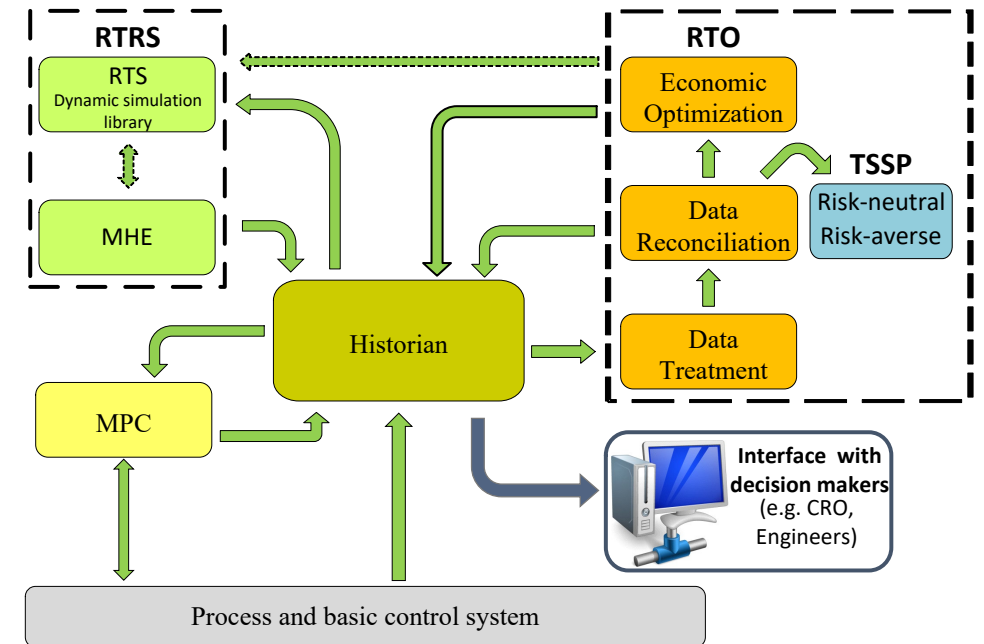
4400 variables  
4700 equations

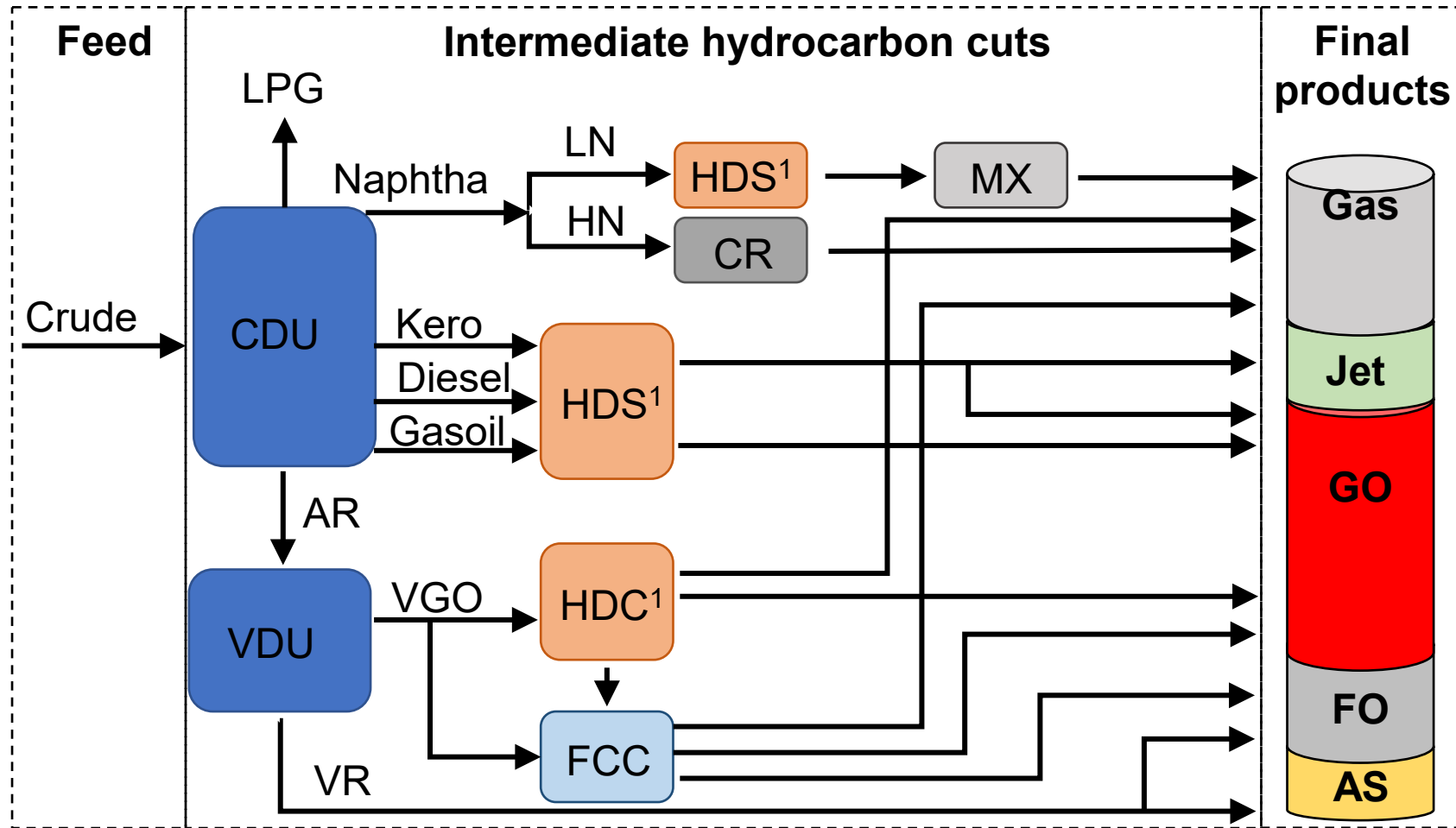
8371 variables  
7789 equations

	A	B	C	D	E	F	G	H
2		Donantes						
3	E03_1_D0_kspasFhc	KspasFhc	15.3817879		P1_1Spl_v_2fn.F_gpl[2] = 0.7832.1772	Me3h de H2 de P1_d1_F	P1_d1_F	87832.82898
4	E03_1_D0g_mn_1fn	bdF_mesta	63.45641071		N1_1_F1005_fm.F_gpl[2] = 0.291.23902	Me3h de H2 de H1C_1101	H1C_1101	4593.25375
5	E03_1_F0004_sgrFC_sgral[1]	bdF_Fa1	96.48072784		N2_1_F1006_fm.F_gpl[2] = 0.489.96942	Me3h de H2 de H2C_N02C2	H2C_N02C2	5187.51648
6	E03_1_F0005_sgrFC_sgral[1]	bdF_Fa2	27.50353842		P2_1_A1122_fm.F_gpl[2] = 73.005	Pureza de P2	P2_F	73.00501192
7	E03_1_F1009_fm.F_gpl[2]	Kgh de gas total + HC del BODFHC_LF78	91.1199556		N2_1_F1010_fm.F_gpl[2] = 68.54318029	Me3h de H2 de n2_d5_d2	n2_d5_d2	72.98229256
8	E03_1_HC_m_Fhc	m3h de carga E03	39.0255445		N2C_1_T11_fm.F_gpl[2] = 15033.12614	Me3h de H2 de H2C_1113	H2C_1113	14602.23638
9	E03_1_HC_m_rh0hc	densidad de carga	500		N2C_1_F0007_fm.F = 132.003359	Me3h de gas total de HODFHC_LFC7	N2C_Fhc_Rc8	150.1525555
10	E03_1_HC_m_rh1hc	PM de carga	140		N2C_1_F0008_fm.F = 339.505288	Me3h de gas total de HODFHC_LFC8	N2C_Fhc_Rc8	365.8419733
11	E03_1_PV015_sgrAV_sgral[1]	bdF_reciclo	0.008466335		B03_1_Dep_mn2_1gm.F = 18.78817887	Me3h de gas total en el HC que entra al dep1	BDF_reciclo	2.303409808
12	E03_1_PV020_sgrAV_sgral[1]	bdF_Fa3	67.87786657		N3_1_T11_fm.F_gpl[2] = 17057.01101	Me3h de H2 de H2C_reciclo	H2C_reciclo	37503.481784
13	E03_1_PV134_sgrAV_sgral[1]	bdF_Fa3	67.87786657		N3_1_F0001_fm.F = 0.054708291	Me3h de gas total en el HC F0001		0.0482811
14	E03_1_PV138_sgrAV_sgral[1]	bdF_Fa3	67.87786657		N3_1_F0003_fm.F = 34.04693008	Me3h de gas total en el HC F0003		45.23146379
15	E03_1_R1_0hc	CE	1.41002013		S04_1_F1004_fm.F_gpl[2] = 57.58916028	Me3h de H2 de F1F_0100_c2	F1F_0100_c2	61.93206372
16	E03_1_R1_0hc	GE	11.62937987		R04_1_0001_fm.F_gpl[2] = -0.016160291	Me3h de H2 de H2C_SF	H2C_SF	-0.01
17					G2_1_mn2_2_fm.F_gpl[2] = 13037.5497	Me3h de H2 de gF2_d3_d2	gF2_d3_d2	12540.80279
18	E06_1_F0001_sgrFC_sgral[1]	bdF_k1	0.000188811		G1_1_lsp_u_6_fm.F_gpl[2] = 52526.41056	Me3h de H2 de gF2_d3_d3	gF2_d3_d3	53998.8874
19	E06_1_F0002_sgrFC_mn_sgral[1]	Kgh de gas total + lgh de HC del F0005	0.086.592395		H03_1_lsp_u_6_fm.F_gpl[2] = 97028.76004	Me3h de H2 de H2C_F1 + H2C_d3_d3 + H2C_d3_d3	H2C_F1	87957.48978
20	E06_1_F0012_sgrFC_sgral[1]	bdF_k12	3.456465.06		G4_1_T13_fm.F_gpl[2] = 84.225	Pureza de gF4_d3_d4	gF4_d3_d4	84.24608845
21	E06_1_F0013_sgrFC_sgral[1]	bdF_k13	3.456465.06		G4_1_F1015_fm.F_gpl[2] = 213.2236843	Me3h de H2 de gF4_d3_d4	gF4_d3_d4	210.0726331
22	E06_1_F0015_sgrFC_sgral[1]	bdF_k15	23.83970007		D0_1_F1016_fm.F_gpl[2] = -0.00949308993	Me3h de H2 de F_03	F_03	-0.009493
23	E06_1_F0111_sgrFC_sgral[1]	bdF_k11	51.85272811		D0_1_F0003_fm.F = 7.70626299-65	Me3h de gas total del F0003		0.0000001
24	E06_1_H4_F	c_b4b6	75.76558487		D0_1_R1_R1_Fhc = 0.0025	m3h de HC de quench		0.0025
25	E06_1_HC_m_Fhc	m3h de carga	6.44093889		B03_1_PV015_fm.F_gpl[2] = 0.00162256	Me3h de H2 de bdf_reciclo	bdF_reciclo	0.001716342
26	E06_1_HC_m_rh0hc	densidad de carga	500		B03_1_FT008_fm.F = 1.530349519	Me3h de gas total de FT008		2.35711542
27	E06_1_HC_m_rh1hc	PM de carga	140		R04_1_F0018_fm.F = 1.07819384-46	Me3h de gas total de F0018		0.0000001
28	E06_1_PV014_sgrAV_sgral[1]	bdF_k10	4.63374E-06		N1_1_F1012_fm.F_gpl[2] = 254.9456317	Me3h de H2 de n1_n5_s1	n1_n5_s1	228.1298196
29	E06_1_PV019_outAV_sgral[1]	bdF_pn0	7.96691E-07		G3_1_lsp_u_6_fm.F_gpl[2] = 34391.32219	Me3h de H2 de gF2_d3_d4	gF2_d3_d4	34589.47879
30	E06_1_PV018_sgrAV_sgral[1]	bdF_pn0	7.96691E-07		G3_1_F1017_fm.F_gpl[2] = 274.3205013	Me3h de H2 de gF2_d3_d4	gF2_d3_d4	273.8090864
31	E06_1_PV024_sgrAV_sgral[1]	bdF_pn0A	51.80454338		G2_1_F1024_fm.F_gpl[2] = 645.2595978	Me3h de H2 de gF2_d7_d9	gF2_d7_d9	632.4665837
32	E06_1_PV028_outAV_sgral[1]	bdF_pn0B	0.121565729		H03_1_F1018_fm.F_gpl[2] = 251.8671194	Me3h de H2 de H2C_d5_d5	H2C_d5_d5	286.963231
33	E06_1_PV028_sgrAV_sgral[1]	bdF_pn0B	0.121565729		G1_1_F1047_fm.F_gpl[2] = 437.4326872	Me3h de H2 de gF2_d7_s1	gF2_d7_s1	463.2489938
34	E06_1_PV020_outAV_sgral[1]	bdF_hc7	51.85272137					
35	E06_1_PV022_sgrAV_sgral[1]	bdF_hc7	51.85272137					
36	E06_1_R1_R2_0hc	CE	2.310609163					
37	E06_1_R1_R2_0hc	GE	1.629584837					

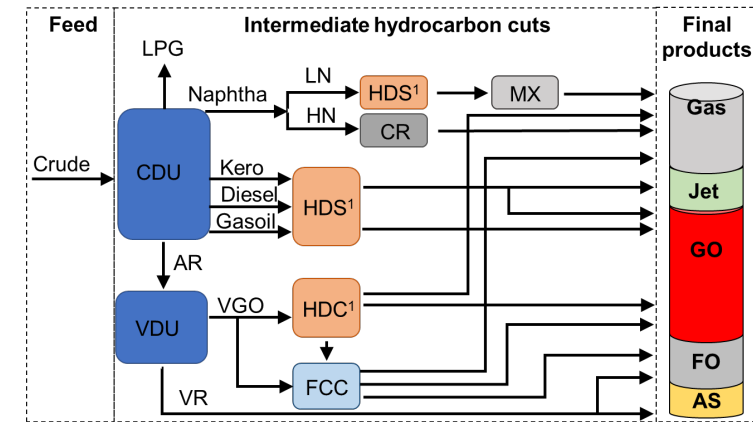
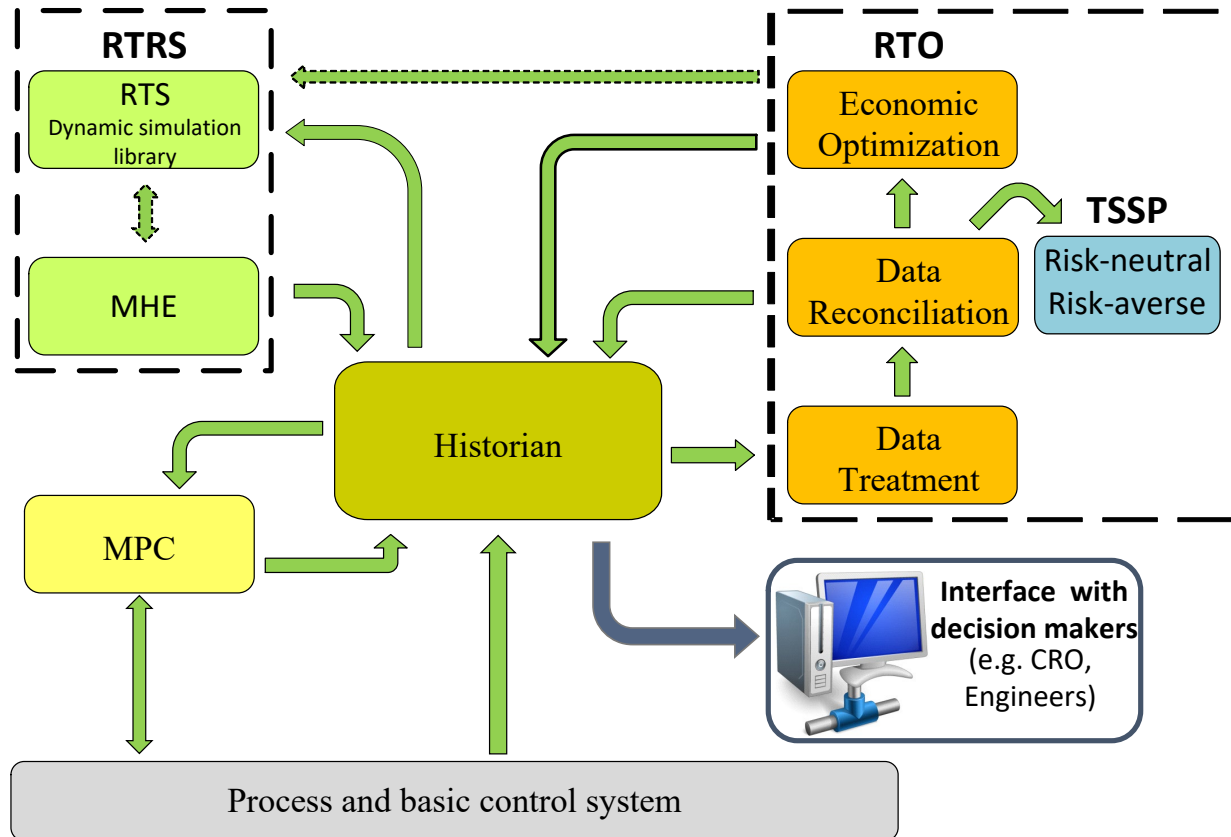


- Dificultad para mantener modelos
  - Parámetros, estados, etc.
  - Cambios en la estructura de la planta
- Especificar grados de libertad
- Interfaces Inteligentes



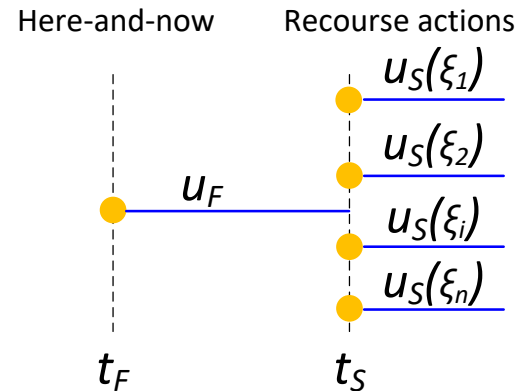


- Crude oil changes every 2-3 days
- Uncertain properties of new feeds impact downstream during changeover periods
- H<sub>2</sub> demand is directly affected by feed chemical properties (mostly unknown)



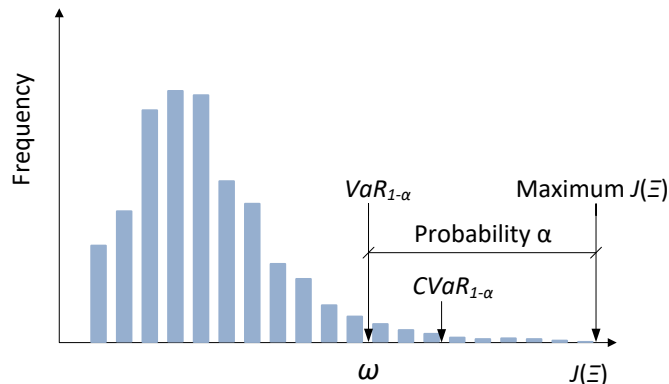
- Crude oil changes every 2-3 days
- Uncertain properties of new feeds impact H<sub>2</sub> demand

## Two-stage stochastic programming



Main assumptions:

- H<sub>2</sub> Producers are decided at first stage
- Rest of the variables (e.g. HC loads) are used for recourse once the uncertainty is realized.
- H<sub>2</sub> demand for each process unit is uncertain, responding to a discrete probability function
- 9 scenarios are represented ( $j = 1 \dots 9$ )



$$\max_{F_{H_2i}, HC_k(\xi_j), R_k(\xi_j)} J_F \left( - \sum_{i=1}^2 p_{H_2i} \cdot F_{H_2i} \right) + \mathbb{E} \left\{ J_S \left( \sum_{k=1}^4 p_{HC_k} \cdot HC_k(\xi_j) - p_{R_k} \cdot R_k(\xi_j) \right) \right\}$$

s.t.

$$h_F(x_F, u_F) = 0,$$

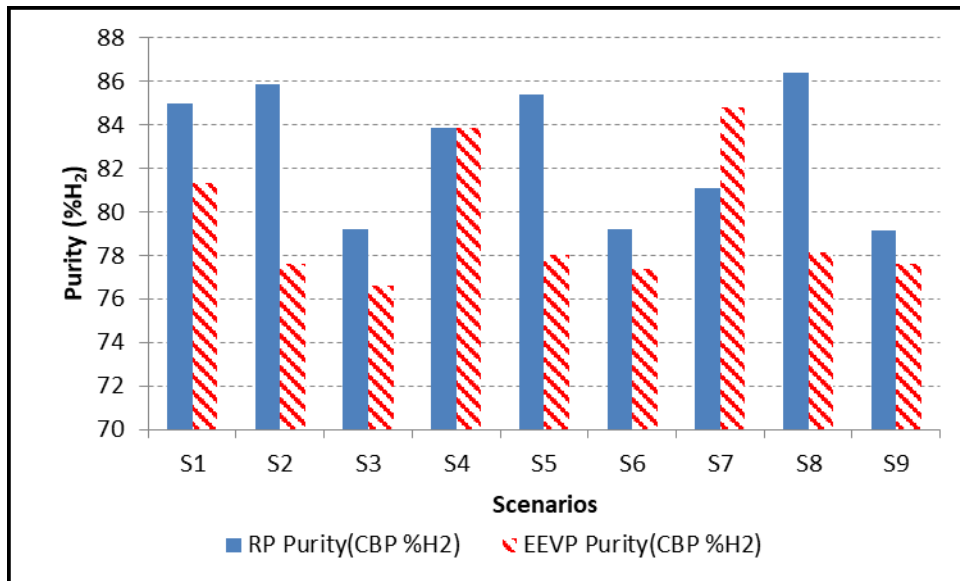
$$g_F(x_F, u_F) \leq 0,$$

$$h_S(x_F, u_F, u_S(\xi), x_S(\xi)) = 0 \quad \forall \xi \in \Xi,$$

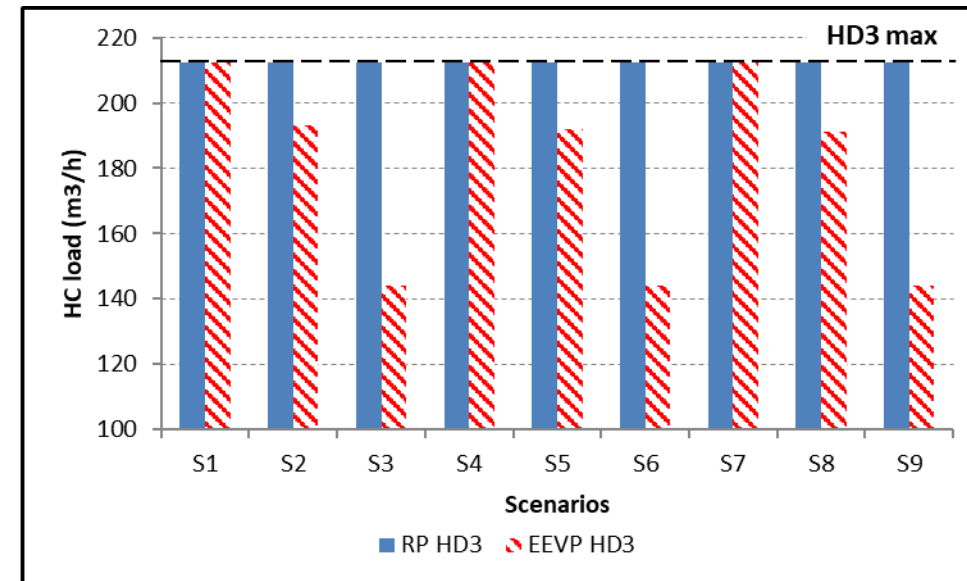
$$g_S(x_F, u_F, u_S(\xi), x_S(\xi)) \leq 0 \quad \forall \xi \in \Xi,$$



## Two-stage stochastic problem Petronor case study – Risk-neutral



Low purity header hydrogen purity at scenarios S1 to S9 applying RP and EEVP



RP and EEVP solutions for HC loads of process unit HD3