

Minimization of the H2 production cost

Operational Optimization - Mathematical formulation

Assumptions

- (1) Cost related to H2O consumption neglected
- (2) Time step of one hour ($\Delta t=1h$)
- (3) Total simulation over N_{day} days
- (4) Linearization of the current voltage (polarization curves) for $j>2500A/m^2$

Parameters

Operating pressure in the stack [bar]	P
Minimum operating temperature [°C]	T_{min}
Maximum operating temperature [°C]	T_{max}
Electrolyte KOH concentration [%wt]	Koh
Dynamic Hydrogen production degradation coefficient [$\text{€}/\text{Nm}^3$]	β_{dyn}
Nominal production capacity of the electrolyzer [Nm^3/h]	C_{nom}
Minimum production capacity to avoid shutdown (in [0,1])	Coeff_buff
Initial Hydrogen storage	S_{t0}
Nominal storage capacity [Nm^3]	S_{vess_nom}
Nominal battery pack capacity [kWh]	S_{batt_nom}
“Big M” method parameter to adjust the production efficiency [kWh]	M1
“Big M” method parameter to adjust the production capacity [Nm^3/h]	M2
“Big M” method parameter to adjust the production efficiency [kWh]	M3

Simulation parameters

Number of hours in the simulation [] (multiple of 24)	N_t
Number of days in the simulation []	N_{day}
Time step duration [h]	Δt
List of time steps	$T=[0, N_t]$
List of days of the simulation	$D=[0, N_{day}]$

Decision variables

Hydrogen production rate [Nm^3/h]	$H2_f$
Hydrogen mass production rate [kg/h]	$H2_{mf}$
Hydrogen stored in at each time step t [Nm^3]	S_{in}
Hydrogen stored out at each time step t [Nm^3]	S_{out}
Electrolyzer turned On/Off [binary variable: 0->Off, 1->On]	y

Other variables

Cost due to degradation of the electrolyzer [$\text{€}/\text{h}$]	K_d
Cost due to electricity purchases [$\text{€}/\text{h}$]	K_e

Oxygen production rate [Nm ³ /h]	O2_f
Oxygen mass production rate [kg/h]	O2_mf
Power consumption [kW]	φ
Actual Power consumption, accounting for cold/hot starts [kW]	φ_eff
Actual Power consumption, accounting for η_conso=η_conso(H2_mf) [kW]	φ_eff2
Power provided by day ahead market contract [kW]	φ_day
Power provided by spot on contract [kW]	φ_spot
Production efficiency [kWh/Nm ³]	η_conso
Hydrogen stored at time t [Nm ³]	S_t
Net amount of hydrogen coming out of the plant [kg]	H2_mf_net
Daily hydrogen contract allocation (flexible contracts) [kg/h]	H2_dc_h
Account for cold starts (binary: 0->Cold start, 1->No cold start)	y1

Inputs

Daily hydrogen delivery contract (flexible contracts) [kg/day]	H2_dc
Hourly hydrogen delivery contract (fixed contracts) [kg/h]	H2_hc
Electricity price on the day ahead market [€/MWh]	π_da
Electricity price on the spot on market [€/MWh]	π_so

Objective function: minimization of the daily H2 production cost

$$\sum_{t \in T} (K_e(t) + K_d(t))$$

Constraints:

- Cost of electricity purchase

$$\text{For } t \in T, K_e(t) = (\phi_{\text{spot}}(t) + \phi_{\text{eff}}(t) - \phi(t)) * \pi_{\text{spot}}(t) + \phi_{\text{reg}}(t) * \pi_{\text{reg}}(t)$$

- Energy balance

$$\text{For } t \in T, \phi(t) = \phi_{\text{day}}(t) + \phi_{\text{spot}}(t)$$

- Cost related to electrolyzer degradation

$$\text{For } t=1, K_d(t) = \beta_{\text{stat}} * H2_f(t)$$

$$\text{For } t \in T, K_d(t) = \beta_{\text{stat}} * H2_f(t) + \beta_{\text{dyn}} * (H2_f(t) - H2_f(t-1))$$

- Limited production capacity (design optimisation)

$$C_{\text{nom}} < C_{\text{nom_max}}$$

$$C_{\text{nom}} > C_{\text{nom_min}}$$

- Limited storage capacity (design optimisation)

$$S_{nom} < S_{nom_max}$$

$$S_{nom} > S_{nom_min}$$

- Detection of whether the electrolyzer is on or off

$$\text{For } t \in T, H2_f(t) = y(t) * H2_f(t)$$

- Detection of cold start (electrolyzer off for the previous 3 time steps)

$$\text{For } t \in T \setminus \{0, 1, 2, 3\}, \sum_{j=t-4}^{t-1} H2_f(j) \geq C_{nom_min} * y1(i)$$

- Limited production and account for cold starts (3 min delay) and hot starts (15 sec delay)

$$\text{For } t \in T, H2_f(t) < C_{nom}$$

$$\text{For } t \in T \setminus \{0, 1, 2, 3\}, H2_f(t) \leq 57/60 * C_{nom} + M2 * y1(t)$$

$$\text{For } t \in T \setminus \{0, 1\}, H2_f(t) \leq (1 - 15/3600) * C_{nom} + M2 * y(t-1)$$

$$\text{For } t \in T, H2_f(t) > \text{Coeff_b} * C_{nom}$$

- Power input, accounting for the loss in efficiency when there is a cold start

$$\text{For } t \in T, \phi(t) \leq \phi_eff(t)$$

$$\text{For } t \in T \setminus \{0, 1, 2, 3\}, 2 * \phi(t) - M1 * y1(t) \leq \phi_eff(t)$$

$$\text{For } t \in T \setminus \{0, 1, 2, 3, 4\}, 5/4 * \phi(t) - M1 * y1(t-1) \leq \phi_eff(t)$$

- Hydrogen net output at each time step

$$\text{For } t \in T, H2_mf_net(t) = H2_mf(t) + S_out(t) - S_in(t)$$

- Flexible Hydrogen delivery contracts ensured

$$\text{For } d \in \mathbf{D}, H2_dc(d) = \sum_{t=24*d}^{24*(d+1)} H2_dc_h(t)$$

- Hydrogen balance between net output of the plant and delivery

$$\text{For } t \in T, H2_mf_net(t) = H2_hc(t) + H2_dc_h(t)$$

- Constraints on the operating Temperature of the electrolyzer
For $t \in T$, $T(t) > T_{\min}$
For $t \in T$, $T(t) < T_{\max}$
- Hydrogen production knowing the inlet power (accounts for initial cold start)
 $\phi(0) = 2 * \eta_{\text{prod}}(t) * H2_{\text{mf}}(0)$
 $\phi(1) = 5/4 \eta_{\text{prod}}(t) * H2_{\text{mf}}(1)$
 $\phi(2) = 4/3 * \eta_{\text{prod}}(t) * H2_{\text{mf}}(2)$
For $t \in T \setminus \{0, 1, 2\}$, $\phi(t) = \eta_{\text{prod}}(t) * H2_{\text{mf}}(t)$
For $t \in T$, $H2_{\text{f}}(t) = \text{Coeff_mff} * H2_{\text{mf}}(t)$
- Hydrogen storage balance
For $t \in T$, $S_{\text{t}}(t+1) = S_{\text{t}}(t) + S_{\text{in}}(t) - S_{\text{out}}(t)$
- Maximum storage capacity
For $t \in T$, $S_{\text{t}}(t) < S_{\text{nom}}$
- Positivity constraints
For $t \in T$, $S_{\text{t}}(t) \geq 0$
For $t \in T$, $S_{\text{in}_t}(t) \geq 0$
For $t \in T$, $S_{\text{out}_t} \geq 0$

Indicators (post-simulation)

- O2 production related to H2 production ($H_2O \rightarrow H_2 + \frac{1}{2} O_2$)
For $t \in T$, $O2_{\text{mf}}(t) = \frac{1}{2} * M(O_2) / M(H_2) * H2_{\text{mf}}(t)$
- Hydrogen production efficiency
For $t \in T$, $\eta_{\text{conso}}(t) = \phi(t) / H2_{\text{f}}(t)$
- Portion of the net Hydrogen outflow of the plant going for flexible contracts
For $t \in T$, $\alpha(t) = H2_{\text{dc}_h}(t) / (H2_{\text{dc}_d}(t) + H2_{\text{hc}}(t))$

Parameters values

$$M(H_2) = 32 \text{ g/mol}$$

$$M(O_2) = 2.016 \text{ g/mol}$$

$$\text{Coeff_mff} = 1/0.0899$$

$$\text{Coeff_f} = 1/(2 \cdot 96\,485) \cdot 44.61 \cdot 3600 \cdot 0.0899$$

Schematic of the steps to evaluate
the production costs of hydrogen

