Supporting Information: Coupling Renewable Energy and Storage Technologies with Hydrogen-Based Steel Production: A Design and Scheduling Optimization Approach

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1 Model formulation

This model formulation builds on the work of Zhang et al. (2016).

1.1 Mass balances

The general equation for the mass balance of the different processes for a given facility is as follows:

$$\overline{Q}_{jht} = \overline{Q}_{jht-1} + B_{jht} - S_{jht} + \sum_{i} \rho_{ij} P_{iht} \quad \forall\, j,\, h,\, t \in \overline{T}_h \tag{S1}$$

In this equation, the amount of resource j stored at time t of season h is represented by $\overline{Q}_{rjht}$. B_{rjht} and S_{rjht} denote the amounts of consumed or discharged resource at each location. The amount of reference resource produced or consumed is denoted by P_{riht}. Finally, the parameter ρ_{ij} denotes the conversion factor between resource j and the reference resource of process i.

The production of the reference resource in each process i is limited by the plant capacity:

$$P_{iht} = \eta_{iht} C_i \quad \forall\, i \in \{PV, WT\},\, h,\, t \in \overline{T}_h \tag{S2}$$

$$P_{iht} \leq \eta_{iht} C_i \quad \forall\, i \in I \setminus \{PV, WT\},\, h,\, t \in \overline{T}_h \tag{S3}$$

The plant capacity is denoted by C_i. The parameter η_{ikt} is used to represent the time-varying process capacity, for instance, wind or solar generation, where the capacity is not only a function of the plant size but also of the wind/solar availability. This parameter is calculated using the solar irradiance/ambient (Sánchez and Martín, 2018; Hlal et al., 2019) temperature or the wind velocity (de la Cruz and Martín, 2016) for each time period and location.

The storage capacity $\overline{C}_j$ is an upper bound for the inventory level in those resources with associated storage.

$$\overline{Q}_{jht} \leq \overline{C}_j \quad \forall\, j \in \hat{S},\, h,\, t \in \overline{T}_h \tag{S4}$$

$$\overline{Q}_{jht} = 0 \quad \forall\, j \notin \hat{S},\, h,\, t \in \overline{T}_h \tag{S5}$$

The set $\hat{S}$ consists of all resources that can be stored (battery power, hydrogen and hydrogenated and dehydrogenated LOHC).

For the specific case of the battery, a minimum level is imposed to avoid problems in the performance and durability of the unit. In this case, a 15% of the capacity is set as minimum level of storage.

$$\overline{Q}_{jht} \geq 0.15\overline{C}_j \quad \forall\, j \in \{\text{Battery}\},\, h,\, t \in \overline{T}_h \tag{S6}$$

There is a maximum value for the capacity ($C_i^{\max}$)for each process involved in the network. The binary variable x_i indicates whether process i is selected in the process network.

$$C_i \leq C_i^{\max} x_i \quad \forall\, i \tag{S7}$$

In this particular case, the process capacities of the battery charge and discharge must be the same (both are determined by the battery specifications):

$$C_{BC} = C_{BD} \tag{S8}$$

Similarly, there is also a maximum value for the storage capacity denoted by $\overline{C}_j^{\max}$. The binary variable $\bar{x}_j$ is equal to 1 if a storage facility for product j is selected.

$$\overline{C}_j \leq \overline{C}_j^{\max} \bar{x}_j \quad \forall\, j \tag{S9}$$

The resource availability is also limited for those resources used as raw materials in the proposed network (indicated by the set $\hat{B}$).

$$B_{jht} \leq B_{jht}^{\max} \quad \forall\, j \in \hat{B},\, h,\, t \in \overline{T}_h \tag{S10}$$

$$B_{jht} = 0 \quad \forall\, j \notin \hat{B},\, h,\, t \in \overline{T}_h \tag{S11}$$

Some resources of the network do not have an associated demand (i.e., they are not in the set $\hat{J}$). Therefore, the outlet flowrate of these species is fixed to 0:

$$S_{jht} = 0 \quad \forall\, j \notin \hat{J},\, h,\, t \in \overline{T}_h \tag{S12}$$

1.2 Mode-based operation

Each of the processes involved can operate in four different operating modes: off, startup, on and shutdown. The binary variable y_{imht} indicates if a process i is operating in a certain mode

m. If a process is selected, one of the operating modes must be assigned:

$$\sum_{m \in M_i} y_{imht} = x_i \quad \forall\, i,\, h,\, t \in \overline{T}_h \tag{S13}$$

The set M_i denotes the set of allowed operating modes for process i.

In the particular case of the battery charge and discharge processes, only one of the two could be in on mode at the same time (it is not possible to charge and discharge the battery simultaneously):

$$\sum_{i \in \{BC, BD\}} y_{imht} \leq 1 \quad \forall\, m \in \{ON\},\, h,\, t \in \overline{T}_h \tag{S14}$$

The amount of reference resource consumed or produced by process i, P_{iht}, must be produced or consumed in one of the different operating modes. The variable $\overline{P}_{imht}$ denotes the quantity of reference resource consumed or produced in mode m:

$$P_{iht} = \sum_{m \in M_i} \overline{P}_{imht} \quad \forall\, i,\, h,\, t \in \overline{T}_h \tag{S15}$$

A maximum ($\widetilde{C}_{im}^{\max}$) and minimum ($\widetilde{C}_{im}^{\min}$) value for the amount of reference resource produced or consumed for each mode is introduced:

$$\widetilde{C}_{im}^{\min} y_{imht} \leq \overline{P}_{imht} \leq \widetilde{C}_{im}^{\max} y_{imht} \quad \forall\, i,\, m \in M_i,\, h,\, t \in \overline{T}_h \tag{S16}$$

The following constraints are related to the transition between operating modes for the same process unit. The maximum rate of change within a mode is limited by an upper bound ($\bar{\Delta}_{im}^{\max}$):

$$\begin{aligned} -\bar{\Delta}_{im}^{\max} - \overline{M}(2 - y_{imht} - y_{imh,t-1}) &\leq \overline{P}_{imht} - \overline{P}_{imh,t-1} \\ &\leq \bar{\Delta}_{im}^{\max} + \overline{M}(2 - y_{imht} - y_{imh,t-1}) \quad \forall\, i,\, m \in M_i,\, h,\, t \in \overline{T}_h \end{aligned} \tag{S17}$$

The binary variable $z_{im'mht}$ is introduced to indicate that process i switches from mode m to mode m' at time t. The possible transitions are defined by the following equation:

$$\begin{aligned} &\sum_{m' \in \overline{TR}_{im}} z_{im'mh,t-1} - \sum_{m' \in \overline{TR}_{im}} z_{imm'h,t-1} = y_{imht} - y_{imh,t-1} \\ &\qquad \forall\, i,\, m \in M_i,\, h,\, t \in \overline{T}_h \end{aligned} \tag{S18}$$

where the set TR_i includes all the possible mode-to-mode transitions for the process i, and $\overline{TR}_{im} = \{m' : (m', m) \in TR_i\}$ and $\widehat{TR}_{im} = \{m' : (m, m') \in TR_i\}$.

A process i must remain for a certain minimum number of time periods ($\theta_{imm'}$) in an operating mode m before switching to another mode m':

$$y_{im'ht} \geq \sum_{k=1}^{\theta_{imm'}} z_{imm'h,t-k} \quad \forall\, i,\, (m, m') \in TR_i,\, h,\, t \in \overline{T}_h \tag{S19}$$

Finally, predefined sequences of modes (from mode m to mode m' to mode m'') for a process i can be defined, establishing a fixed stay time for each of the modes involved in the sequence.

$$z_{imm'h,t-\bar{\theta}_{imm'm''}} = z_{im'm''ht} \quad \forall\, i,\, (m,m',m'') \in SQ_i,\, h,\, t \in \overline{T}_h \tag{S20}$$

The set SQ_i denotes the set of predefined sequences for process i and $\bar{\theta}_{imm'm''}$ is the fixed stay time in mode m' in the predefined sequence.

1.3 Continuity constraints

Continuity constraints ensure the feasible transition between seasons. A cyclic schedule is imposed; therefore, the initial mode of a season must be the same as the final one.

$$y_{imh,0} = y_{imh,|\overline{T}_h|} \quad \forall\, i,\, m \in M_i,\, h \tag{S21}$$

$$z_{imm'ht} = z_{imm'h,t+|\overline{T}_h|} \quad \forall\, i,\, (m,m') \in TR_i,\, h,\, -\theta_i^{\max} + 1 \le t \le -1 \tag{S22}$$

For the transitions between seasons, the state at the final time of one season and at the initial time of the next season must be the same.

$$y_{imh,|\overline{T}_h|} = y_{im,h+1,0} \quad \forall\, i,\, m \in M_i,\, h \in H \setminus |H| \tag{S23}$$

$$\begin{aligned} &z_{imm'h,t+|\overline{T}_h|} = z_{imm',h+1,t} \\ &\forall\, i,\, (m,m') \in TR_i,\, h \in H \setminus |H|,\, -\theta_i^{\max} + 1 \le t \le -1. \end{aligned} \tag{S24}$$

The storage is allowed between seasons. The following equations determine the change in inventory levels from one season to the next.

$$\hat{Q}_{jh} = \overline{Q}_{jh,|\overline{T}_h|} - \overline{Q}_{jh,0} \quad \forall\, j \in \hat{S},\, h \tag{S25}$$

$$\overline{Q}_{jh,0} + n_h\, \hat{Q}_{jh} = \overline{Q}_{j,h+1,0} \quad \forall\, j,\, h \in H \setminus |H| \tag{S26}$$

$$\overline{Q}_{j,|H|,0} + n_{|H|}\, \hat{Q}_{j,|H|} = \overline{Q}_{j,1,0} \quad \forall\, j \tag{S27}$$

1.4 Objective function

The objective of this work is to meet a given demand for hydrogen and power $D_{j,h,t}$ using the different proposed technologies (including storage).

$$S_{jht} = D_{jht} \quad \forall\, j \in \hat{J},\, h,\, t \in \overline{T}_h \tag{S28}$$

The goal is to minimize the following objective function:

$$
\begin{aligned}
OC = &\sum_{i}\sum_{m\in M_i}\sum_{h}\sum_{t} J_{imht} + \sum_{i}\sigma_i\left(\delta_i x_i + \gamma_i C_i\right) + \\
&\sigma_j\left(\overline{Q}_{LOHC_0,1,0} + \overline{Q}_{LOHC_n,1,0}\frac{MW_{LOHC_0}}{MW_{LOHC_n}}\right)C_{LOHC_0} + \\
&\sum_{j\in\hat{S}}\left(\alpha_j\bar{x}_j + \beta_j\overline{C}_j\right) + \sum_{i}\sum_{j}\sum_{h}\sum_{t}\xi_{ij}\rho_{ij}P_{iht}
\end{aligned}
\tag{S29}
$$

which comprises the costs of production and storage.

The piece-wise linear approximation used to compute the first term of equation (S29), J_{imht}, is as follows:

$$P_{imht} = \sum_{l\in L_i}\left(\lambda_{imhtl}\left(\hat{P}_{im,l-1} - \hat{P}_{im,l}\right) + \hat{P}_{iml}\omega_{imhtl}\right) \quad \forall\, i,\, m\in M_{ri},\, h,\, t \tag{S30}$$

$$J_{imht} = \sum_{l\in L_i}\left(\lambda_{imhtl}\left(\hat{J}_{im,l-1} - \hat{J}_{im,l}\right) + \hat{J}_{iml}\omega_{imhtl}\right) \quad \forall\, i,\, m\in M_{ri},\, h,\, t \tag{S31}$$

$$\lambda_{imhtl} \le \omega_{imhtl} \quad \forall\, i,\, m\in M_i,\, h,\, t,\, l\in L_i \tag{S32}$$

$$\sum_{l\in L_i}\omega_{iktl} = y_{ikt} \quad \forall\, i,\, m\in M_i,\, h,\, t \tag{S33}$$

2 Modeling Parameters

The optimization problem incorporates multiple parameters, including the different yields, maximum capacity constraints, and cost coefficients. For the LOHC systems, two parameter sets are presented to reflect the two systems studied: N-ethylcarbazole (LOHC1) and an indole-based mixture (LOHC2).

Parameter $\rho_{i,j}$

Process	Resource	Yield (kW/kW or kg/kW)	Process	Resource	Yield (kW/kW or kg/kW)
PV	Solar	-1	FC	Heat	7.80278E-01
PV	Power	1	C	Power	-1
WT	Wind	-1	C	H_2	-0.277777778
WT	Power	1	C	Heat	33069.7
BC	Power	-1	LOHC-H	Power	-1 / -1
BC	Battery power	0.97	LOHC-H	H_2	-3.26E-03/-2.15E-03
BD	Power	1	LOHC-H	Heat	-1.53E+00/-2.23E+00
BD	Battery power	-1.1494	LOHC-H	LOHC0	-6.81E-02/-5.73E-02
EL	Power	-1	LOHC-H	LOHCn	7.13E-02/5.95E-02
EL	Water	-4.48263608E-05	LOHC-DH	Power	-1/-1
EL	H_2	5.12612885E-06	LOHC-DH	H_2	1.58E-03/1.62E-03
FC	Power	1	LOHC-DH	Heat	-4.99E+01/-6.27E+01
FC	H_2	-1.63859E-05	LOHC-DH	LOHC0	3.30E-02/4.35E-02
			LOHC-DH	LOHCn	-3.46E-02/-4.52E-02

Maximum process capacity C_i^{max}

Process	C_i^{max} (area or kW)	Process	C_i^{max} (area or kW)
PV	5% of total area of the region	FC	220000
WT	5% of total area of the region	C	10
BC	10000	LOHC-H	700/1100
BD	10000	LOHC-dH	3000/3000
EL	1000000.0		

Maximum storage capacity $\overline{C}_i^{max}$

Resource	$\overline{C}_i^{max}$ (kJ or kg)
Battery	3.6e8
H_2	1e6
LOHC0	1.23e8/1.23e8
LOHCn	1.23e8/1.23e8

Process capital cost contribution δ_i, γ_i

Resource	δ_i (MM$)	γ_i (MM$ / area or MM$/kW)
PV	0.0001	1.24216E-04
WT	0.0001	4.91000000E-04
BC	0	0
BD	0	0
EL	17.72062345	0.00161936
FC	9.4377e-2	1.9593e-3
C	0.3753	2.8024
LOHC-H	0.5144/0.5089	0.0022/0.0014
LOHC-DH	0.5191/0.5353	0.0024/0.0014

Storage capital cost α_i, β_i

Resource	α_i ($)	β_i ($/kJ or $/kg)
Battery	0	0.07111
H_2	0.0001	500
LOHC0	0.0001/0.0001	0.137/0.152
LOHCn	0.0001/0.0001	0.160/0.152

Piece-wise linear approximation $\hat{P}_{iml}$, $\hat{J}_{iml}$

Resource	(kW)	(MM$/year)	Resource	(kW)	(MM$/year)
PV	0	0	EL	2000000	-25.57117624
PV	5.00E+09	0	FC	0	0
WT	0	0	FC	220000	19.25
WT	5.00E+09	0	C	0	0
BC	0	0	C	10	0
BC	10000	0	LOHC-H	0	0
BD	0	0	LOHC-H	700/1100	3.9282/4.0399
BD	10000	0	LOHC-DH	0	0
EL	0	0	LOHC-DH	3000/3000	1.9446E-01/3.6887E-01

Storage O&M cost ξ_j

Resource	ξ_j ($/kJ or $/kg)
Battery	83.3333 e-9
H_2	0
LOHC0	0
LOHCn	0

3 Operating Results

The scheduling results have been presented for three specific locations among the provinces of mainland Spain. For the electricity scheduling of the LOHC1 (N-ethylcarbazole), the results for Córdoba have been presented. Here, the results for the provinces of A Coruña and Guadalajara are also shown.

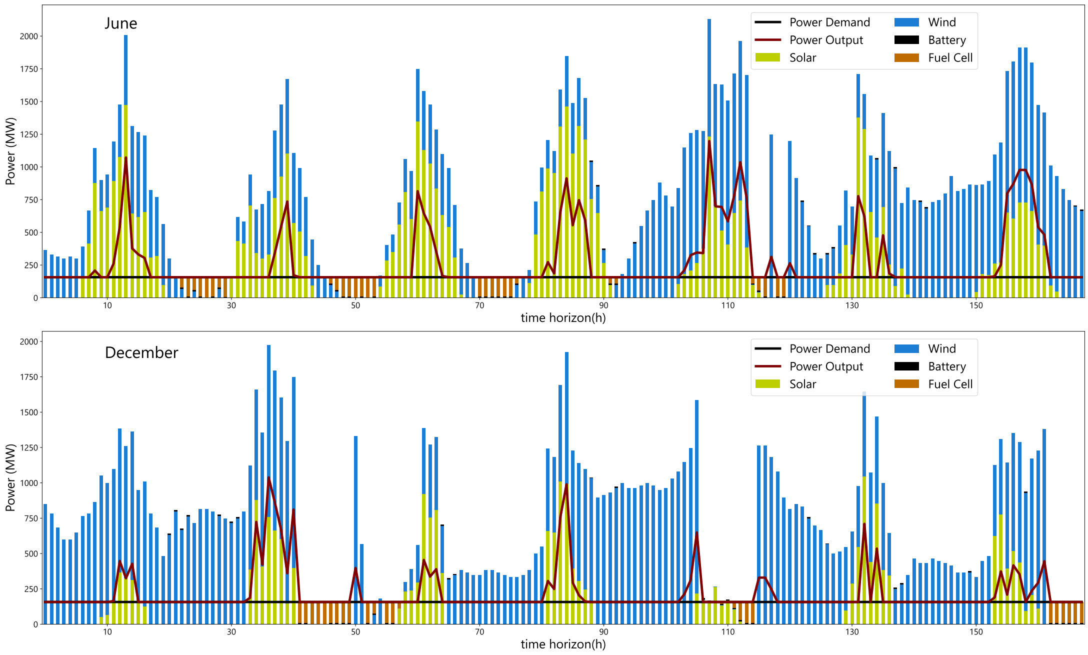

Figure S1: Electricity scheduling results in the province of A Coruña for the system with N-ethylcarbazole as LOHC

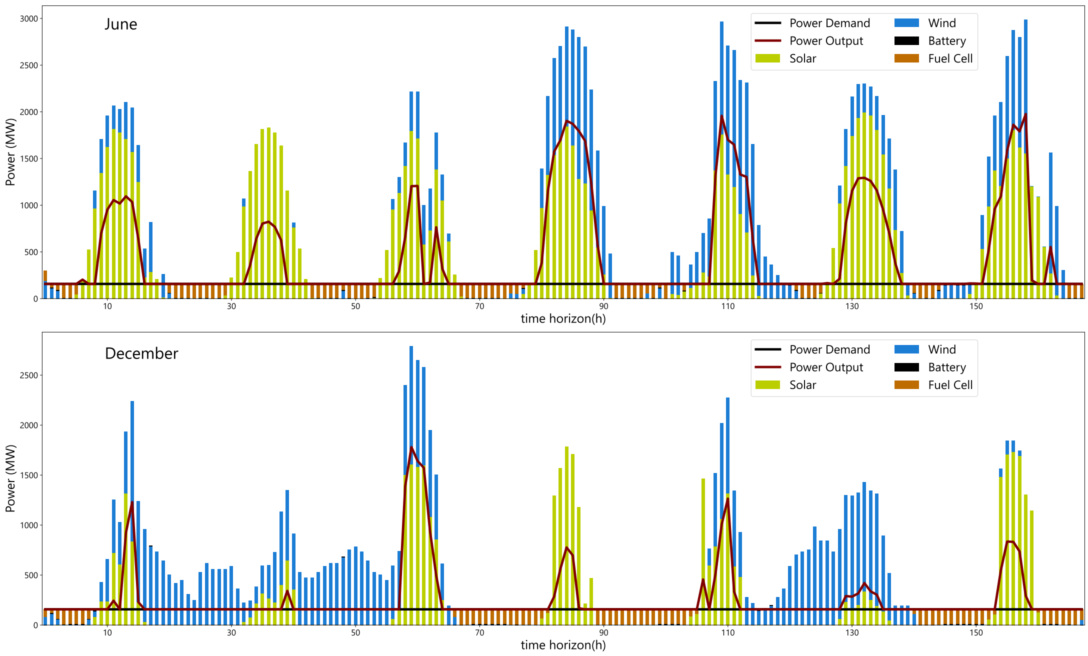

Figure S2: Electricity scheduling results in the province of Guadalajara for the system with N-ethylcarbazole as LOHC

For the electricity scheduling of the LOHC2 (indoles mixture), the results for A Coruña have been presented. Here, the results for the provinces of Córdoba and Guadalajara are also shown.

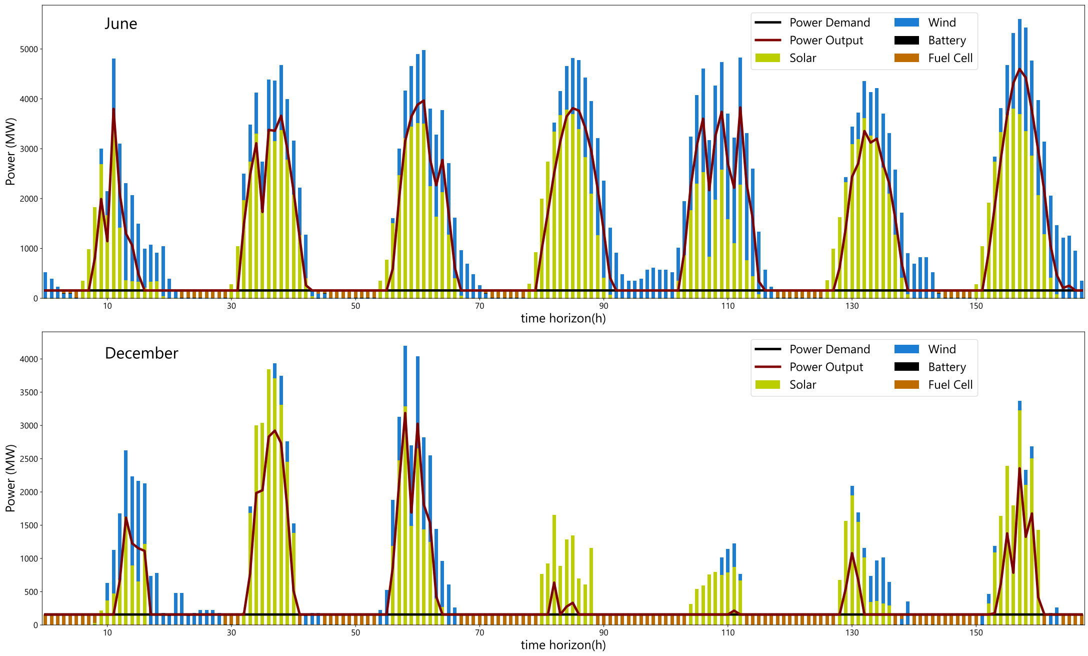

Figure S3: Electricity scheduling results in the province of Córdoba for the system with indoles mixture as LOHC

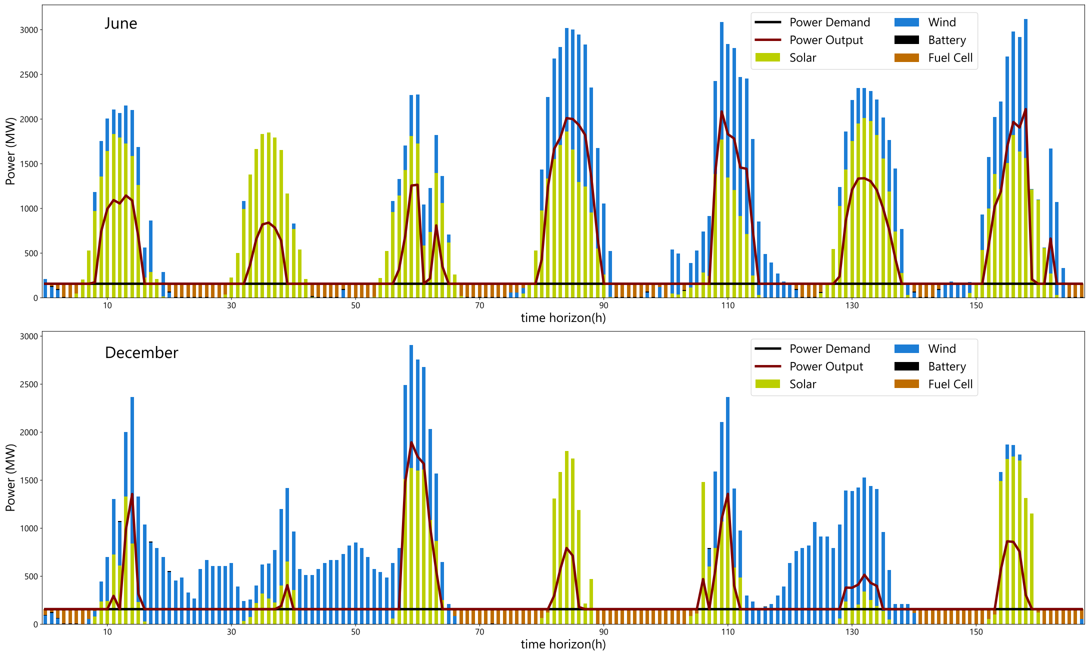

Figure S4: Electricity scheduling results in the province of Guadalajara for the system with indoles mixture as LOHC

For the hydrogen scheduling of the LOHC1 (N-ethylcarbazole), the results for Guadalajara have been presented in the manuscript. Here, the results for the provinces of Córdoba and A Coruña are also shown.

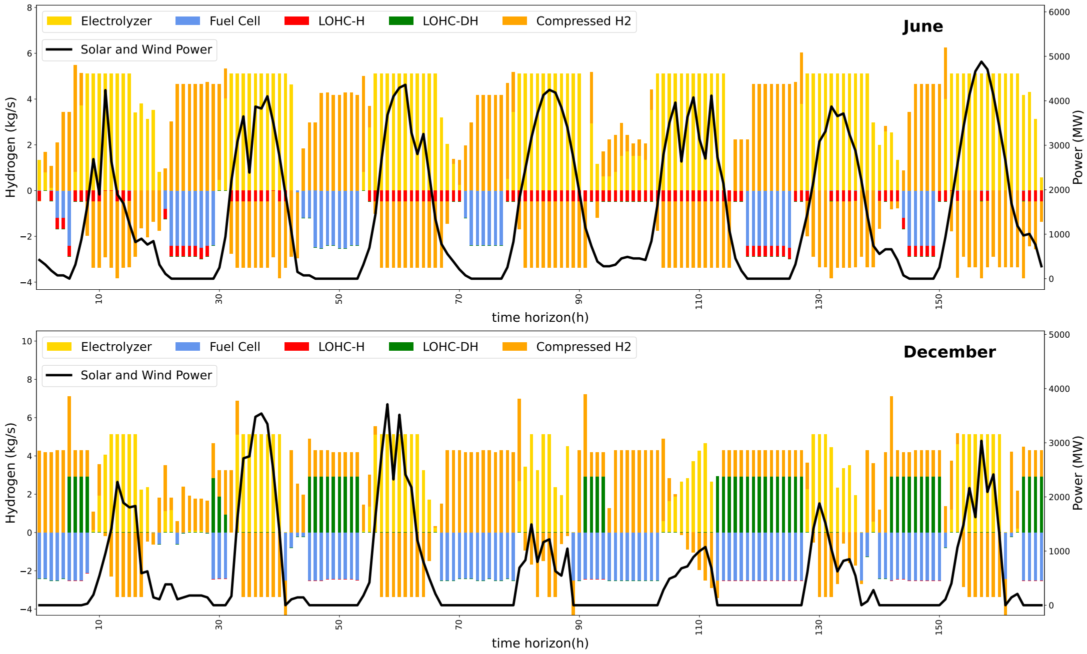

Figure S5: Hydrogen scheduling results in the province of Córdoba for the system with N-ethylcarbazole as LOHC

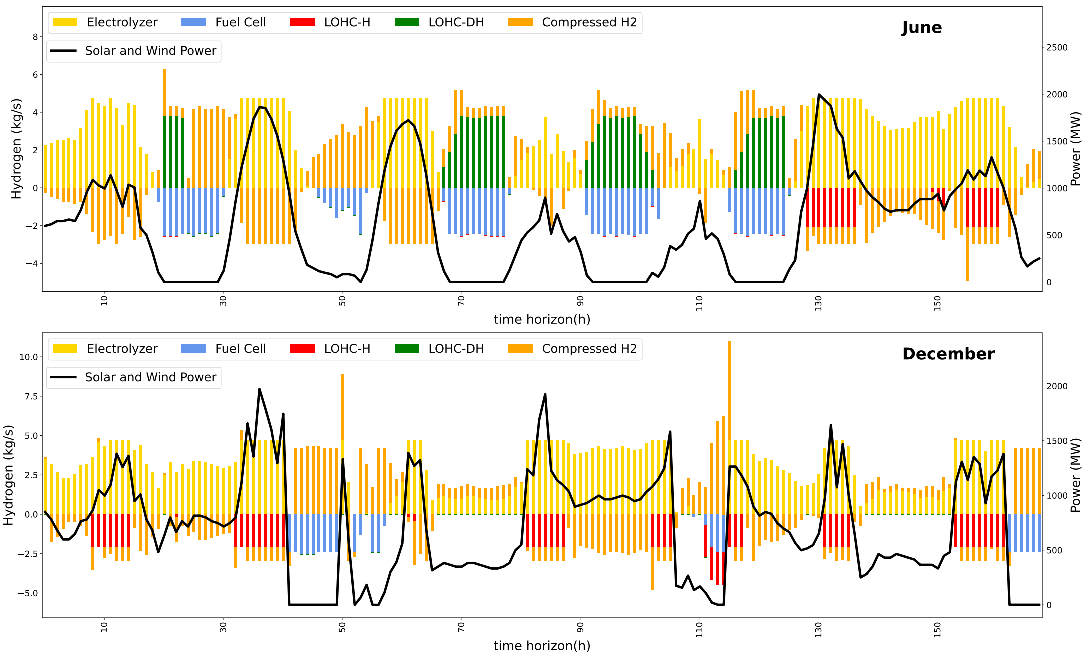

Figure S6: Hydrogen scheduling results in the province of A Coruña for the system with N-ethylcarbazole as LOHC

For the hydrogen scheduling of the LOHC2 (indoles mixture), the results for A Coruña are presented in the manuscript. Here, the results for Córdoba and Guadalajara are also shown.

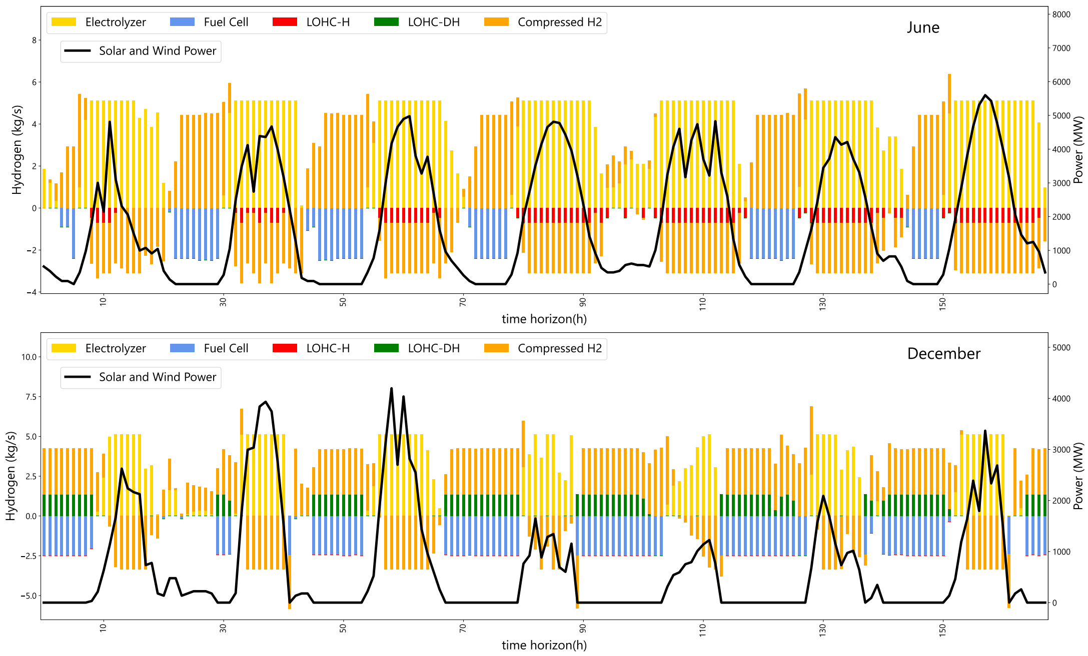

Figure S7: Hydrogen scheduling results in the province of Córdoba for the system with indoles mixture as LOHC

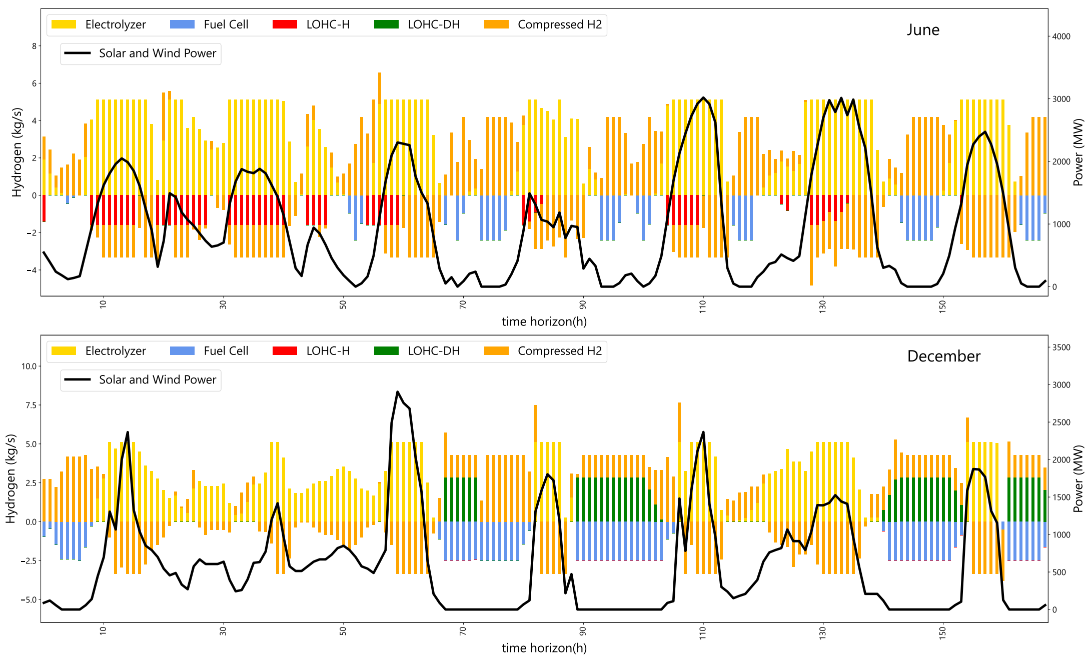

Figure S8: Hydrogen scheduling results in the province of Guadalajara for the system with indoles mixture as LOHC

Nomenclature

Indices / sets/ subsets

$\hat{B}$	resources use as raw material of the network
$\tilde{B}$	resources with a maximum annual availability
$h \in H$	seasons in the multiscale time representation
$i \in I$	processes evaluated in the power to fuel network
$j \in J$	resources involved in the network
$\hat{J}$	product with associated demand
$l \in L$	segments in operating cost piecewise-linear approximations
L_i	segments in piecewise-linear approximation
$m \in M$	operating modes for each of the process
M_i	operating modes for a process
$\hat{S}$	resources that could be stored
$t \in T$	time periods in the multiscale time representation
$\overline{T}_h$	time periods in season h
$\overline{TR}_{im}$	mode transitions to reach mode m
$\widehat{TR}_{im}$	mode transtions to progress from mode m
TR_i	predefined sequences of mode transitions

Parameters

$\overline{B}_j^{max}$	maximum annual resource than can be consumed
$C_i^{\max}$	maximum production capacity
$\overline{C}_i^{\max}$	maximum storage capacity
$\widetilde{C}_{im}^{\max}$	maximum production in a given mode
$\widetilde{C}_{im}^{\min}$	minimum production in a given mode
$D_{power,h,t}$	power demand
$\hat{J}_{iml}$	operating cost for piecewise-linear approximation
$\overline{M}$	big-M parameter
n_h	number of repetition of the horizon scheduling for a season
$\hat{P}_{iml}$	production level for piecewise-linear approximation
ρ_{ij}	conversion factor of the different products with respect to the reference resource
η_{iht}	availability of production capacity for wind/solar
$\bar{\Delta}_{im}^{\max}$	maximum rate of change
$\theta_{imm'}$	minimum stay time in a certain mode
$\bar{\theta}_{imm'm''}$	fixed stay time for a predefined sequence
$\theta^{\max}$	stay time in a mode
σ_i	conversion factor between capital and operating cost for a process
δ_i	fixed capital cost coefficient

γ_i	unit capital cost coefficient
α_j	annualized fixed capital cost for storing
β_j	annualized unit capital cost for storing
Δt	length of one time period
λ_{imhtl}	coefficient for piecewise-linear approximation
ξ_j	O&M cost for storing

Variables

B_{jht}	amount of resource consumed
C_i	production capacity for different processes
$\overline{C}_j$	storage capacity for different resources
J_{imht}	process operating cost not related to capital cost
OC	Operating cost
P_{iht}	amount of reference resource produced
$\overline{P}_{imht}$	reference resource produced in certain mode
$\overline{Q}_{jht}$	inventory level
$\hat{Q}_{jh}$	net inventory in a season
S_{jht}	amount of resource release
x_i	binary variable to select process units
$\overline{x}_i$	binary variable to select storage units
y_{imht}	binary variable to select a mode for a specific process
$z_{imm'ht}$	binary variable for mode transitions
w_{rimhtl}	binary variable for piecewise-linear aproximation

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