Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supplemental Material 1.0

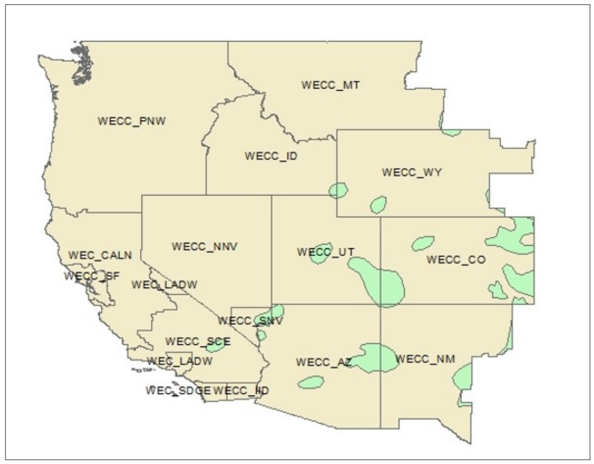

Figure S1: Western states with possible salt domes/deposits

Table S1: Delivery pathways available in SERA

Pathway	Stage	Technology
Liquid hydrogen (LH2) truck	1	LH2 truck terminal with liquefaction and storage
	2	LH2 truck
	3	End use point (city gate/refueling station)
Gaseous hydrogen (GH2) pipeline	1	Pipeline compressor and salt cavern storage
	2	Pipeline (transmission)
	3	End use point (city gate/refueling station)
Gaseous hydrogen (GH2) truck	1	GH2 truck terminal with storage
	2	GH2 truck
	3	End use point (city gate/refueling station)

Table S2: Breakdown of hydrogen demand (other than on-road transportation) by location

Location	Aggregated Non-transport Demand types
San Diego	Aviation, Residential/Commercial, others
Los Angeles	Marine, Refinery, Biofuel, Aviation, Residential/Commercial, others
San Jose	Aviation, Residential/Commercial, others
San Francisco	Marine, Refinery, Biofuel, Aviation, Residential/Commercial, others

Sacramento	Aviation, Residential/Commercial, others
Bakersfield	Refinery, Biofuel, Aviation, Residential/Commercial, others

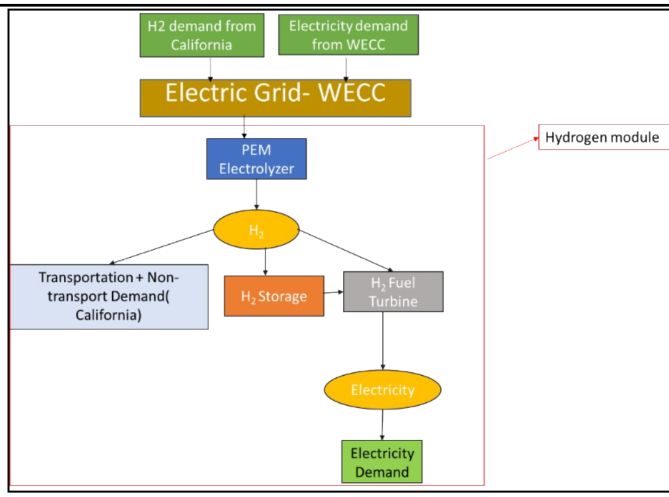

Figure S2: Hydrogen module in GOOD

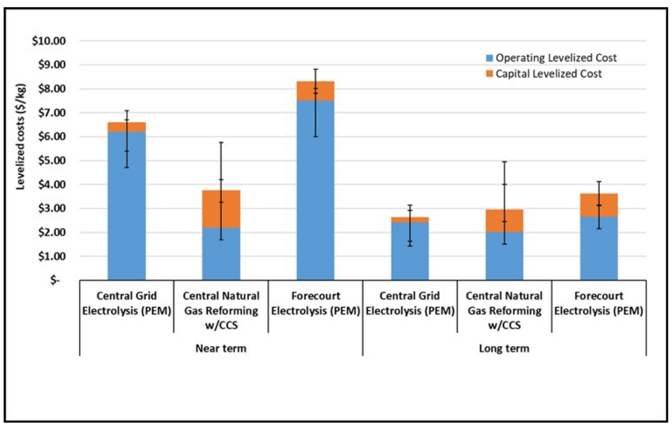

Figure S3: Levelized cost of hydrogen production

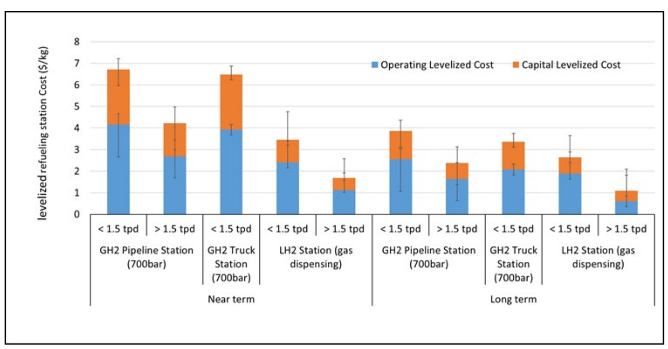

Figure S4: Levelized refueling station costs

	Distance (km)													
Capacity (tpd)	5	10	30	50	100	150	200	300	400	500	700	1000	1200	1500
0.5	$ 13.57	$13.59	$10.79	$13.63	$13.70	$13.76	$13.86	$13.96	$14.09	$14.22	$14.54	$14.87	$15.19	$ 15.52
1	$ 10.76	$10.77	$ 8.51	$10.81	$10.86	$10.92	$11.00	$11.09	$11.20	$11.31	$11.59	$11.87	$12.15	$ 12.43
2	$ 7.94	$ 7.96	$ 6.23	$ 7.73	$ 8.03	$ 8.08	$ 8.15	$ 8.22	$ 8.31	$ 8.41	$ 8.64	$ 8.88	$ 9.11	$ 9.35
3	$ 5.13	$ 5.14	$ 3.96	$ 4.50	$ 5.20	$ 5.24	$ 5.29	$ 5.35	$ 5.43	$ 5.50	$ 5.69	$ 5.88	$ 6.07	$ 6.27
10	$ 4.89	$ 4.90	$ 3.61	$ 4.00	$ 4.97	$ 5.01	$ 5.07	$ 5.14	$ 5.22	$ 5.30	$ 5.51	$ 5.72	$ 5.76	$ 5.81
15	$ 4.65	$ 4.67	$ 3.26	$ 3.51	$ 4.35	$ 4.79	$ 4.85	$ 4.92	$ 5.02	$ 5.09	$ 5.13	$ 5.18	$ 5.22	$ 5.27
20	$ 4.42	$ 4.43	$ 2.91	$ 3.02	$ 3.37	$ 3.72	$ 4.26	$ 4.50	$ 4.52	$ 4.54	$ 4.59	$ 4.64	$ 4.69	$ 4.74
30	$ 4.30	$ 4.31	$ 2.85	$ 2.93	$ 3.20	$ 3.47	$ 3.88	$ 4.28	$ 4.39	$ 4.41	$ 4.46	$ 4.51	$ 4.57	$ 4.62
50	$ 4.17	$ 4.17	$ 2.79	$ 2.84	$ 3.03	$ 3.22	$ 3.50	$ 3.78	$ 4.16	$ 4.28	$ 4.33	$ 4.39	$ 4.45	$ 4.50
75	$ 4.55	$ 4.55	$ 2.77	$ 2.81	$ 2.98	$ 3.14	$ 3.38	$ 3.62	$ 3.95	$ 4.27	$ 4.74	$ 4.81	$ 4.88	$ 4.94
100	$ 4.93	$ 4.94	$ 2.75	$ 2.79	$ 2.92	$ 3.06	$ 3.26	$ 3.46	$ 3.74	$ 4.01	$ 4.68	$ 5.23	$ 5.31	$ 5.38
150	$ 4.20	$ 4.21	$ 2.72	$ 2.75	$ 2.85	$ 2.95	$ 3.11	$ 3.26	$ 3.46	$ 3.67	$ 4.17	$ 4.45	$ 4.51	$ 4.58
200	$ 3.47	$ 3.48	$ 2.69	$ 2.71	$ 2.78	$ 2.85	$ 2.95	$ 3.05	$ 3.19	$ 3.32	$ 3.62	$ 3.67	$ 3.72	$ 3.77
300	$ 3.82	$ 3.82	$ 2.69	$ 2.71	$ 2.77	$ 2.83	$ 2.92	$ 3.01	$ 3.13	$ 3.25	$ 3.55	$ 3.85	$ 4.10	$ 4.16
400	$ 4.16	$ 4.17	$ 2.68	$ 2.70	$ 2.75	$ 2.80	$ 2.88	$ 2.96	$ 3.07	$ 3.17	$ 3.44	$ 3.70	$ 3.97	$ 4.23

Mode of Delivery
GH2 Pipeline
GH2 Truck
LH2 Truck

Figure S5: Least-cost delivery mode to a 1.5 metric ton per day refueling station (station costs included)

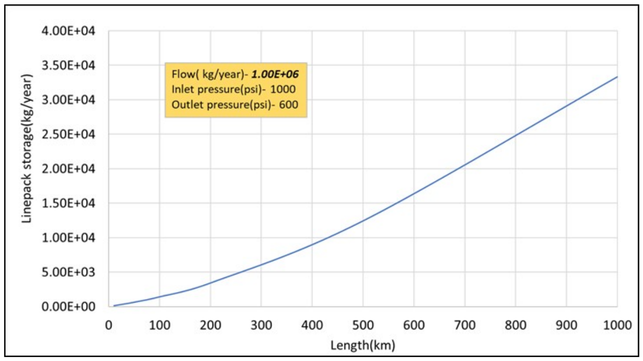

Figure S6: Storage limits for line-packed hydrogen pipelines

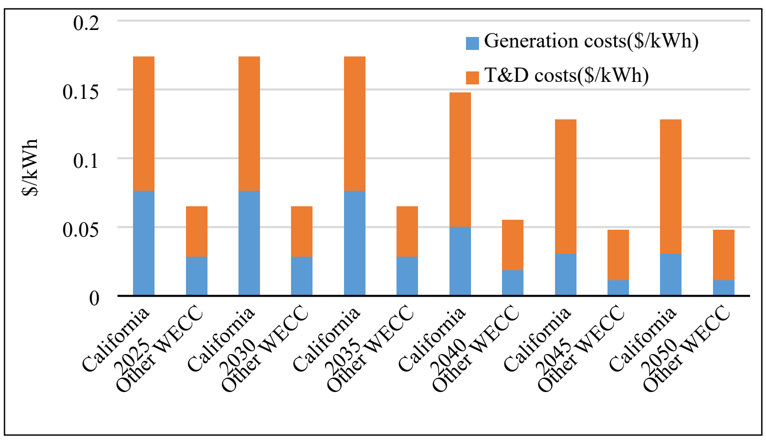

Figure S7: Breakdown of industrial electricity prices ($/kWh)

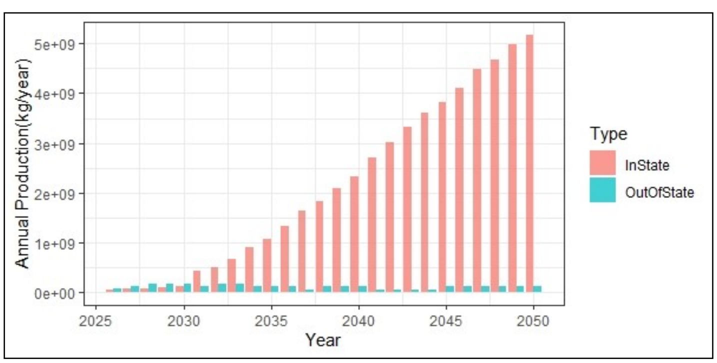

Figure S8: Distribution of in state and out-of-state production/regional imports for scenario POL_0perc_hub

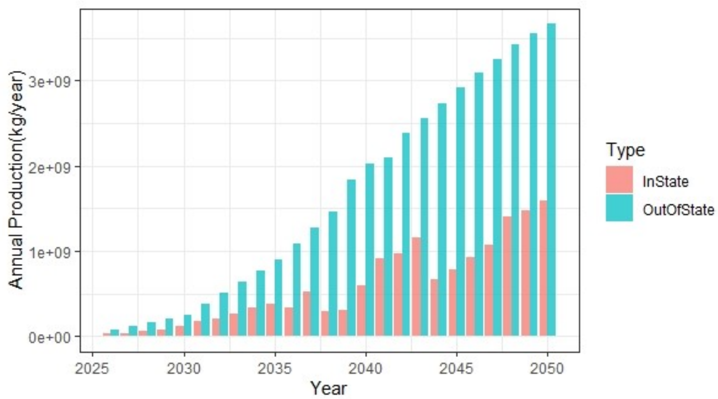

Figure S9: Distribution of in-state and out-of-state production/regional imports for scenario POL_75perc_hub

1. Nomenclature

1.1. Sets

N: the set of all nodes

T: the set of all intra-year time periods

Y: the set of all years

PT: the set of all production technologies

PW: the set of all pathways

L: the set of all links

L_n: the set of all links connected to node n

PT_{clean}: the set of clean H_2 production technologies

S_{pw}: the set of all stages in pathway pw

S_{pw}^{unext}: the set of all un-extended stages in pathway pw

S_{pw}^{ext} : the set of all extended stages in pathway pw

1.2. Decision Variables

All decision variables are non-negative, unless stated otherwise.

1.2.1. Planning Variables

$K^{pt,new}_{n,y}$: New capacity of production technology pt added at node n in year y

$K^{s,pw,new}_{n,y}$: New capacity of unextended stage s of pathway pw added at node n in year y

$K^{s,pw,new}_{l,y}$: New capacity of extended stage s of pathway pw added at link l in year y

$K^{stor,s,pw,new}_{n,y}$: New capacity of storage at unextended stage s of pathway pw added at node n in year y

1.2.2. Operations Variables

$p^{pt}_{n,t,y}$: Total hydrogen produced by production technology pt at node n in time-period t in year y

$f^{s,pw}_{n,t,y}$: Total hydrogen flowing through stage s of pathway pw at node n in time – period t in year y

$f^{stor_{in},s,pw}_{n,t,y}$: Total hydrogen flowing into storage at stage s of pathway pw at node n in time – period t in year y

$f^{stor_{out},s,pw}_{n,t,y}$: Total hydrogen flowing out of storage at stage s of pathway pw at node n in time – period t in year y

$x^{stor,s,pw}_{n,t,y}$: Total hydrogen stored at at stage s of pathway pw at node n in time – period t in year y

$f^{s,pw}_{l,n\rightarrow n_l',t,y}$: Total hydrogen flowing from node n across link l at stage s of pathway pw in time – period t in year y

$f^{s,pw}_{l,n_l'\rightarrow n,t,y}$: Total hydrogen flowing into node n across link l at stage s of pathway pw in time – period t in year y

$f^{stor_{in},s,pw}_{l,n\rightarrow n_l',t,y}$: Total hydrogen flowing into storage in extended stage s of pathway pw across link l in time-period t in year y

$f^{stor_{out},s,pw}_{l,n\rightarrow n_l',t,y}$: Total hydrogen flowing out of storage in extended stage s of pathway pw across link l in time-period t in year y

$x^{stor,s,pw}_{l,n\rightarrow n_l',t,y}$: Total hydrogen stored in extended stage s of pathway pw across link l in time-period t in year y

1.3. Parameters

$IC^{stor,s,pw}$: Investment cost of storage at un-extended stage s of pathway pw ($/kg)
FC^{pt}: Annual fixed cost of production technology pt ($/kg)
$FC^{s,pw}$: Annual fixed cost of un-extended stage s of pathway pw ($/kg)
$FC^{stor,s,pw}$: Annual fixed cost of storage at un-extended stage s of pathway pw ($/kg)
$FC^{l,s,pw}$: Annual fixed cost of extended stage s of pathway pw across link l ($/kg)

IC^{pt}: Investment cost of production technology pt($/kg)

$IC^{s,pw}$:Investment cost of stage s of pathway pw ($/kg)

$IC^{l,s,pw}$: Investment cost of extended stage s of pathway pw across link l($/kg)

OC^{pt}: Operating cost of hydrogen production technology pt ($/kg)

$OC^{f,s,pw}$: Operating cost of hydrogen owing through unextended stage s of pathway pw ($/kg)

$OC^{stor_{in},s,pw}$: Operating cost of hydrogen sent to storage at unextended stage s of pathway pw ($/kg)

$OC^{stor_{out},s,pw}$: Operating cost of hydrogen withdrawn from storage at unextended stage s of pathway pw ($/kg)

$OC^{l,s,pw}$: Operating cost of hydrogen owing across link l through extended stage s of pathway pw ($/kg)

$D_{n,t,y}$: Total hydrogen demand at node n in time-period t in year y (kg)

$Y^{s,pw}$: Hydrogen yield across stage s of pathway pw

$K^{pt,grid_{req}}_{n,y}$: Production capacity requirement determined by the grid model for production technology pt, at node n, in year t.

$K^{stor,grid_{req}}_{y}$: Total system wide H_2 storage capacity requirement determined by the grid model for year t.

α^{clean}_{y} : Fraction of total H_2 demand in year y to be satisfied by clean production technologies.

K^{pt}_{max}: Maximum annual capacity addition limit for production technology pt

$K^{s,pw}_{max}$: Maximum annual capacity addition limit for stage s of pathway pw

$K^{stors,pw}_{max}$: Maximum annual storage capacity addition limit for un-extended stage s of pathway pw

β^{pt}_{min}: Minimum utilization factor for production technology pt

$\beta^{s,pw}_{min}$: Minimum utilization factor for stage s of pathway pw

r: Discount Rate

2. Formulation

2.1. Objective function

Minimize the total investment and operating costs of producing and storing hydrogen and transporting it across the pathways to demand nodes. This is a NPV based cost minimization.

$$\text{Min} \sum_{y\epsilon Y}\left(\frac{1}{1+r}\right)^{y}(I+F+O) \quad (1)$$

where,

$$I = \sum_{n\epsilon N}\left(\sum_{pt\epsilon PT} IC^{pt}K^{pt,\,new}_{n,y} + \sum_{pw\epsilon PW}\sum_{s\epsilon S^{unext}_{pw}}\left(IC^{s,pw}K^{s,pw,\,new}_{n,y} + IC^{stor,s,pw}K^{stor,s,pw,\,new}_{n,y}\right)\right) + \sum$$

$$F = \sum_{n\epsilon N}\left(\sum_{pt\epsilon PT} FC^{pt}K^{pt}_{n,y} + \sum_{pw\epsilon PW}\sum_{s\epsilon S^{unext}_{pw}} \left(FC^{s,pw}K^{s,pw}_{n,y} + FC^{stor,s,pw}K^{stor,s,pw}_{n,y}\right)\right) + \sum_{l\epsilon L}\sum_{pw\epsilon PW}\sum_{s\epsilon S^{ext}_{pw}} FC^{l,s,pw}K^{s,pw}_{l,y}$$

$$O$$

$$= \sum_{n\epsilon N}\sum_{t\epsilon T}\left(\sum_{pt\epsilon PT} OC^{pt}_{n,y,t}p^{pt}_{n,y,t} + \sum_{pw\epsilon PW}\left(\sum_{s\epsilon S^{unext}_{pw}}\left(OC^{s,pw}_{n,y,t}f^{s,pw}_{n,y,t} + OC^{stor_{in},pw}_{n,y,t} f^{stor_{in},s,pw}_{n,y,t} + OC^{s}\right.\right.\right.$$

2.2. Constraints

- Sum of H2 flowing through the first stage of all pathways at node n should be equal to the total H2 production at node n:

$$\sum_{pw\epsilon PW} f^{1,pw}_{n,t,y} = \sum_{pw\epsilon PW} p^{pt}_{n,t,y}, \quad \forall n, \forall t, \forall y \qquad (2)$$

- Hydrogen balance at un-extended stages which are not the last stage of the pathway

$$Y^{s,pw} f^{s,pw}_{n,t,y} + f^{stor_{out},s,pw}_{n,t,y} - f^{stor_{in},s,pw}_{n,t,y} = f^{s+1,pw}_{n,t,y}, \quad \forall pw, \forall s \in S^{unext}_{pw} \mid s \neq last, \forall n, \forall t, \forall y \qquad (3)$$

- Hydrogen storage evolution at un-extended stages:

$$x^{stor,s,pw}_{n,t,y} = x^{stor,s,pw}_{n,t-1,y} + f^{stor_{in},s,pw}_{n,t,y} - f^{stor_{out},s,pw}_{n,t,y}, \quad \forall pw, \forall s \in S^{unext}_{pw}, \forall n, \forall t, \forall y \qquad (4)$$

- Hydrogen balance at extended stages:

$$f^{s,pw}_{n,t,y} + \sum_{l\epsilon L_n}\left(Y^{s,pw} f^{s,pw}_{l,n\to n_l,t,y} - f^{s,pw}_{l,n_l\to n t,y} + f^{stor_{out},s,pw}_{l,n_l\to n,t,y} - f^{stor_{in},s,pw}_{l,n_l\to n,t,y}\right) = f^{s,pw}_{n,t,y}, \ \forall pw, \forall s\epsilon S^{pw}_{ext}, \forall n, \forall t, \forall y$$

(5)

- Hydrogen storage evolution at extended stages:

$$x^{stor,s,pw}_{l,n\to n_l,t,y} = x^{stor,s,pw}_{l,n\to n_l,t-1,y} + f^{stor_{in},s,pw}_{l,n\to n_l,t,y} - f^{stor_{out},s,pw}_{l,n\to n_l,t,y}, \ \forall l, \forall pw, \forall s\epsilon S^{pw}_{ext}, \forall n, \forall t, \forall y \qquad (6)$$

- Sum of net hydrogen flowing through the last stage of all pathways at node n should be equal to the total H2 demand at node n:

$$D_{n,t,y} = \sum_{pw \in PW}\left(Y^{last,pw} f^{last,pw}_{n,t,y} + f^{stor_{out},last,pw}_{n,t,y} - f^{stor_{in},last,pw}_{n,t,y}\right), \quad \forall n, \forall t, \forall y \qquad (7)$$

- Hydrogen production capacity limits:

$$p^{pt}_{n,t,y} \leq K^{pt}_{n,y} \quad \forall pt, \forall n,\ \forall t,\ \forall y \qquad (8)$$

- Hydrogen un-extended stage flow limits:

$$f^{s,pw}_{n,t,y} \leq K^{s,pw}_{n,y} \ ,\ \ \forall pw,\ \forall s \in S^{unext}_{pw}\ ,\ \forall n, \forall t, \forall y \qquad (9)$$

- Hydrogen un-extended stage storage limits:
-

$$x^{stor,s,pw}_{n,t,y} \leq K^{stor,s,pw}_{n,y}, \forall pw, \forall s \epsilon S^{unext}_{pw}, \forall n, \forall t, \forall y \qquad (10)$$

- Hydrogen extended stage storage limits:

$$x^{stor,s,pw}_{n,t,y} \leq K^{stor,s,pw}_{n,y}, \forall pw, \forall s \epsilon S^{ext}_{pw}, \forall n, \forall t, \forall y \qquad (11)$$

- Hydrogen extended stage flow limits

$$f^{s,pw}_{l,n \rightarrow n'_l,t,y} \leq K^{s,pw}_{l,y} \qquad \forall l,\ \forall pw, \forall s \in\ S^{ext}_{pw}\ , \forall n, \forall t, \forall y \qquad (12)$$

- Total production capacity evolution:

$$K^{pt}_{n,y} = K^{pt}_{n,y-1} + K^{pt,new}_{n,y} \quad \forall pt, \forall n,\ \forall t,\ \forall y \qquad (13)$$

- Total un-extended stage capacity evolution:

$$K^{s,pw}_{n,y} = K^{s,pw}_{n,y-1} + K^{s,pw,new}_{n,y}\ ,\ \ \forall pw,\ \forall s \in S^{unext}_{pw}\ ,\ \forall n, \forall t, \forall y \qquad (14)$$

- Total extended stage capacity evolution:

$$K^{s,pw}_{l,y} = K^{s,pw}_{l,y-1} + K^{s,pw,new}_{l,y} \quad \forall l,\ \forall pw, \forall s \in\ S^{ext}_{pw}\ , \forall n, \forall t, \forall y \qquad (15)$$

- Total un-extended stage storage capacity evolution:

$$K^{stor,s,pw}_{n,y} = K^{stor,s,pw}_{n,y-1} + K^{stor,s,pw,\ new}_{n,y} \qquad (16)$$

- Total extended stage storage capacity: There is a max cap on the amount of hydrogen storage possible for a given length of pipeline

$$K^{stor,s,pw}_{l,y} = f\left(K^{s,pw}_{l,y}\right) \qquad (17)$$

Where f is a polynomial function of the installed extended stage capacity.

Grid connected constraints

- Nodal Production Capacity Constraint: may be turned off or on depending on the scenario

$$K^{pt}_{n,y} \geq K^{pt,grid_{req}}_{n,y}, \forall n, \forall pt, \forall y \qquad (18)$$

- System-wide Storage Capacity Constraint: may be turned off or on depending on the scenario
-

$$\sum_{n\epsilon N}\sum_{pw\epsilon PW}\sum_{s\epsilon S_{pw}^{unext}} K_{n,y}^{stor,s,pw} + \sum_{l\epsilon L}\sum_{pw\epsilon PW}\sum_{s\epsilon S_{pw}^{ext}} K_{l,y}^{stor,s,pw} \geq K_{y}^{stor,\, grid_{req}}, \forall y \quad (19)$$

Renewable hydrogen policy constraint

$$\sum_{n\epsilon N}\sum_{pt\epsilon PT_{clean}}\sum_{t\epsilon T} p_{n,t,y}^{pt} \geq \alpha_{y}^{clean}\sum_{n\epsilon N}\sum_{t\epsilon T} D_{n,t,y}, \forall y \quad (20)$$

Onsite Production Constraints:

$$\sum_{pt\epsilon PT_{onsite}} p_{n,t,y}^{pt} \leq D_{n,t,y}, \quad \forall n, \forall t, \forall y \quad (21)$$