Supplementary: Multiperiod Multiscale Modeling and Optimization of Hydrogen-based Dense Energy Carrier Supply Chains

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S 1 Multi-scale model formulation

S 1.1 Sets

$\mathcal{I}$	all processes (i)
$\mathcal{J}$	all resources (j)
$\mathcal{A}$	all locations (a)
$\mathcal{Y}$	years (y) , $\{\underline{y}..\overline{y}\}$
$\mathcal{D}$	representative days (d), $\{\underline{d}..\overline{d}\}$
$\mathcal{H}$	hours (h), $\{\underline{h}..\overline{h}\}$
$\mathcal{S}$	cost scenarios (s), $\{$*conservative*, *moderate*, *advanced*$\}$

S 1.2 Subsets

$\{\mathcal{I}_y\}_{y\in\mathcal{Y},a\in\mathcal{A}}$	processes (i) available in year (y) at location (a)
$\{\mathcal{J}_y\}_{y\in\mathcal{Y},a\in\mathcal{A}}$	resources (j) available in year (y)
$\mathcal{I}_{cc}$	processes (i) earning carbon credits
$\mathcal{J}_{sell}$	marketable resources (j)
$\mathcal{J}_{nosell}$	resources (j) that cannot be discharged
$\mathcal{J}_{store}$	resources (j) that can be stored
$\mathcal{J}_{nostore}$	resources (j) that cannot be stored
$\mathcal{J}_{H_2-demand}$	resources (j) that meet the H_2 demand
$\mathcal{J}_{mile-demand}$	resources (j) that meet mileage demand

S 1.3 Variables

S 1.3.1 Binary

$x^{P}_{a,i\in\mathcal{I},y\in\mathcal{Y}}$	1 if process is built, 0 otherwise
x^{S}	1 if storage facility is built, 0 otherwise

S 1.3.2 Annual location level: $y \in Y, a \in A$

$opex^{fix-total}$	total fixed operational expenditure (\$/year)
$opex^{var-total}$	total variable operational expenditure (\$/year)
$opex^{total}$	total operational expenditure (\$/year)
$capex^{total}$	total capital expenditure (\$/year)
$credit^{total}$	total credits earned (\$/year)
$cost^{total}$	total expenditure (\$/year)
b^{total}	total expenditure on purchase of resources (\$/year)
gwp^{total}	total annualized global warming potential ($kg.CO_2eq$/year)
$land^{total}$	total land use (acres/year)
$emission^{total}$	total carbon emitted ($kg.CO_2eq$/year)
$miles^{total}$	total mileage provided by all fuel sources (miles/year)

S 1.3.3 Annual production facility level: $i \in I, y \in Y, a \in A$

$opex^{fix}$	fixed operational expenditure of process (\$/year)
$opex^{var}$	variable operational expenditure of process (\$/year)
$capex$	capital expenditure of process (\$/year)
$opex$	total operational expenditure of process (\$/year)

$credit$	annual carbon credits earned by process (\$/year)
p^{annual}	annual production by process (unit/year)
cap^P	production capacity of process (unit/year)
gwp	global warming potential of process ($kg.CO_2eq$/year)
$land$	land use by process (acres/year)

S 1.3.4 Annual storage facility level: $j \in J, y \in Y, a \in A$

b^{annual}	annual expenditure on purchase of resource (\$/year)
s^{annual}	annual sale of resource (unit/year)
c^{annual}	annual sale of resource (unit/year)
cap^S	capacity of storage facility (unit/year)
$miles^{annual}$	annual miles provided by fuel source (miles/year)

S 1.3.5 Hourly inventory and resource scheduling: $j \in J, h \in H, D \in D, y \in Y, a \in A$

c	resource consumed (unit/hour)
s	resource sold (unit/hour)
inv	inventory level of storage facility (unit/hour)

S 1.3.6 Hourly production scheduling: $i \in I, h \in H, D \in D, y \in Y, a \in A$

p	production by process (unit/hour)

S 1.4 Parameters

$Opex^{fix}_{s\in\mathcal{S},i\in\mathcal{I},y\in\mathcal{Y}}$	fixed operating cost for process
$Opex^{var}_{s\in\mathcal{S},i\in\mathcal{I},y\in\mathcal{Y}}$	variable operating cost for process
$Capex_{s\in\mathcal{S},i\in\mathcal{I},y\in\mathcal{Y}}$	capital cost for process
$Opex^{fix}_{s\in\mathcal{S},i\in\mathcal{I},y\in\mathcal{Y}}$	fixed operating cost of unit
$\nabla Cap^{P-max}_{a\in\mathcal{A},i\in\mathcal{I},y\in\mathcal{Y}}$	maximum production capacity increase allowed
$\nabla Cap^{P-min}_{a\in\mathcal{A},i\in\mathcal{I},y\in\mathcal{Y}}$	minimum production capacity increase allowed
$\nabla Cap^{S-max}_{a\in\mathcal{A},j\in\mathcal{J},y\in\mathcal{Y}}$	maximum storage capacity increase allowed
$\nabla Cap^{S-min}_{a\in\mathcal{A},j\in\mathcal{J},y\in\mathcal{Y}}$	minimum storage capacity increase allowed
$C^{max}_{a\in\mathcal{A},j\in\mathcal{J},h\in\mathcal{H},d\in\mathcal{D},y\in\mathcal{Y}}$	maximum resource availability
$Loss^{store}_{j\in\mathcal{J}}$	storage losses
$Credit_{p\in\mathcal{P},i\in\mathcal{I}}$	credit provided for process in planning period
$Cost^{purchase}_{a\in\mathcal{A},j\in\mathcal{J}}$	purchase cost of resource
$Mileage_{j\in\mathcal{J}}$	mileage provided by resource
$Demand$	daily demand for product
A^f	annualization factor
$Cap^f_{a\in\mathcal{A},i\in\mathcal{I},d\in\mathcal{D},h\in\mathcal{H},y\in\mathcal{Y}}$	capacity utilization factor
$\eta_{a,i\in\mathcal{I},j\in\mathcal{J}}$	conversion factor
$wt_{d\in\mathcal{D}}$	weight of each cluster

S 2 Constraints

S 2.1 Network design

The network design constraints resolve the capacity sizing for both production and storage facilities. The binary variables provide decisions on whether a facility is located.

S 2.1.1 Production capacity sizing

There is a minimum capacity enforced to set up production units. The minimum capacity for modular technologies, such as AWE and Li-ion batteries, is lower compared to SMR and PSH.

$$\nabla Cap^{P-min}_{a,i,y} \cdot x^P_{a,i,y} \leq cap^P_{a,i,y} \leq \nabla Cap^{P-max}_{a,i,y} \cdot x^P_{a,i,y} \tag{1}$$

$$\forall\ a \in \mathcal{A}, i \in \mathcal{I}_y, y \in \{\underline{y}\}$$

$$\nabla Cap^{P-min}_{a,i,y} \cdot x^P_{a,i,y} \leq cap^P_{a,i,y} - cap^P_{a,i,y-1} \leq \nabla Cap^{P-max}_{a,i,y} \cdot x^P_{a,i,y} \tag{2}$$

$$\forall\ a \in \mathcal{A}, i \in \mathcal{I}_y, y \in \mathcal{Y} \setminus \{\underline{y}\}$$

S 2.1.2 Production capacity expansion

These constraints restrict the maximum capacity that can be increased in a particular year while also ensuring that the capacities do not decrease as compared to previous years.

S 2.1.3 Storage capacity sizing

The storage capacity and facility location decisions are determined using these constraints.

$$\nabla Cap^{S-min}_{a,j,y} \cdot x^S_{a,j,y} \leq cap^S_{a,j,y} \leq \nabla Cap^{S-max}_{a,j,y} \cdot x^S_{a,j,y} \tag{3}$$

$$\forall\ a \in \mathcal{A}, j \in \mathcal{J}_p, y \in \{\underline{y}\}$$

$$\nabla Cap^{S-min}_{a,j,y} \cdot x^S_{a,j,y} \leq cap^S_{a,j,y} - cap^S_{a,j,y-1} \leq \nabla Cap^{S-max}_{a,j,y} \cdot x^S_{a,j,y} \tag{4}$$

$$\forall\ a \in \mathcal{A}, j \in \mathcal{J}_p, y \in \mathcal{Y} \setminus \{\underline{y}\}$$

S 2.2 Resource balance

These constraints determine the flow of resources through the network and provide optimal scheduling decisions. Scheduling decisions are determined at a finer temporal scale (hours). Nonetheless, the resource balance utilizes the network decision made at longer temporal resolutions (years) from constraints 2 and 4

S 2.2.1 Nameplate production capacity

The realized production rates for each hour are determined using the following constraints. To account for the intermittent availability of solar and wind, the solar DNI and wind speed power outputs are normalized to generated capacity utilization factors.

$$p_{a,i,h,d,y} \leq Cap^f_{a,i,d,h,y} \cdot cap^P_{a,i,y} \tag{5}$$

$$\forall\ a \in \mathcal{A}, i \in \mathcal{I}_y, h \in \mathcal{H}, d \in \mathcal{D}, y \in \mathcal{Y}$$

S 2.2.2 Nameplate storage capacity

The inventory levels at every hour are restricted to the nameplate storage capacity using the following constraints.

$$inv_{a,j,h,d,y} \leq cap^S_{a,j,y} \tag{6}$$

$$\forall\, a \in \mathcal{A}, j \in \mathcal{J}_y, h \in \mathcal{H}, d \in \mathcal{D}, y \in \mathcal{Y}$$

S 2.2.3 Resource consumption capacity

These constraints restrict the amount of resource that can be consumed.

$$c_{a,j,h,d,y} \leq C^{max}_{a,j,h,d,y} \tag{7}$$

$$\forall\, a \in \mathcal{A}, j \in \mathcal{J}_p, h \in \mathcal{H}, d \in \mathcal{D}, y \in \mathcal{Y}$$

S 2.2.4 Inventory balance

The inventory balance constraints 8, 9, 10, 11 are applied over exhaustive subsets of the planning horizon to determine both the resource flow through the network, and account for inventory cycling.

Start-up inventory balance

This constraint is only applied to the first hour of the planning horizon. The starting inventory levels are assumed to be zero.

$$inv_{a,j,h,d,y} \leq \sum_{\forall i \in \mathcal{I}_p} \eta_{i,j} \cdot p_{a,i,h,d,y} + c_{a,j,h,d,p} - s_{a,j,h,d,y} \tag{8}$$

$$\forall\, a \in \mathcal{A}, j \in \mathcal{J}_p, h \in \{\underline{h}\}, d \in \{\underline{d}\}, y \in \{\underline{y}\}$$

Daily start-up inventory balance

The inventory at the start of the day is determined using the following constraints. The inventory from the previous day is cycled.

$$inv_{a,j,h,d,y} \leq (1 - Loss_j) \cdot inv_{a,j,h',d-1,y} + \sum_{\forall i \in \mathcal{I}_p} \eta_{i,j} \cdot p_{a,i,h,d,y} + c_{a,j,h,d,p} - s_{a,j,h,d,y} \tag{9}$$

$$\forall\, a \in \mathcal{A}, j \in \mathcal{J}_p, h \in \{\underline{h}\}, h' \in \{\overline{h}\}, d \in \mathcal{D} \setminus \{\underline{d}\}, y \in \mathcal{Y}$$

Annual start-up inventory balance

The inventory at the start of the year is evaluated by the following constraints wherin the inventory from the end of the previous year is cycled.

$$inv_{a,j,h,d,y} \leq (1 - Loss_j) \cdot inv_{a,j,h',d',y-1} + \sum_{\forall i \in \mathcal{I}_p} \eta_{i,j} \cdot p_{a,i,h,d,y} + c_{a,j,h,d,p} - s_{a,j,h,d,y} \tag{10}$$

$$\forall\, a \in \mathcal{A}, j \in \mathcal{J}_p, h \in \{\underline{h}\}, h' \in \{\overline{h}\}, d \in \{\underline{d}\}, d' \in \{\overline{d}\}, y \in \mathcal{Y} \setminus \{\underline{y}\}$$

General inventory balance

Thee following constraints provide the inventory balance for the rest of the planning horizon.

$$inv_{a,j,h,d,y} = (1 - Loss_j) \cdot inv_{a,j,h-1,d,y} + \sum_{\forall i \in \mathcal{I}_p} \eta_{i,j} \cdot p_{a,i,h,d,y} + c_{a,j,h,d,p} - s_{a,i,h,d,y} \tag{11}$$

$$\forall\, a \in \mathcal{A}, j \in \mathcal{J}_p, h \in \mathcal{H} \setminus \{\underline{h}\}, d \in \mathcal{D} \setminus \{\underline{d}\}, y \in \mathcal{Y}$$

S 2.2.5 Demand constraints

The demand constraints 12 ensure that the daily demand for hydrogen is satisfied. 13 meet an equivalent mileage. Should be noted that these constraints are applied as a part of separate case studies.

Hydrogen demand

$$\sum_{\forall h \in \mathcal{H}} s_{a,j,h,d,y} = Demand_{a,j,d,y} \tag{12}$$

$$\forall\ a \in \mathcal{A}, j \in \mathcal{J}_{H_2-demand} \cap \mathcal{J}_p, d \in \mathcal{D}\, y \in \mathcal{Y}$$

Equivalent miles demand

$$\sum_{\forall h \in \mathcal{H}} s_{a,j,h,d,y} = Demand_{a,j,d,y} \cdot Mileage(H_2) \tag{13}$$

$$\forall\ a \in \mathcal{A}, j \in \mathcal{J}_{miles-demand} \cap \mathcal{J}_p, d \in \mathcal{D}\, y \in \mathcal{Y}$$

S 2.2.6 No selling constraints

These constraints ensure that resources that cannot be discharged are not sold.

$$s_{a,j,h,d,y} = 0 \tag{14}$$

$$\forall\ a \in \mathcal{A}, j \in \mathcal{J}_{nosell} \cap \mathcal{J}_p, h \in \mathcal{H}, d \in \mathcal{D}, y \in \mathcal{Y}$$

S 2.3 Annual resource utilization constraints

The constraints 15, 16 calculate the annual sale, consumption of resources, respectively. The obtained values are multiplied by the cluster weights (wt_d) to adjust the values to the annual scale.

Annual sales

$$s^{annual}_{a,j,y} = \sum_{\forall d \in \mathcal{D}} \sum_{\forall h \in \mathcal{H}} wt_d \cdot s_{a,j,h,d,y} \tag{15}$$

$$\forall\ a \in \mathcal{A}, j \in \mathcal{J}_p, y \in \mathcal{Y}$$

Annual consumption

$$c^{annual}_{a,j,y} = \sum_{\forall d \in \mathcal{D}} \sum_{\forall h \in \mathcal{H}} wt_d \cdot c_{a,j,h,d,y} \tag{16}$$

$$\forall\, a \in \mathcal{A}, j \in \mathcal{J}_p, y \in \mathcal{Y}$$

S 2.4 Annual production

Constraints 17 calculate the re-scaled production on nominal basis for all production facilities. Consequently, the variable operational expenditure is calculated for the re-scaled output.

$$p^{annual}_{a,i,y} = \sum_{\forall d \in \mathcal{D}} \sum_{\forall h \in \mathcal{H}} wt_d \cdot p_{a,i,h,d,y} \tag{17}$$

$$\forall\, a \in \mathcal{A}, i \in \mathcal{I}_p, y \in \mathcal{Y}$$

S 2.5 Annual production cost

We consider three costing components. Variable operational and maintenance (O&M) which are calculated based on the amount of basis resource produced by a process (18). Whereas, annualized capital expenditure(21), and fixed (O&M) costs (19) are evaluated based on the capacity sizing of the processes. Moreover, we can consider three distinct cost scenarios $s \in \mathcal{S}$

S 2.5.1 Variable O&M expenditure

$$opex^{var}_{a,i,y} = Opex^{var}_{s,i,y} \cdot p^{annual}_{a,i,y} \tag{18}$$

$$\forall\, a \in \mathcal{A}, i \in \mathcal{I}_p, y \in \mathcal{Y}$$

S 2.5.2 Fixed O&M expenditure

$$opex^{fix}_{a,i,y} = Opex^{fix}_{s,i,y} \cdot cap^{P}_{a,i,y} \tag{19}$$

$$\forall\ a \in \mathcal{A}, i \in \mathcal{I}_p, y \in \mathcal{Y}$$

S 2.5.3 O&M expenditure

$$opex_{a,i,y} = opex^{fix}_{a,i,y} + opex^{var}_{a,i,y} \tag{20}$$

$$\forall\ a \in \mathcal{A}, i \in \mathcal{I}_p, y \in \mathcal{Y}$$

S 2.5.4 Capital expenditure

$$capex_{a,i,y} = \alpha^{f} \cdot Capex_{s,i,y} \cdot cap^{P}_{a,i,y} \tag{21}$$

$$\forall\ i \in \mathcal{I}_p, y \in \mathcal{Y}$$

S 2.6 System production cost

The cost to the entire system, as the sum of expenditure of individual process units, is calculated using the following constraints.

S 2.6.1 Total variable O&M expenditure

$$opex^{var-total}_{y} = \sum_{\forall i \in \mathcal{I}_p} opex^{var}_{a,i,y} \tag{22}$$

$$\forall\ y \in \mathcal{Y}$$

S 2.6.2 Total fixed O&M expenditure

$$opex^{fix-total}_{y} = \sum_{\forall i \in \mathcal{I}_p} opex^{fix}_{a,i,y} \tag{23}$$

$$\forall\ y \in \mathcal{Y}$$

S 2.6.3 Total O&M expenditure

$$opex_y^{total} = opex_y^{fix-total} + opex_y^{var-total} \tag{24}$$

$$\forall\, y \in \mathcal{Y}$$

S 2.6.4 Total capital expenditure

$$capex_y^{total} = \sum_{\forall i \in \mathcal{I}_p} capex_{a,i,y} \tag{25}$$

$$\forall\, y \in \mathcal{Y}$$

S 2.7 Carbon credits earned

Carbon credits are assigned as per the 45Q amendment (Jones and Sherlock, 2021) using the constraints 26. Furthermore, the total credits earned at the system level are calculated using 27. Here, it should be noted that planning periods $p \in \mathcal{P}$ have different credit rates.

S 2.7.1 Annual carbon credits

$$credit_{a,i,y} = Credit_{p,i,y} \cdot p_{a,i,y}^{annual} \tag{26}$$

$$\forall\, i \in \mathcal{I}_p, y \in \mathcal{Y}$$

S 2.7.2 System carbon credits

$$credit_y^{total} = \sum_{\forall i \in \mathcal{I}_p} credit_{p,i,y} \tag{27}$$

$$\forall\, y \in \mathcal{Y}$$

S 2.8 Resource purchase expenditure

The annual expenditure on resource purchase is evaluated using the constraints 28. The total system-wide expenditure on resource purchase is ascertained using 29

S 2.8.1 Annual purchase expenditure

$$b^{annual}_{a,j,y} = Cost^{purchase}_{p,i,y} \cdot c^{annual}_{a,i,y} \tag{28}$$

$$\forall\ i \in \mathcal{I}_p, y \in \mathcal{Y}$$

S 2.8.2 System purchase expenditure

$$b^{total}_{y} = \sum_{\forall j \in \mathcal{J}_p} b^{annual}_{a,j,y} \tag{29}$$

$$\forall\ y \in \mathcal{Y}$$

S 2.9 Mileage

The annual mileage achieved through the use of different fuel sources is determined using 30. The system total is given by 31

S 2.9.1 Annual mileage

$$miles^{annual}_{a,j,y} = Mileage_{a,j} \cdot s^{annual}_{a,j,y} \tag{30}$$

$$\forall\ j \in \mathcal{J}_{miles-demand} \cap \mathcal{J}_p, y \in \mathcal{Y}$$

S 2.9.2 System mileage

$$miles^{total}_{y} = \sum_{\forall j \in \mathcal{J}_{miles-demand} \cap \mathcal{J}_p} miles^{annual}_{a,j,y} \tag{31}$$

$$\forall\ y \in \mathcal{Y}$$

S 2.10 Objective

The objective of the model is to minimize the total cost incurred by the system. If the hydrogen demand is met, the objective value divided by the total hydrogen production indicates the levelized cost of hydrogen (LCOH). If the system is optimized to meet the mileage demand, then the objective value can be divided by the total mileage determined by constraints 31 to indicate levelized cost per mile travelled.

$$min\ \ cost_y^{total} = capex_y^{total} + opex_y^{total} + b_y^{total} - credit_y^{total} \tag{32}$$

$$\forall\, y \in \mathcal{Y}$$

S 2.11 Costing data

The sources for the costing data is summarized in table 1

Process	**Source**	**Notes**
Li-ion battery	(National Renewable Energy Laboratory, 2021)	8hr storage
Compressed air energy storage (CAES)	(Authority, 2017)	
Pumped storage hydropower (PSH)	(National Renewable Energy Laboratory, 2021)	Class 3
Solar photovoltaics (PV) array	(National Renewable Energy Laboratory, 2021)	Class 5
Wind mill array	(National Renewable Energy Laboratory, 2021)	Class 4
Alkaline water electrolysis	(Yates et al., 2020)	
Steam methane reforming (SMR)	(Parkinson et al., 2018)	90% capture
Hydrogen local storage (Liquefied)	(Papadias and Ahluwalia, 2021)	
Hydrogen geological storage	(Papadias and Ahluwalia, 2021)	
Direct air capture	(Fasihi et al., 2019; Keith et al., 2018)	
Enhanced oil recovery		
Offshore saline aquifer	(Global CCS Institute, 2010)	EU data
Catalytic methanol production	(Bellotti et al., 2017)	

Table 1: Sources for cost data

References

Authority, P. R. P., 2017: Battery energy storage technology assessment. *Platte River Power Authority: Fort Collins, CO, USA*.

Bellotti, D., M. Rivarolo, L. Magistri, and A. Massardo, 2017: Feasibility study of methanol production plant from hydrogen and captured carbon dioxide. *Journal of CO2 utilization*, **21**, 132–138.

Fasihi, M., O. Efimova, and C. Breyer, 2019: Techno-economic assessment of co2 direct air capture plants. *Journal of Cleaner Production*, **224**, 957–980, doi:10.1016/j.jclepro.2019.03.086, URL https://dx.doi.org/10.1016/j.jclepro.2019.03.086.

Global CCS Institute, 2010: The costs of co2 storage. URL https://www.globalccsinstitute.com/archive/hub/publications/119816/costs-co2-storage-post-demonstration-ccs-eu.pdf.

Jones, A. C., and M. F. Sherlock, 2021: The tax credit for carbon sequestration (section 45q). URL https://sgp.fas.org/crs/misc/IF11455.pdf.

Keith, D. W., G. Holmes, D. St. Angelo, and K. Heidel, 2018: A process for capturing co2 from the atmosphere. *Joule*, **2 (8)**, 1573–1594, doi:10.1016/j.joule.2018.05.006, URL https://dx.doi.org/10.1016/j.joule.2018.05.006.

National Renewable Energy Laboratory, 2021: National renewable energy laboratory: 2021 annual technology baseline. URL https://atb.nrel.gov/.

Papadias, D., and R. Ahluwalia, 2021: Bulk storage of hydrogen. *International Journal of Hydrogen Energy*, **46 (70)**, 34 527–34 541, doi:10.1016/j.ijhydene.2021.08.028.

Parkinson, B., M. Tabatabaei, D. C. Upham, B. Ballinger, C. Greig, S. Smart, and E. McFarland, 2018: Hydrogen production using methane: Techno-economics of decarbonizing fuels and chemicals. *International Journal of Hydrogen Energy*, **43 (5)**, 2540–2555.

Yates, J., R. Daiyan, R. Patterson, R. Egan, R. Amal, A. Ho-Baille, and N. L. Chang, 2020: Techno-economic analysis of hydrogen electrolysis from off-grid stand-alone photovoltaics incorporating uncertainty analysis. *Cell Reports Physical Science*, **1 (10)**, 100 209.