

Supplemental Information: Multi-Scale Design for Clean Energy Systems: Industrial Electrification and Flexible Operation of Ammonia Synthesis

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PARAMETERS & ASSUMPTIONS

The parametric assumptions for our analysis are explained here. In addition to this, all separations were assumed to be sharp splits, reactors and separators have linear behavior, and all gases and fluids are ideal.

Unit Operations

General equipment costing guidelines were adapted from [1, 2, 3]. All environmental costs associated with unit construction and decommissioning were assumed to be zero.

Table 1: Unit Costing Parameters

Unit Operation	Price (\$)	Reference	Scale Factor
Compressors & Turbines	1,000,000	1 MW	1
Expanders	1,000	1 kmol/hr	0.5
Electrolyzer	2,000,000	1 MW	1
Haber-Bosch Reactor	7,500,000	1 kmol/hr	0.5
Hydrogen Tank	550,000	1 m ³	0.75
Flash Column	10,000	1 kmol/hr	0.5
Air Separation Unit	3,000,000	1 kmol/hr	0.5
Heat Exchanger	70,000	1 MW	0.5
Pumps	100,000	1 MW	0.5
Photovoltaics	100 · 10 ⁶	1 km ²	1
Concentrating Solar	30 · 10 ⁶	1 km ²	1
Turbo-Generator	1,000,000	1 MW	1
Heat Storage	30,000	1 MWh	1
Batteries	200,000	1 MWh	1

Table 2: Unit Efficiency Parameters

Efficiency Parameters	Value
Compressor Efficiency	0.8
Turbine Efficiency	0.8
Pump Efficiency	0.8
Battery Efficiency (One-Way)	0.95
Heat Storage Efficiency (One-Way)	0.95
Heat to Electricity Efficiency	0.5
Electricity to Heat Efficiency	0.9
Light to Electricity Efficiency	0.3
Light to Heat Efficiency	0.4
Heating Efficiency	0.8
Cooling Efficiency	0.8
Nitrogen Conversion (Haber-Bosch)	0.3
Water Conversion (Electrolysis)	1

Unit operations have constraints which enforce mass balance, energy balance, thermodynamic relations, and operational flexibility. These constraints are outlined in [3]. The Haber-Bosch reactor has an operating temperature and pressure of 425 °C and 250 bar.

Net Present Value

Capital expenditure is amortized over the course of the horizon. The capital recovery factor (*CRF*) is calculated as follows.

$$CRF = \frac{\iota(\iota+1)^n}{(\iota+1)^n - 1} \quad (\text{SI.1})$$

Here ι is the annual interest rate (5%) and n is the investment lifetime (30 years). The initial capital investment (*CI*) is calculated as:

$$CI = \sum_{i \in \mathbf{I}} \rho_i \left(\frac{C_i}{\kappa_i} \right) \psi_i \quad (\text{SI.2})$$

Here, ρ_i is the price, κ_i is the reference capacity, C_i is the design capacity, and ψ_i is the scale factor for a unit i . The capital expenditure for a period (*CAPEX_p*) is then

$$CAPEX_p = \tau_p \cdot CRF \cdot CI \quad \forall p \in \mathbf{P} \quad (\text{SI.3})$$

where τ_p is the duration of a period (5-years). We then calculate the revenue (*RE_p*) generated from the sale of ammonia and the expenses (*EX_p*) due to electricity purchase and emissions penalties.

$$RE_p = C_{NH_3} \sum_{t \in T_p^P} \omega_t M_{t,NH_3} \quad \forall p \in \mathbf{P} \quad (\text{SI.4})$$

$$EX_p = \sum_{t \in T_p} \omega_t (\rho_t^{EL} + \rho_t^{CO2} \gamma_t) Q_{t,G} \quad \forall p \in \mathbf{P} \quad (\text{SI. 5})$$

Where C_{NH3} is the levelized cost of ammonia, $M_{t,NH3}$ is the ammonia produced, ρ_t^{EL} is the price of electricity, ρ_t^{CO2} is the emissions penalty (300 \$/ton), γ_t is grid emissions, $Q_{t,G}$ is the electricity purchased from the grid, and ω_t is the weight, at time t . Corporate taxes (TX_p) are accounted for using:

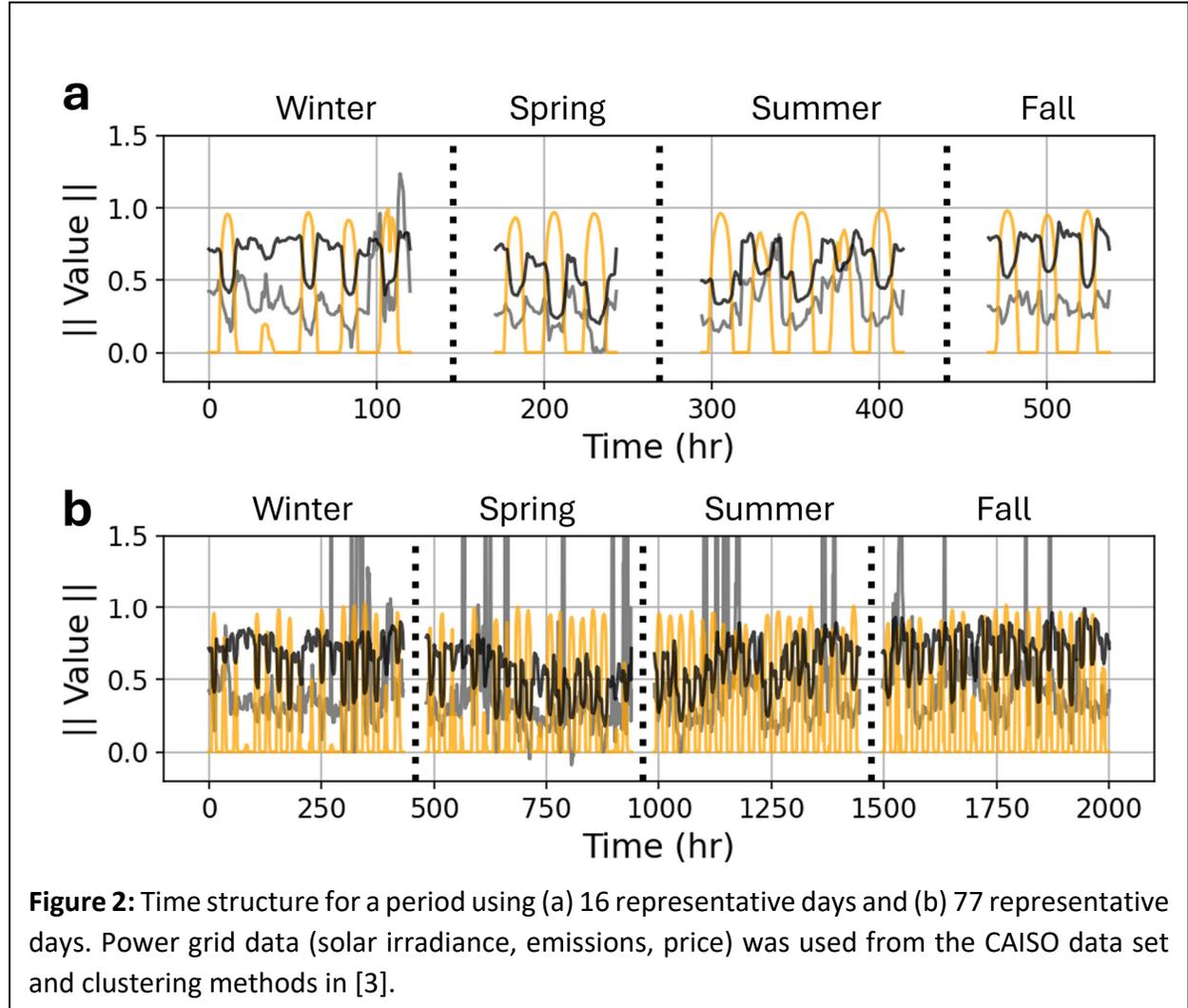
$$TX_p \geq \xi (RE_p - EX_p) \quad \forall p \in \mathbf{P} \quad (\text{SI. 6})$$

where ξ is the corporate tax rate (21%). Finally, we calculate the NPV as:

$$NPV = \sum_{p \in \mathbf{P}} \frac{1}{(1+\alpha)^p} (RE_p - EX_p - TX_p - CAPEX_p) \quad (\text{SI. 7})$$

where α is the discount rate (0.1).

Time Structure



REFERENCES

1. McCabe W, Smith J, Harriott P. Unit Operations of Chemical Engineering. McGraw-Hill Education. 2005.
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3. Kalamaris NN, Maravelias CT. A General optimization framework for designing chemical & energy systems subject to multi-scale Temporal Variability. *Comput. Chem. Eng.* 203:109315 (2025) <https://doi.org/10.1016/j.compchemeng.2025.109315>