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Green Chemical Engineering: Tackling Discontinuities for a More Sustainable Future

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Introduction to discontinuity

1. The Foundational Principles

Since the XIX century, **chemical processes** have been **designed to be continuous and operated under steady-state conditions**. Engineers are conventionally trained to pursue **stability** and consistency in process operations, as this approach facilitates control, optimization, and scale-up. **Steady-state processes are ideal, ensuring product quality, efficiency, and safety**.

"Nihil novi sub sole" (Ecclesiaste 1:9)

2. Advancements and Innovations

However, **the chemical industry gradually introduced intentionally discontinuous processes**, driven by **human intervention** and innovation. In addition to **Matros reactors** and simulated moving bed reactors (**SMBRs**), other examples of **anthropogenic discontinuities** include:

- Batch and semi-batch processes for specialty chemicals and pharmaceuticals
- Pressure swing adsorption (PSA) for gas separation and purification
- Periodic operation of reactors to enhance selectivity or suppress side reactions
- Pulsed flow in multiphase reactors to improve mass transfer and mixing

These **human-imposed discontinuities** showcased the potential advantages of deviating from the steady-state paradigm, such as **increased flexibility, improved performance, and reduced equipment size**.

3. Future Perspectives and Applications

In recent years, the growing adoption of **renewable energy sources**, like **solar, wind, and hydro/tidal power**, has introduced new **exogenous discontinuities to chemical processes**. The intermittent and variable nature of these energy sources has compelled chemical engineers to confront and adapt to **externally imposed fluctuations** in process conditions.

Moreover, the availability and **price volatility of raw materials** can also contribute to process discontinuities. **Economic factors and market dynamics** add another layer of complexity. Fluctuations in demand, changes in product specifications, and supply chain disruptions can all lead to process discontinuities.

The increasing emphasis on sustainability, circular economy principles, and carbon footprint reduction further drives the need for more flexible and adaptive processes.

Paradigm shift

The shift from steady-state to discontinuous processes represents a significant paradigm change in chemical engineering.

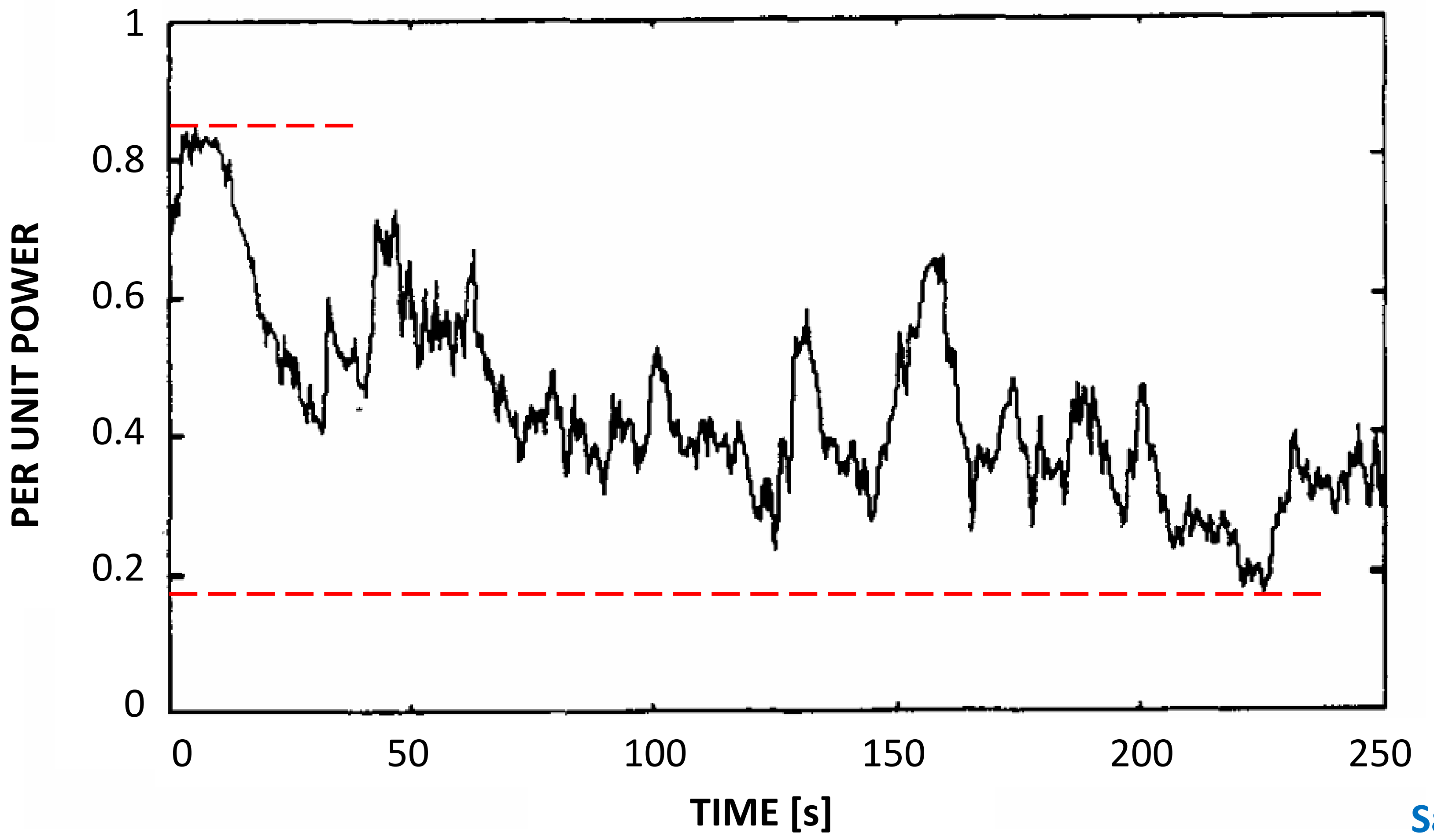
It necessitates a reassessment of core principles and the development of **new tools and strategies to manage variability**. This shift impacts not only process operation but also the **conceptual design of chemical plants**, as flexibility and resilience become critical design criteria.

By embracing the **challenges and opportunities presented by discontinuous processes**, the chemical industry can evolve and contribute to a **more sustainable, agile, and resilient future**.

This paradigm shift sparks new research and innovation, driving the development of more adaptive, environmentally friendly, and economically viable chemical processes.

Variability of wind energy production

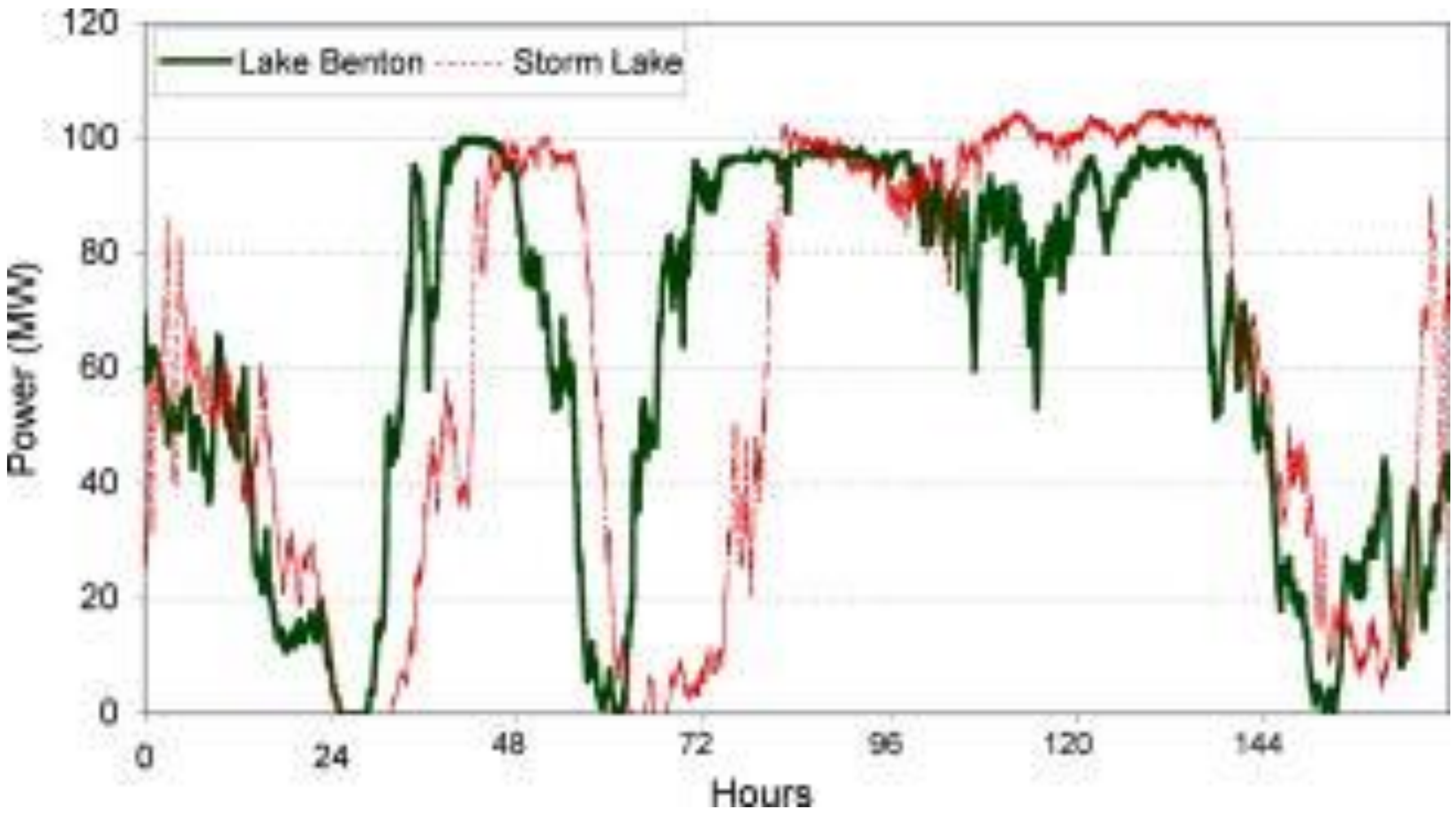
Wind power measurements [@ 1 Hz sampling]



San Francisco, USA

G. McNerney and R. Richardson, "The Statistical Smoothing of Power Delivered to Utilities by Multiple Wind Turbines", (1992).

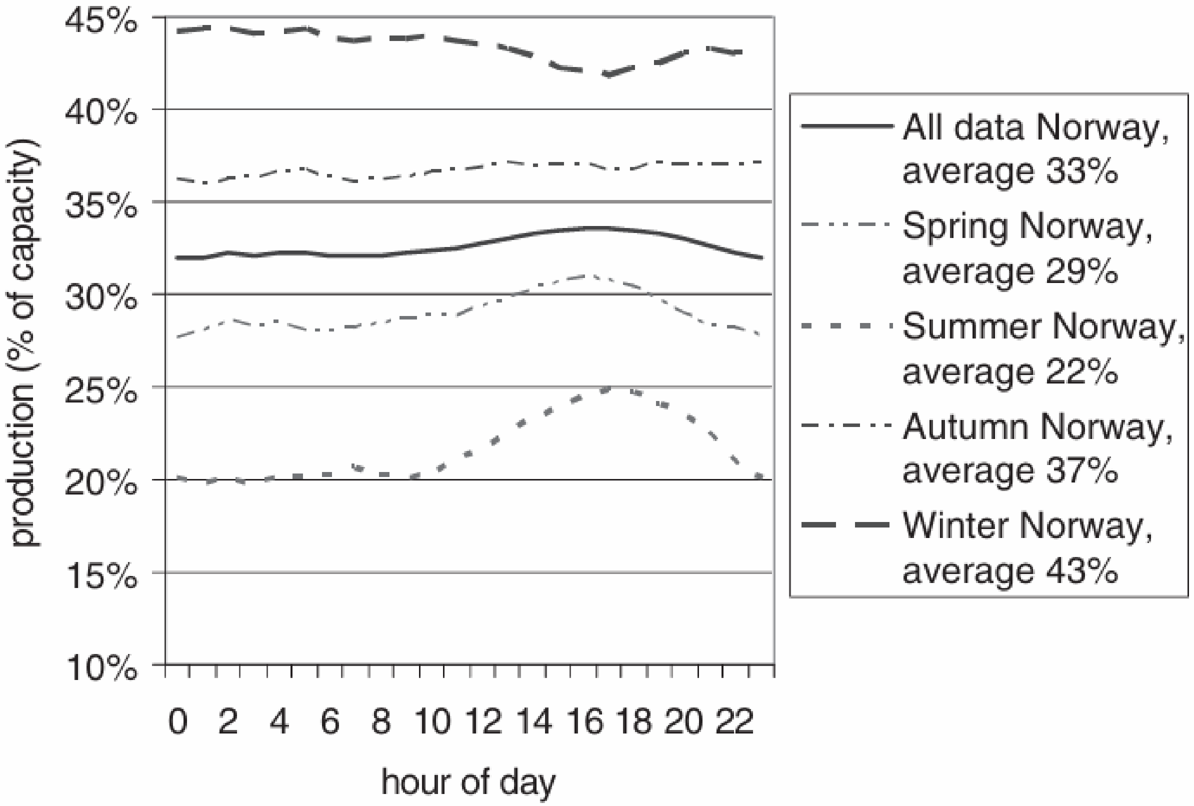
Wind production of two plants in the USA (200 km distance)



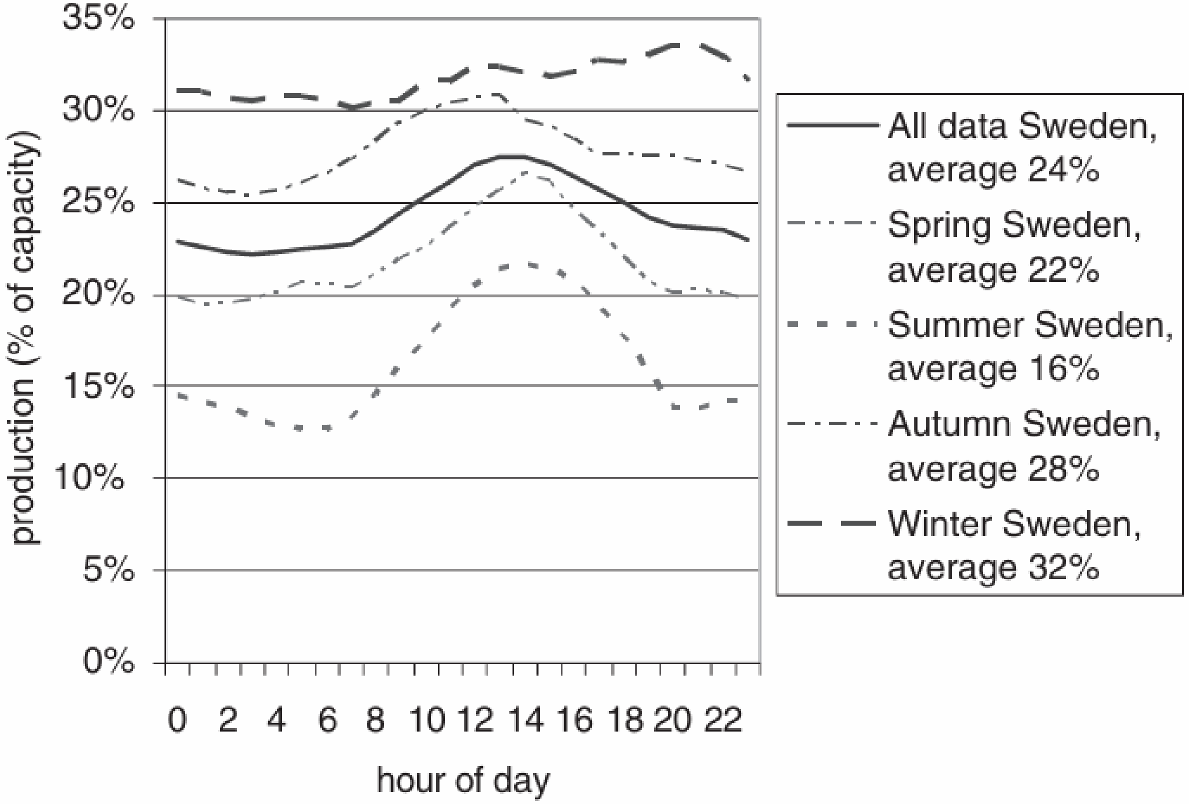
Y.H. Wan, M. Milligan, B. Parsons, “Output Power Correlation Between Adjacent Wind Power Plants”, J. Sol. Energy Eng, (2003).

Seasonal effect in wind production in Nordic Regions

NORWAY

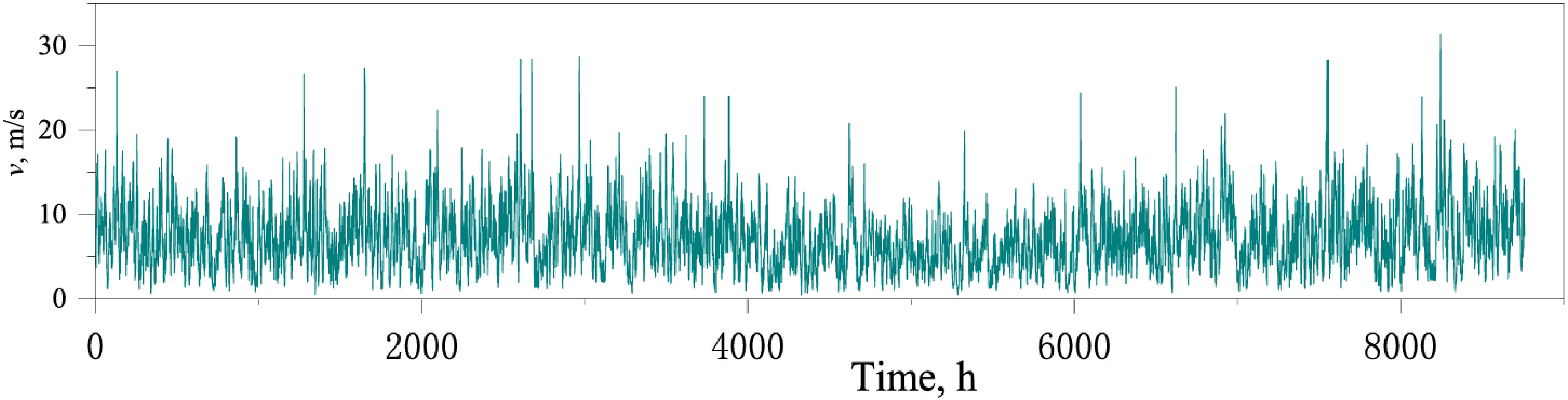


SWEDEN



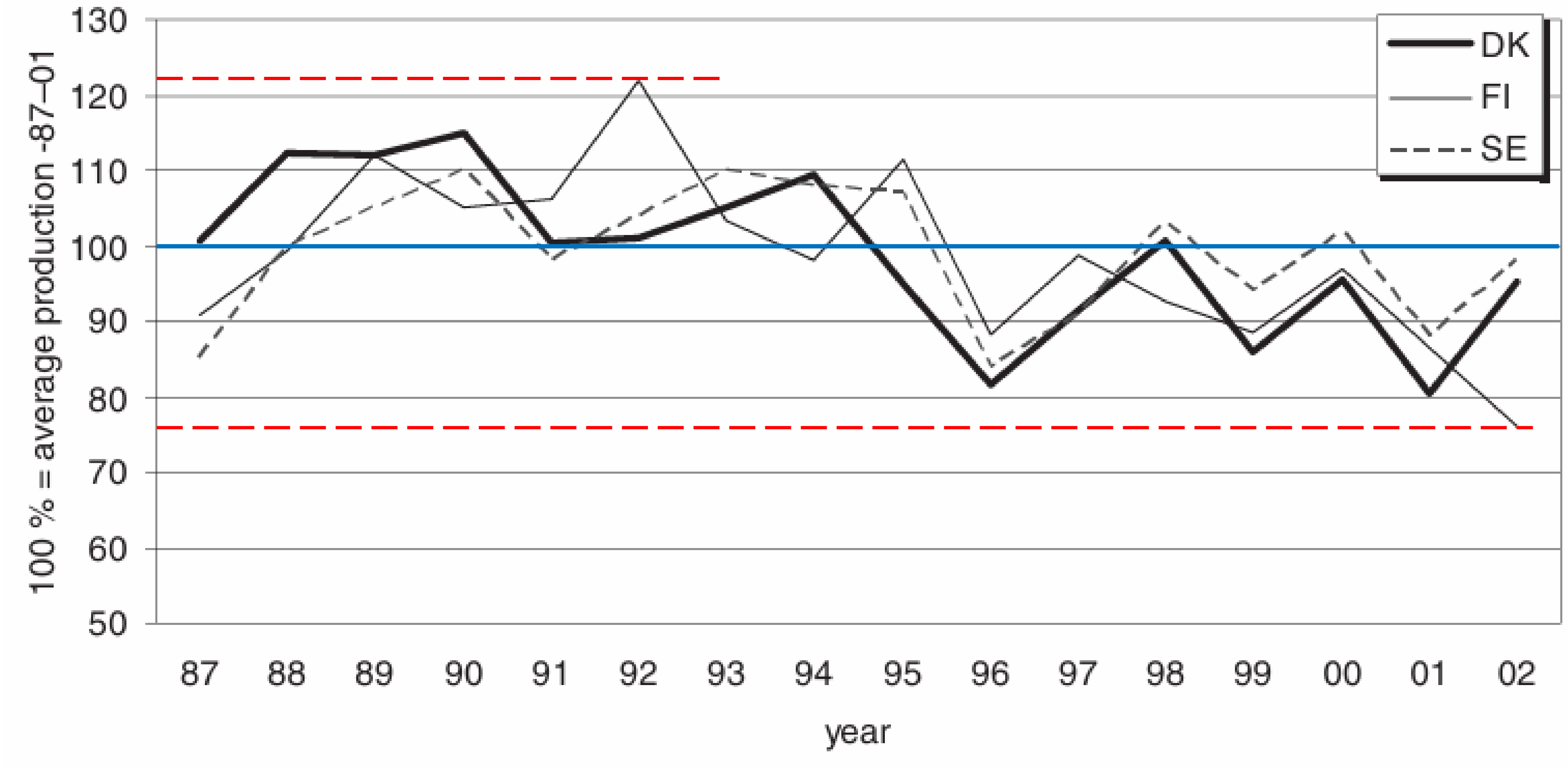
Hannele Holttinen, "Hourly Wind Power Variations in the Nordic Countries", (2004).

Wind speed in China [1 y]



X. Shi, Y. Qian, S. Yang, "Fluctuation Analysis of a Complementary Wind–Solar Energy System and Integration for Large Scale Hydrogen Production", (2020).

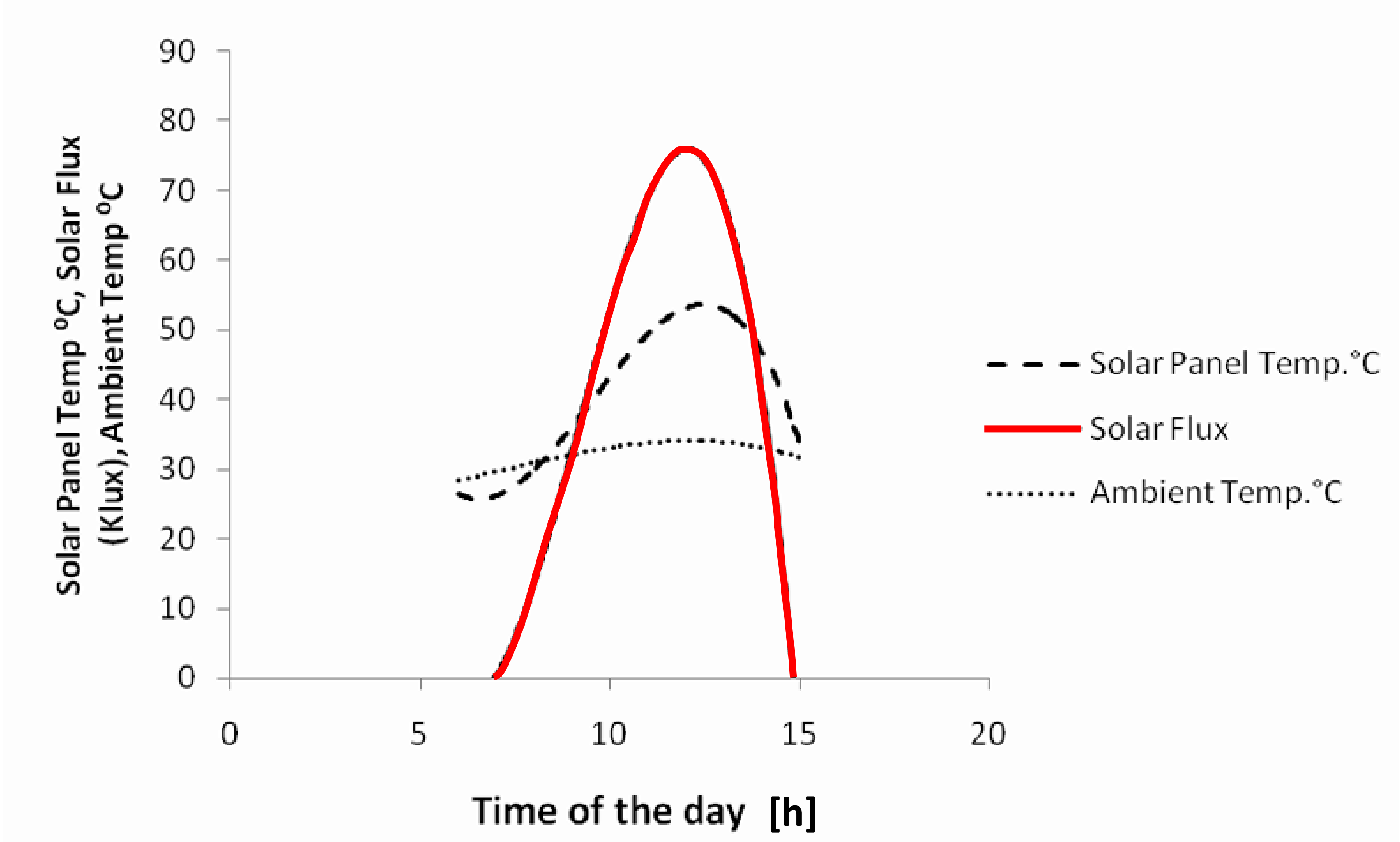
Wind production along years in Nordic Regions [DK, FI, SE]



Hannele Holttinen, "Hourly Wind Power Variations in the Nordic Countries", (2004).

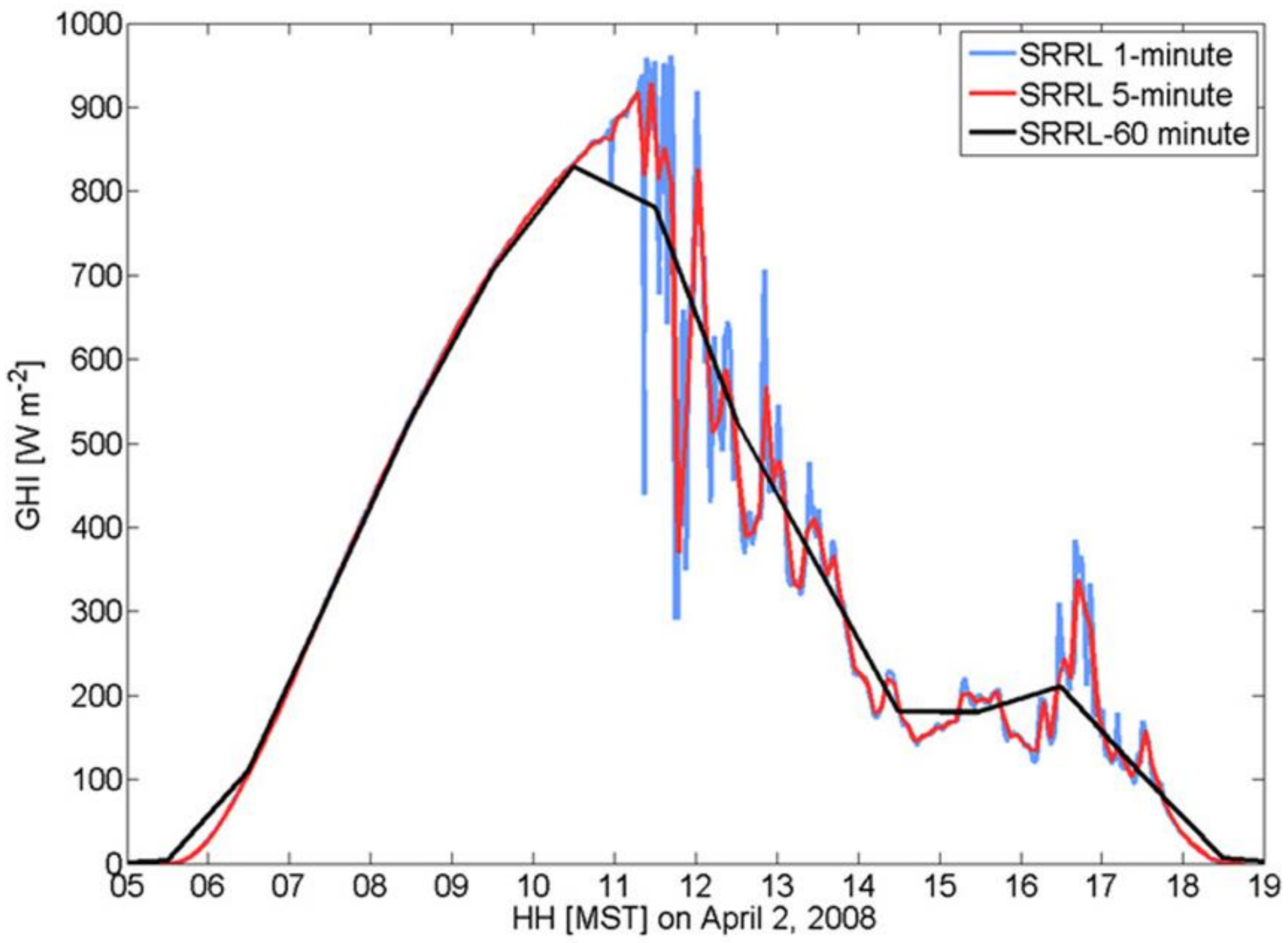
Variability of solar energy production

Solar energy in Nigeria [1 d]



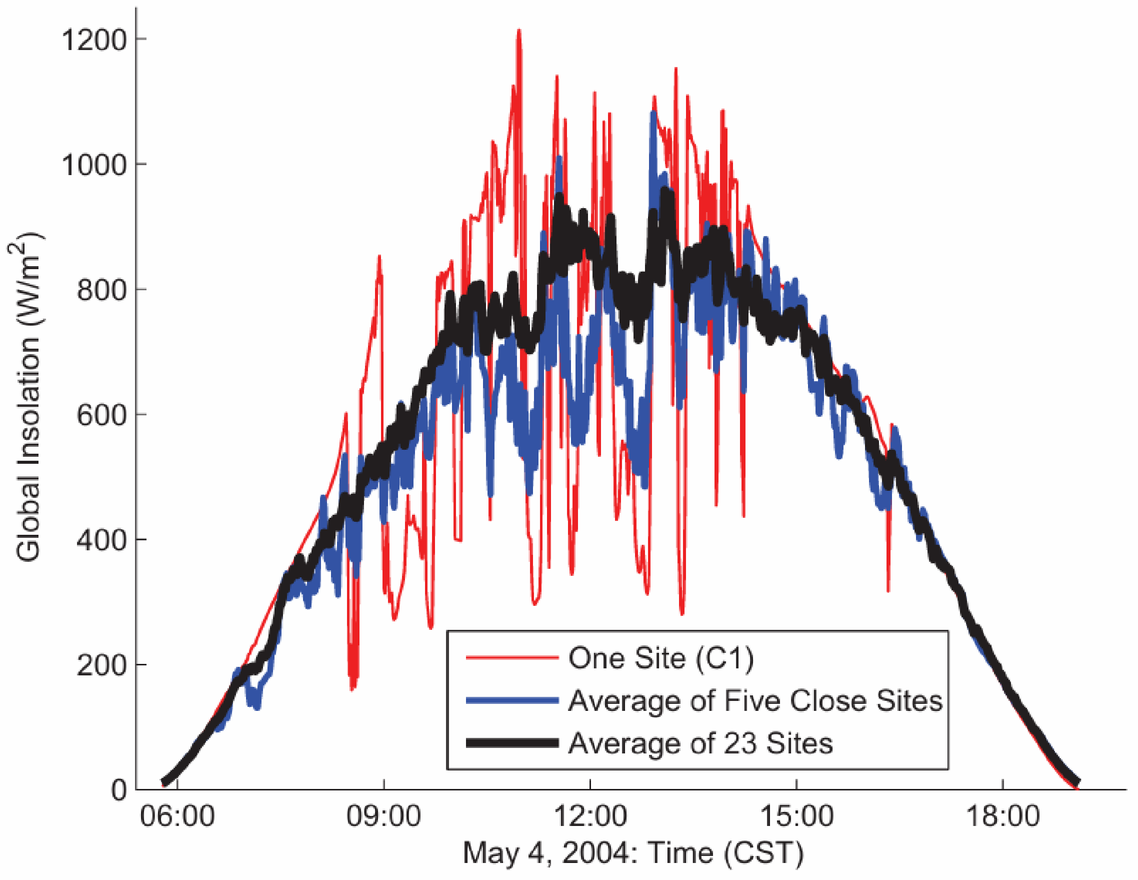
V. B. Omubo-Pepple, C. Israel-Cookey, G. I. Alaminokuma, "Effects of Temperature, Solar Flux and Relative Humidity on the Efficient Conversion of Solar Energy to Electricity", (2009).

Irradiation in Colorado [1 d]



M. Lave, J. Kleissl, "Solar variability of four sites across the state of Colorado", (2010).

Solar radiation in Oklahoma [1 d]

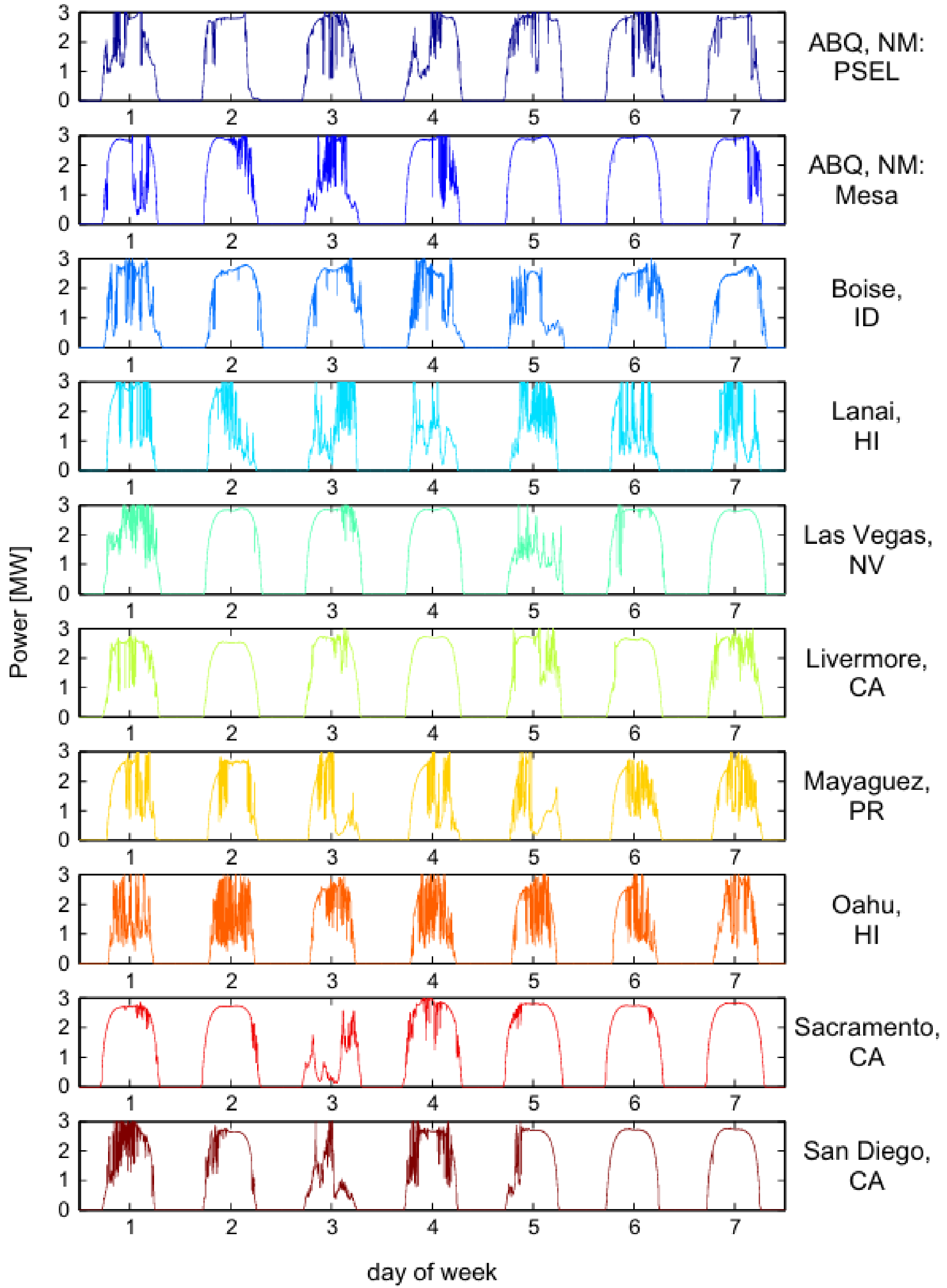


A.D. Mills, R.H. Wiser, "Implications of Geographic Diversity for Short-Term Variability and Predictability of Solar Power", (2011).

Weekly variability of solar radiation

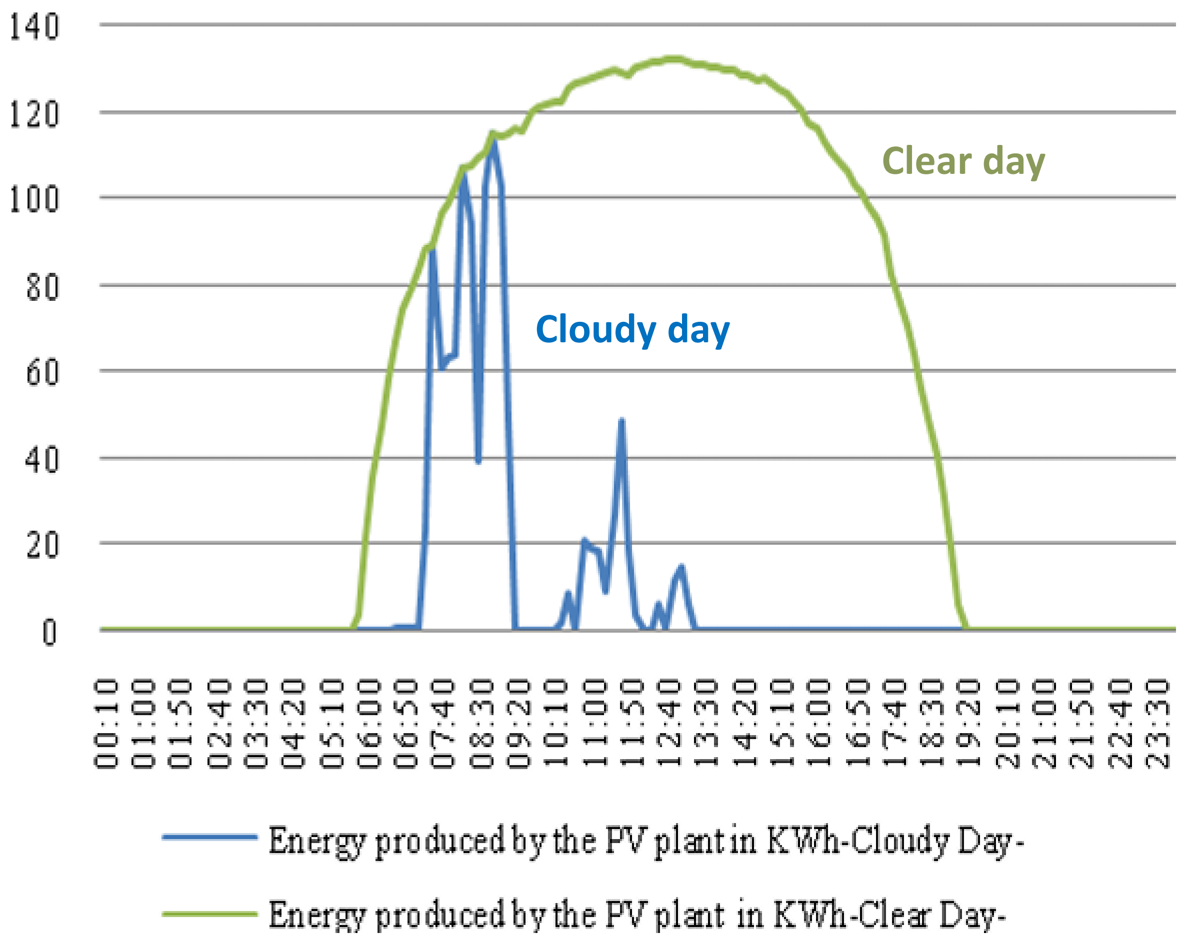
Weekly variability in 10 sites in the western USA

(30 s sampling time)



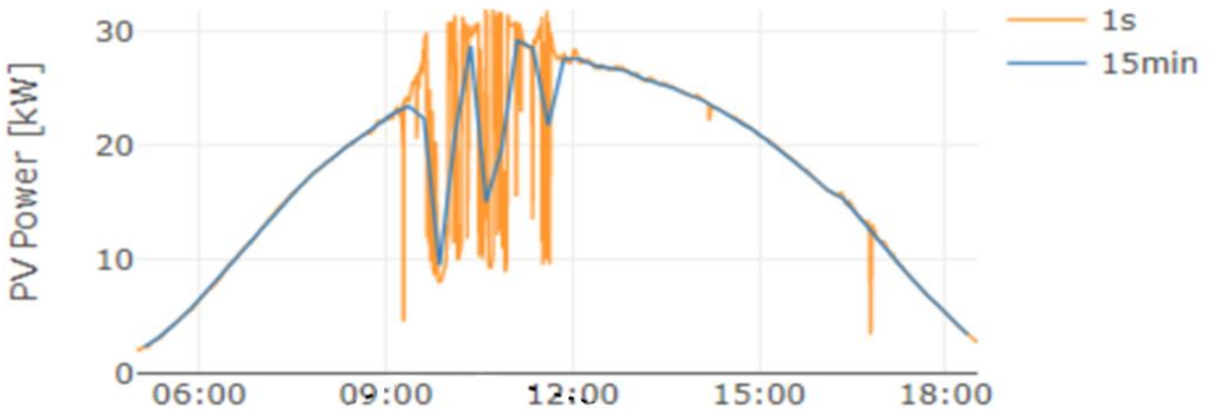
M. Lave, M.J. Reno, R.J. Broderick, "Characterizing local high-frequency solar variability and its impact to distribution studies", (2015).

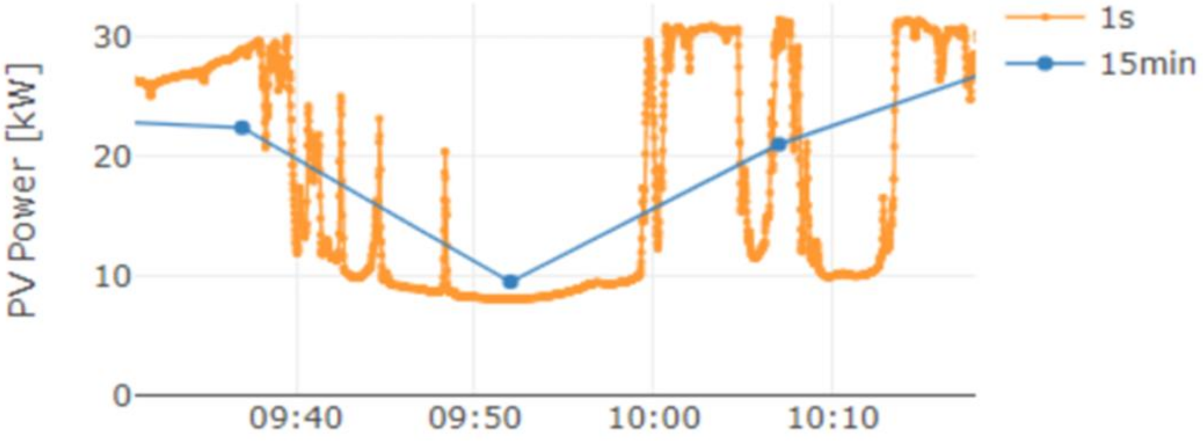
Cloud effect on solar energy production in Morocco



N. Kebir, M. Maaroufi, "Predictive Evaluation of Cloud Motion Impact on a Medium Voltage Solar PV Power System Output", (2015).

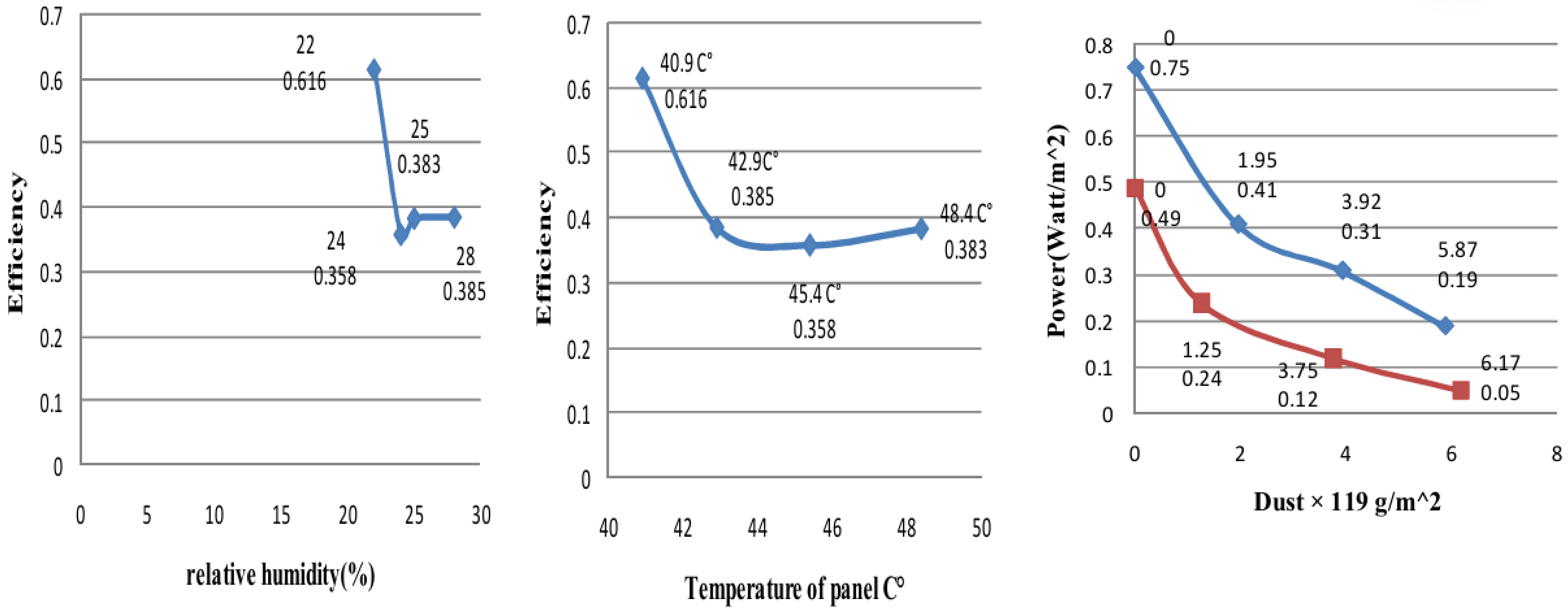
Risk of average [1 s vs 15 min]





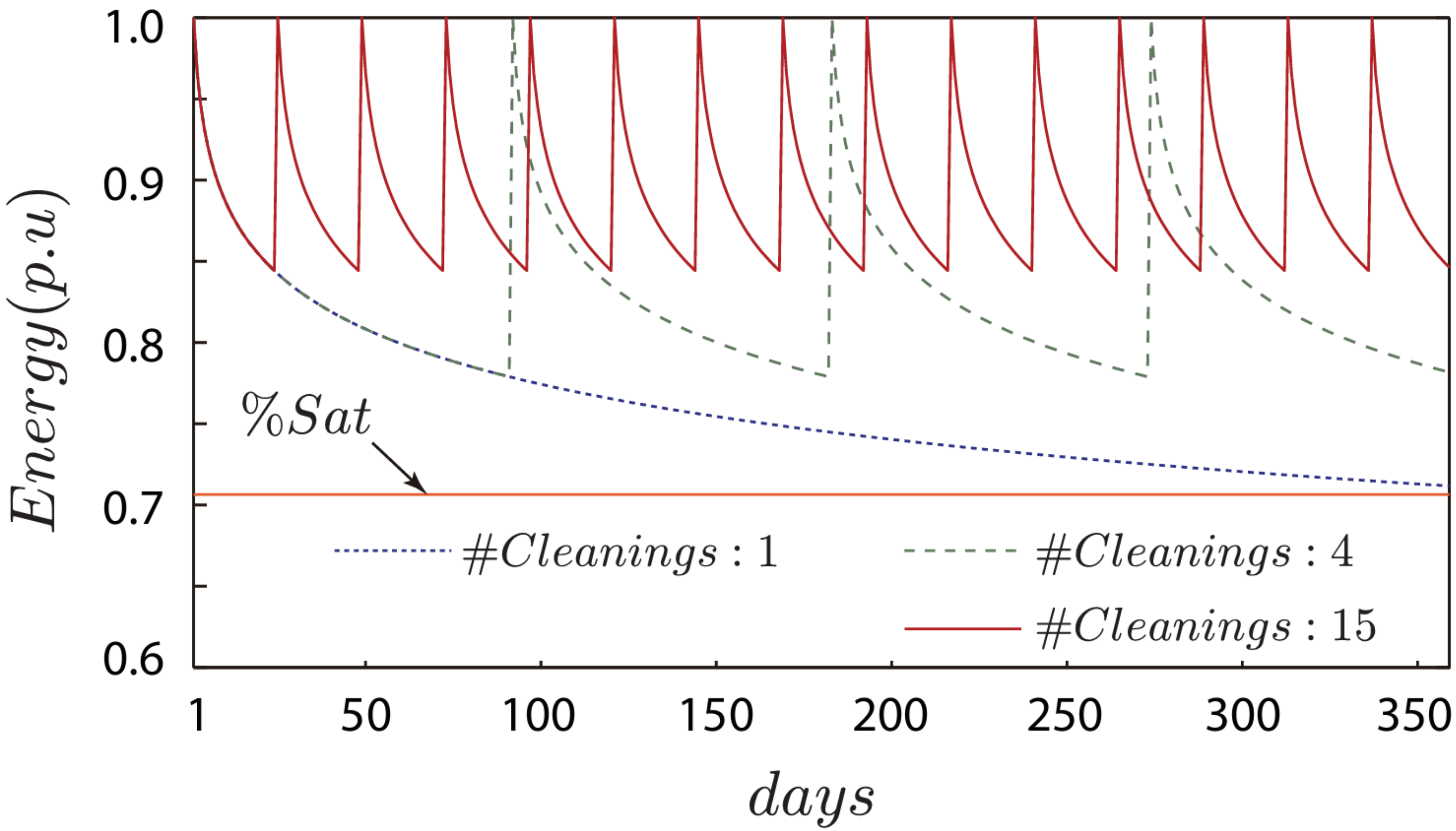
F.P.M. Kreuwela, W.H. Knap, L.R. Visser, W. van Sark, J. Vilà-Guerau de Arellano, C.C. van Heerwaarden. "Analysis of high frequency photovoltaic solar energy fluctuations", (2020).

Weather effects on solar panel efficiency [Qatar]



F. Touati, M. Al-Hitmi, H. Bouchech, "Towards Understanding the Effects of Climatic and Environmental Factors on Solar PV Performance in Arid Desert Regions (Qatar) for Various PV Technologies", (2012).

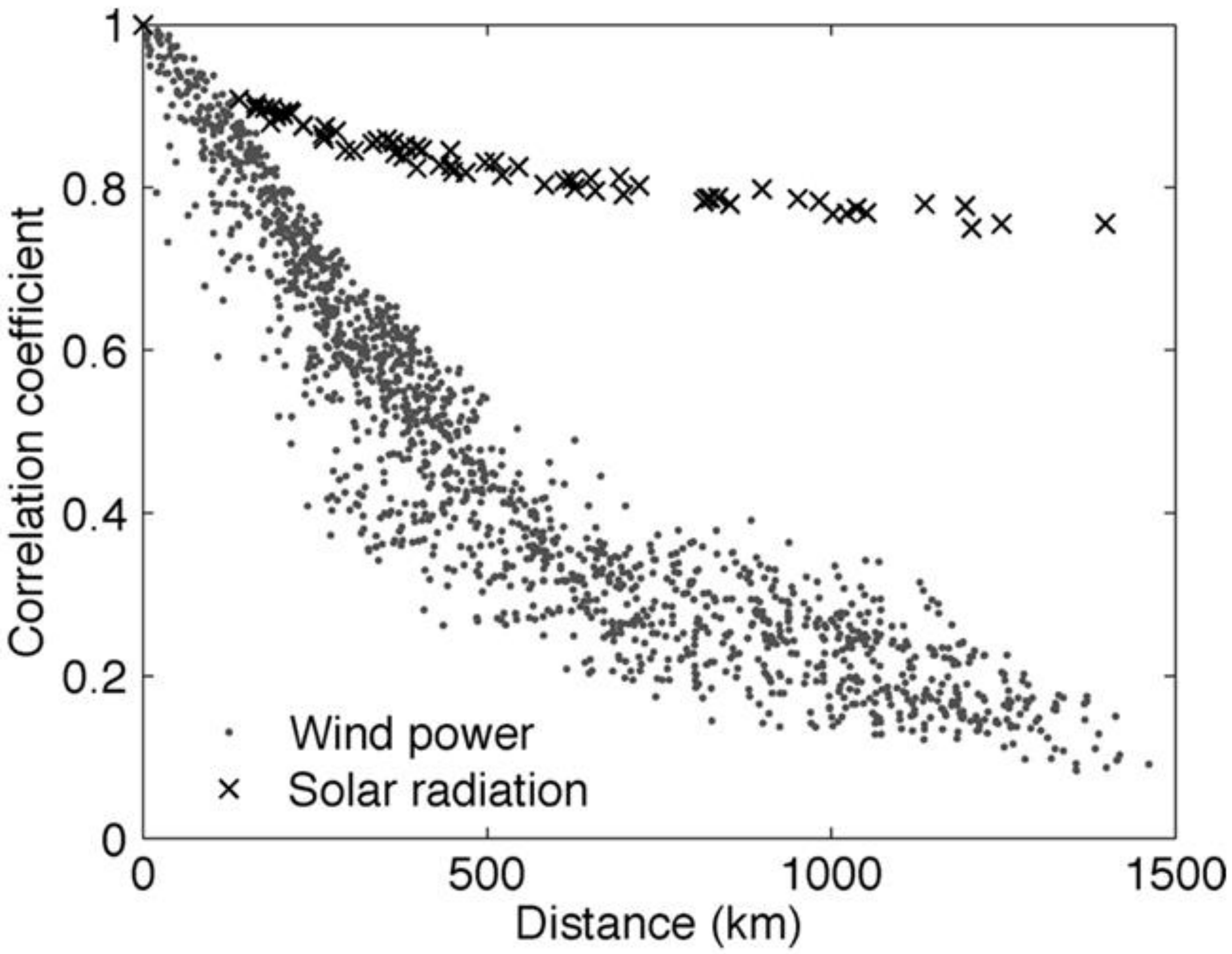
Anthropic variability [cleaning]



J.W. Zapata, M.A. Perez, S. Kouro. "Design of a cleaning program for a PV plant based on the analysis of short-term and long-term effects", (2015).

Solar and wind energy variability

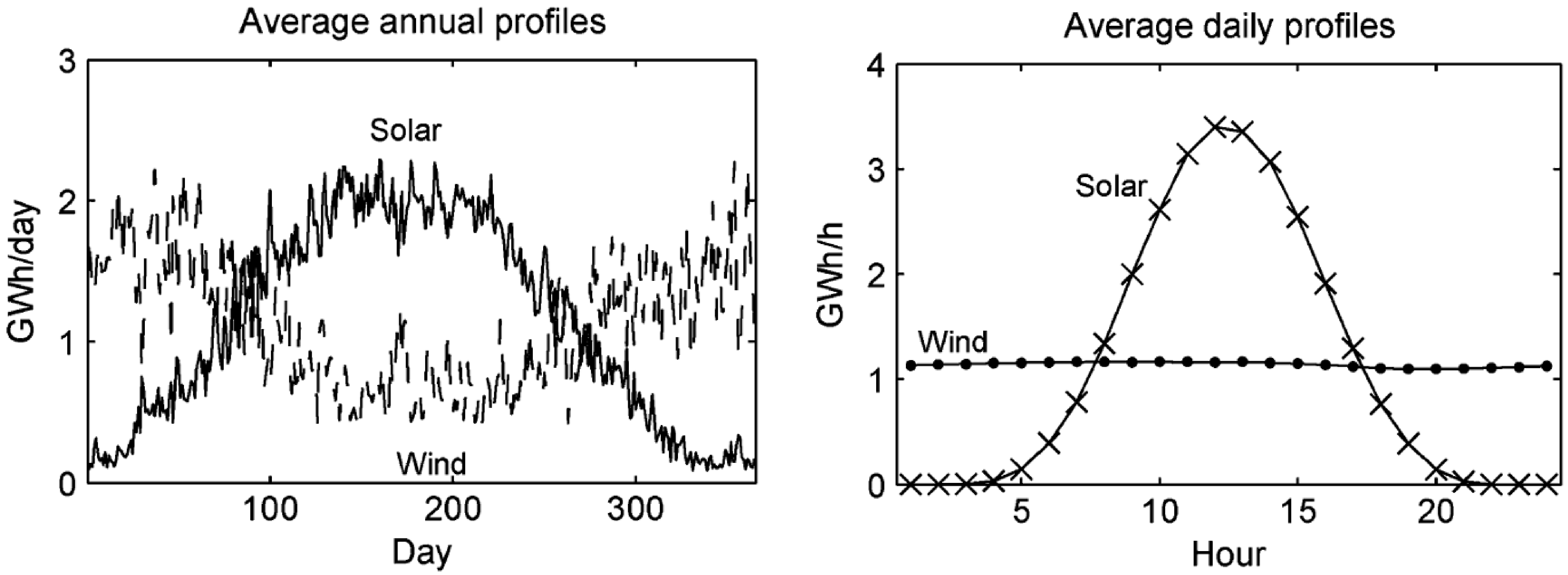
Distance correlation for wind and solar production



Solar radiation is less affected by the distance between sites with respect to wind power.

J. Widén, "Correlations Between Large-Scale Solar and Wind Power in a Future Scenario for Sweden", (2011).

Wind and solar energy in Sweden

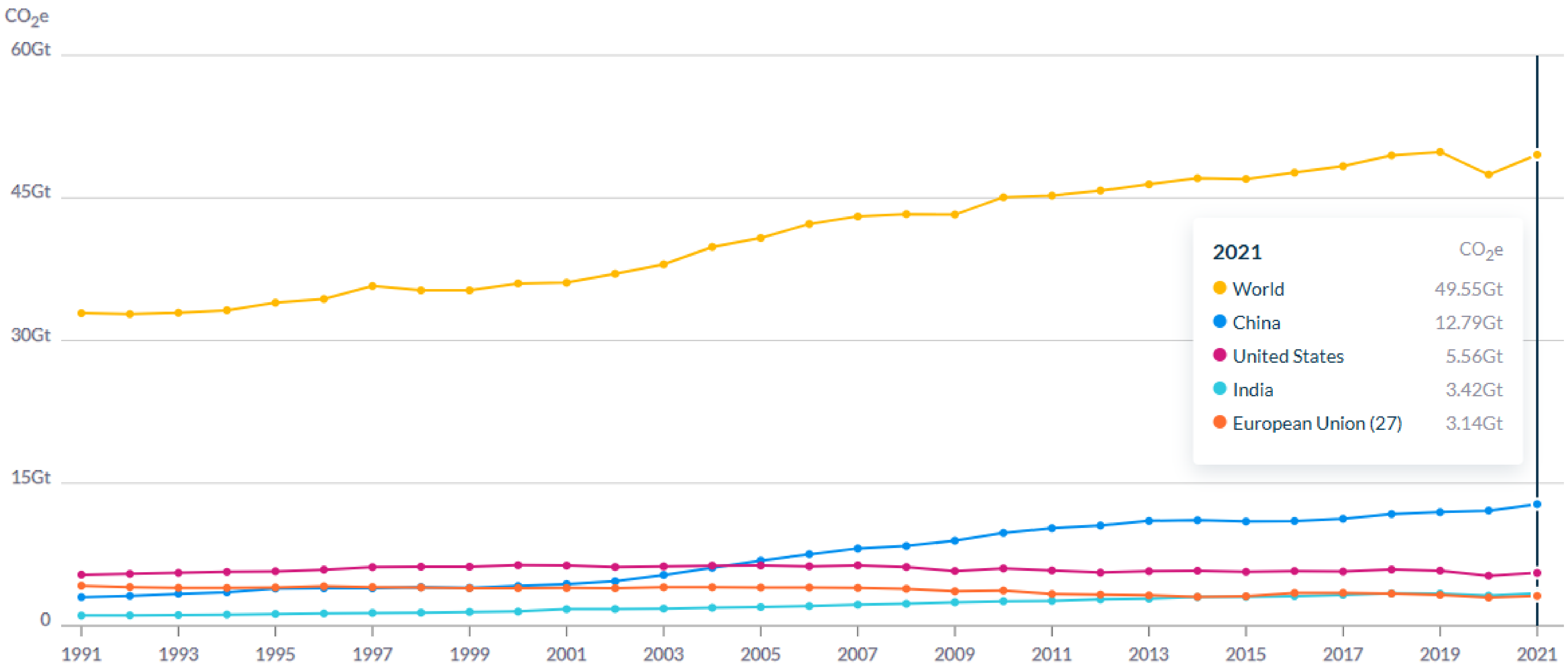


Comparison of wind and solar profiles [year and day].
On an hourly average, wind appears more stable and less variable, while solar follows the usual daylight trend.
During the year, wind is higher in winter, while solar is higher in summer. Average data on all plants.

J. Widén, "Correlations Between Large-Scale Solar and Wind Power in a Future Scenario for Sweden", (2011).

Chemical processes and greenhouse gas emissions

Greenhouse gas (GHG) emissions in the last three decades

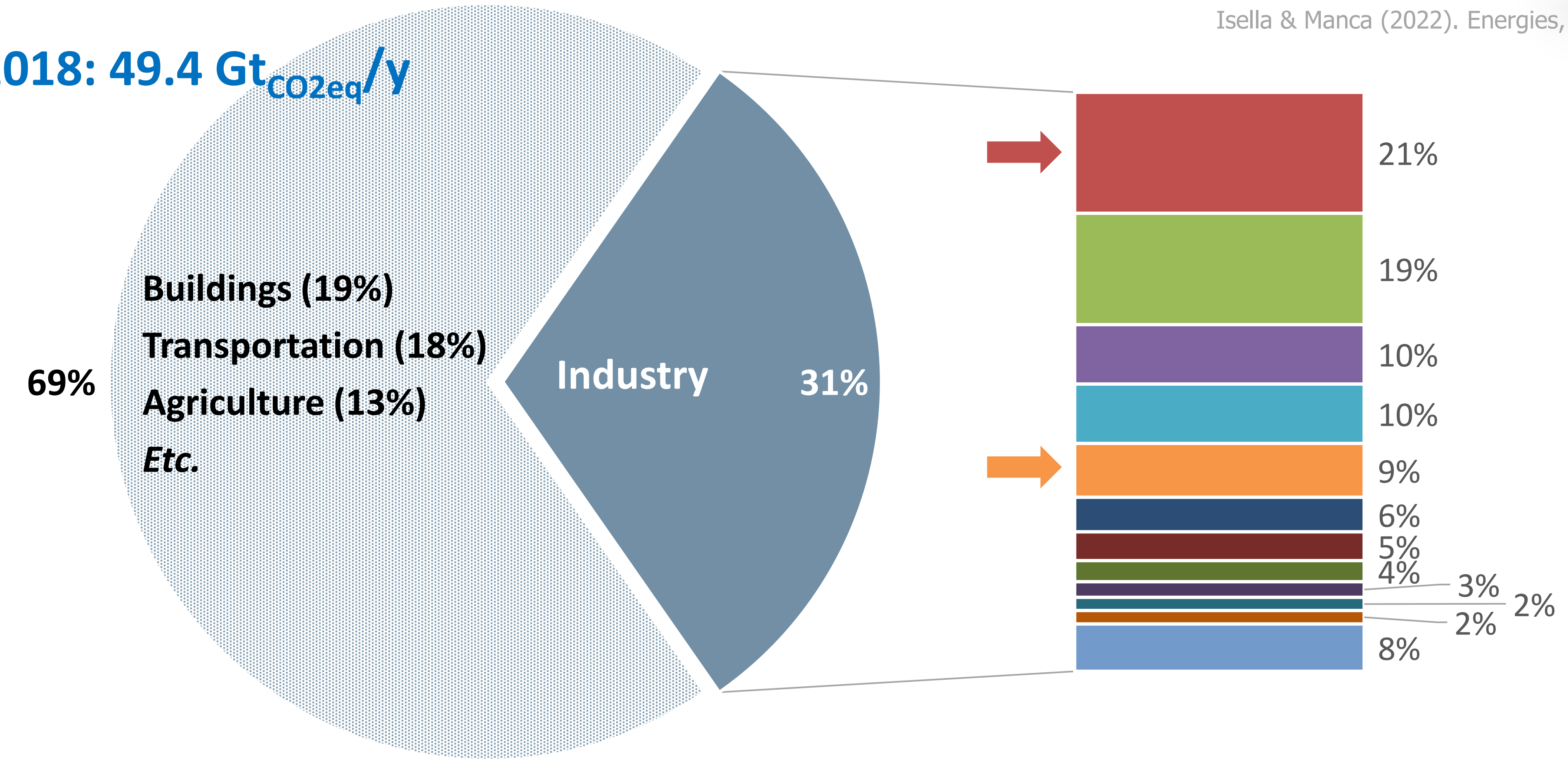


Climate Watch (2024) https://www.climatewatchdata.org/

World GHG emissions by "end-user" (2018)

Isella & Manca (2022). Energies, 15(20), 7560

TOTAL 2018: 49.4 Gt_{CO2eq}/y

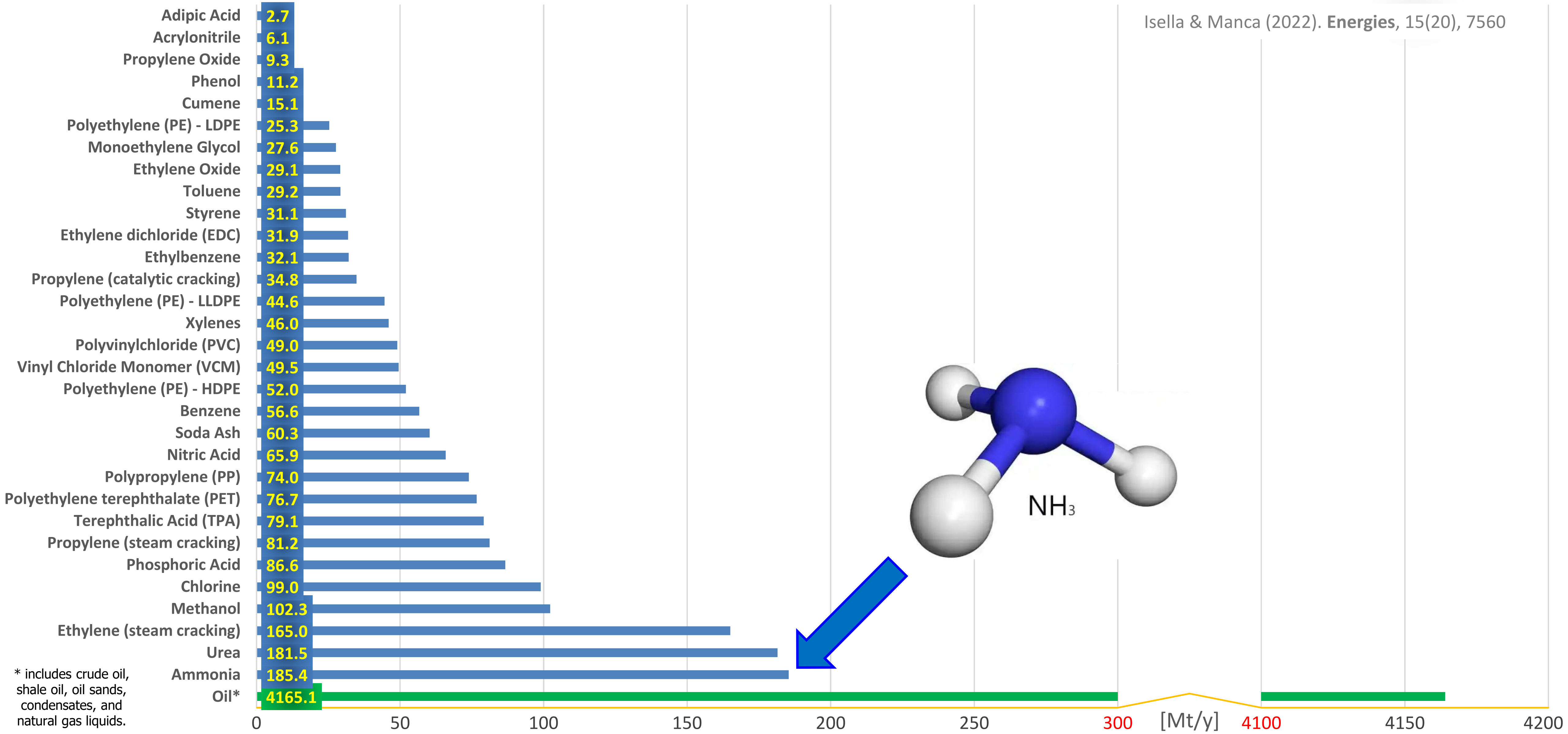


- **Chemical and petrochemical (21%)**
- Iron and steel (19%)
- Cement (10%)
- Non-metallic minerals (10%)
- **Oil refining (9%)**
- Non-ferrous metals (6%)
- Machinery (5%)
- Food and tobacco (4%)
- Paper, pulp, and printing (3%)
- Mining and quarrying (2%)
- Textile and leather (2%)
- Other industries* (8%)

* includes Wood industry and products, Electronics, Other.

Ammonia

Production volumes in the chemical and refining sector (2020)

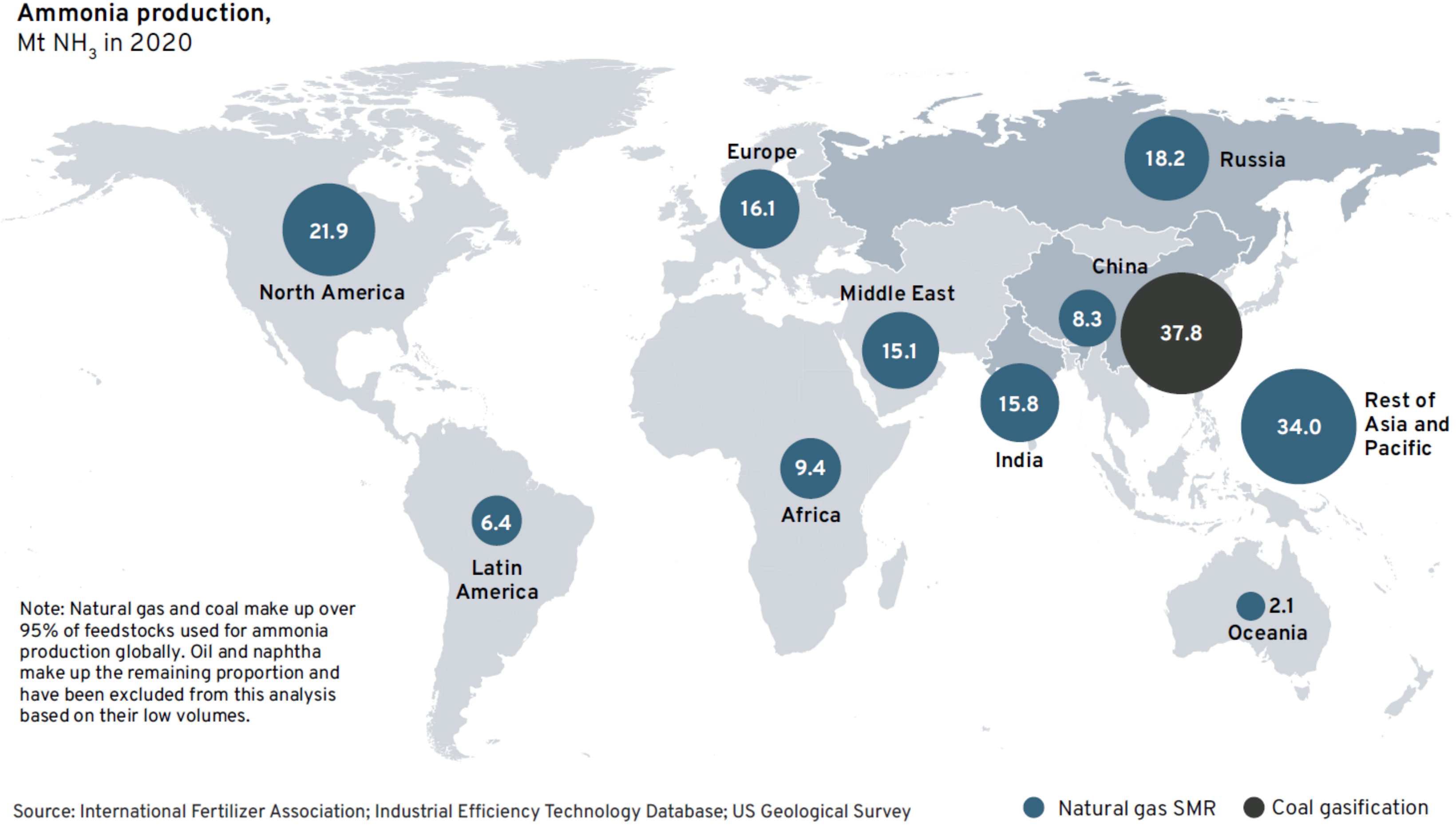


* includes crude oil, shale oil, oil sands, condensates, and natural gas liquids.

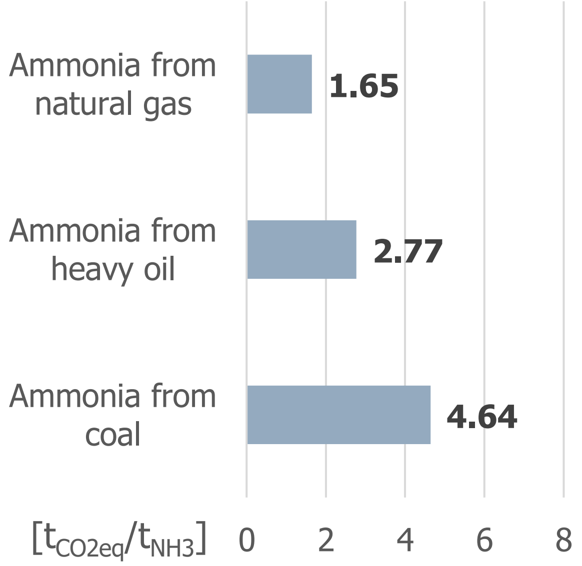
Worldwide ammonia production

2020: 185 Mt_{NH3}/y

- 70% → Fertilizers → 2010–20 growth rate at 1% per year
- 30% → Industrial applications → 2010–20 growth rate at 4% per year

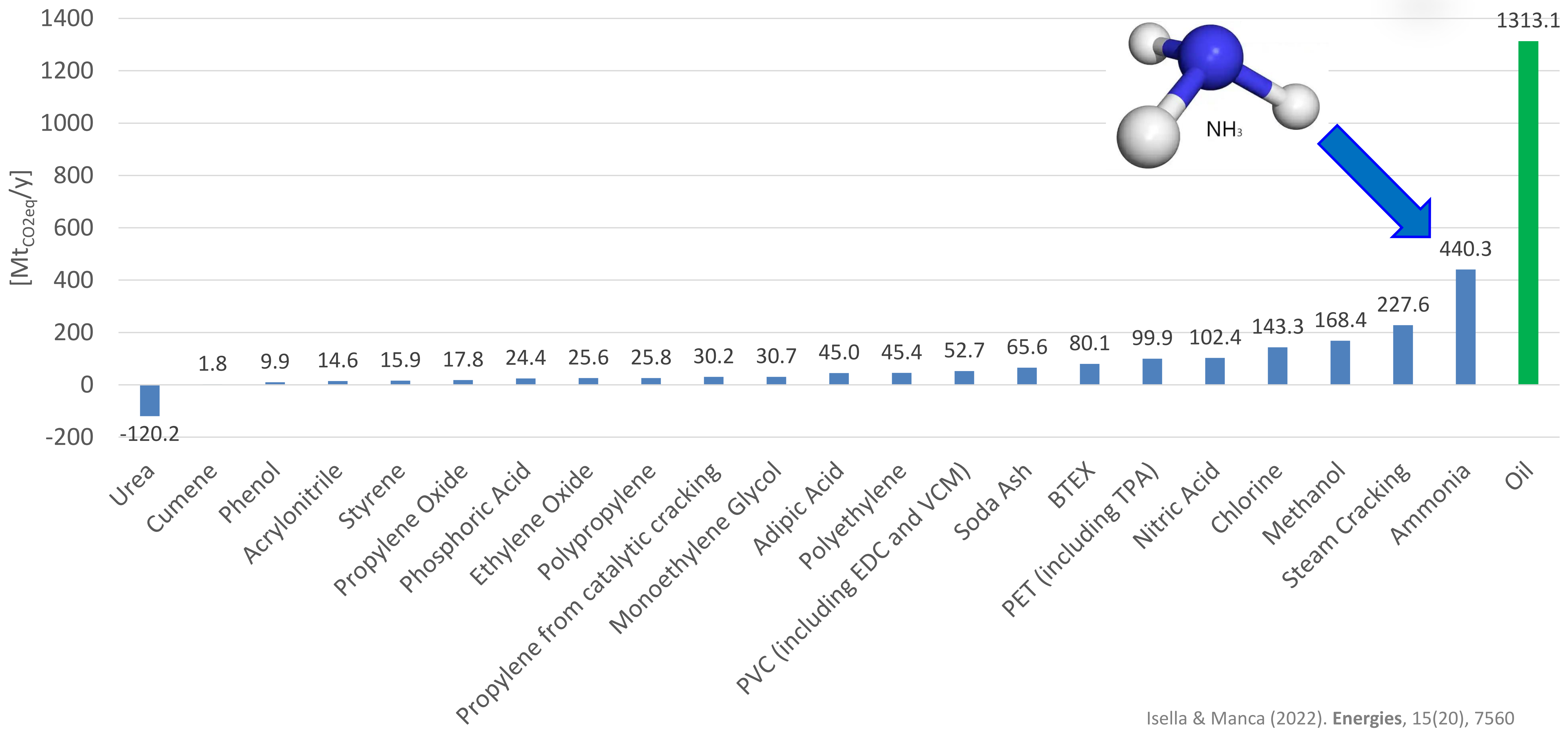


Average gate-to-gate GHG emissions



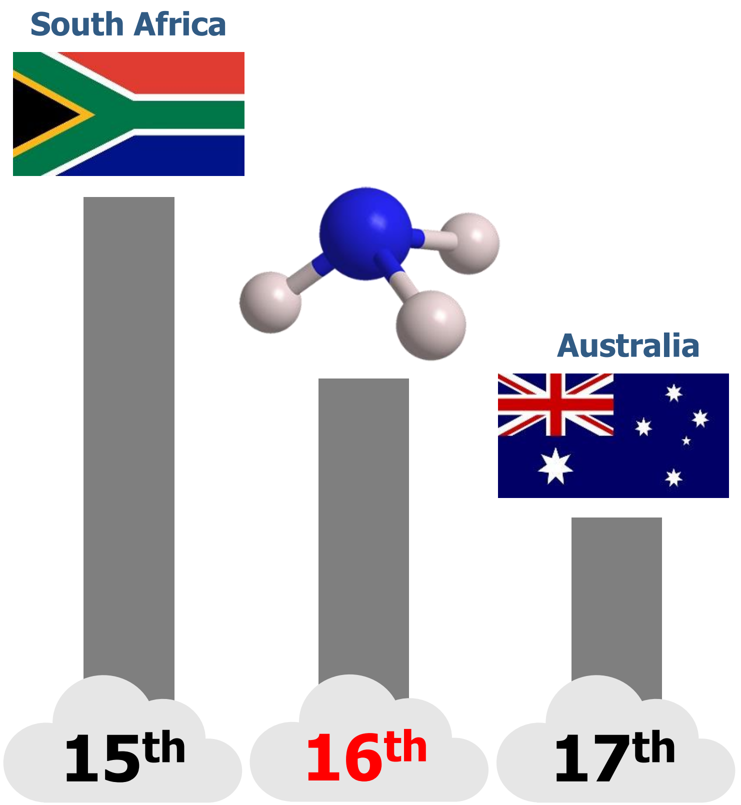
Isella & Manca (2022). **Energies**, 15(20), 7560

Chemical and oil refining GHG emissions (2020)



Isella & Manca (2022). **Energies**, 15(20), 7560

The urgent drive to ammonia decarbonization



«If the ammonia industry were a country, it would be the **16th largest CO_2 emitter**»

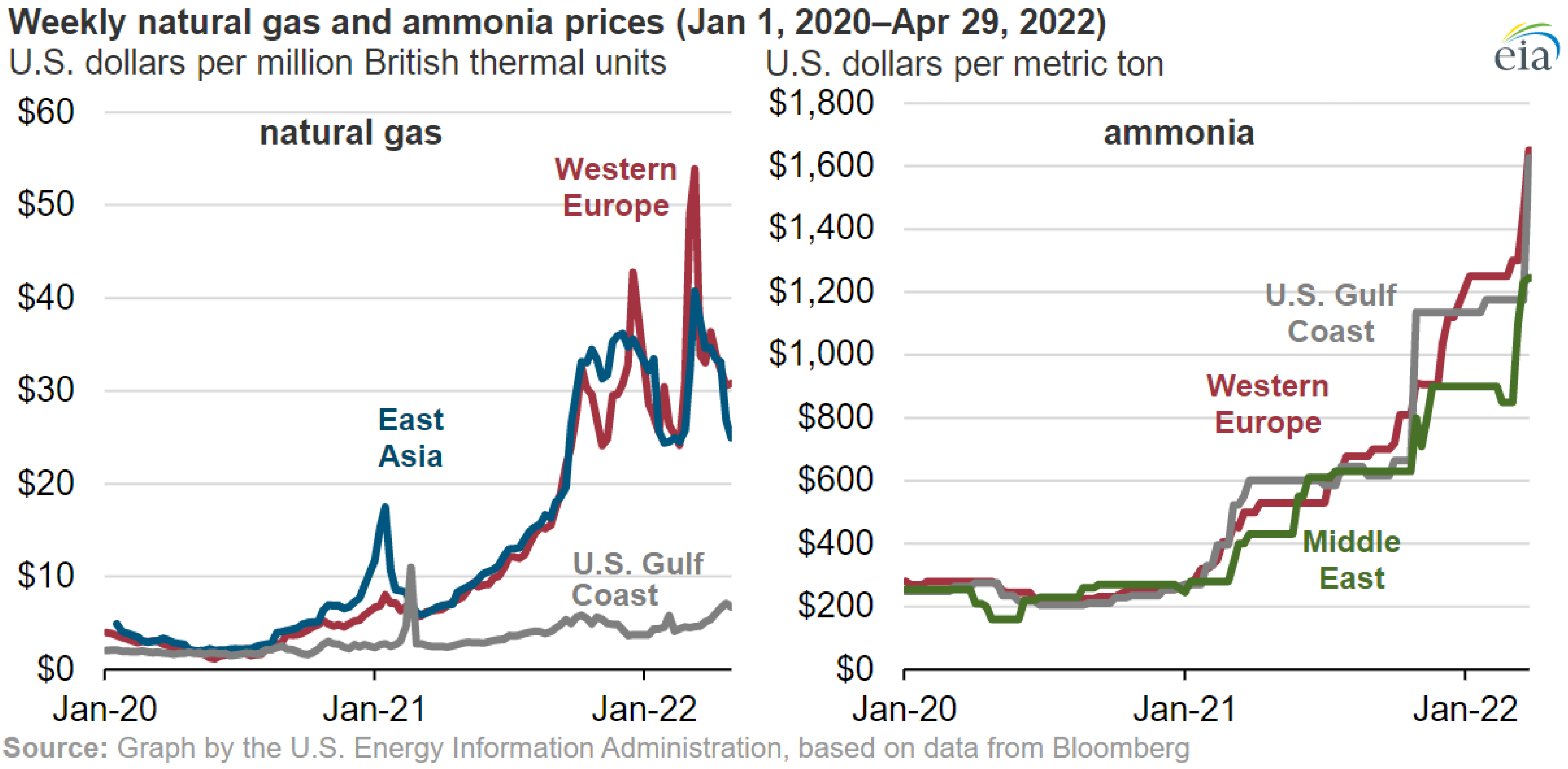
Alexandra McIntosh

Director at Australian Renewable Energy Agency (ARENA), September 2022

	Near-zero-emissions technologies				Transitional technologies	
Technology	**Green ammonia**	**Blue ammonia**	**Biomass-based**	**Methane pyrolysis**	**Revamp electrolyzer**	**Partial CCS**
Feedstock	Water	Natural gas, Oil, Coal	Biomass	Natural gas	Natural gas, Oil, Coal	Natural gas
2020 levelized cost [USD/t_{NH3}]	550~1,400	350~770	770~1,350	480~840	300~670	300~560
Direct CO_2 emissions abatement potential	100%	96%	100%	100%	10%	67%

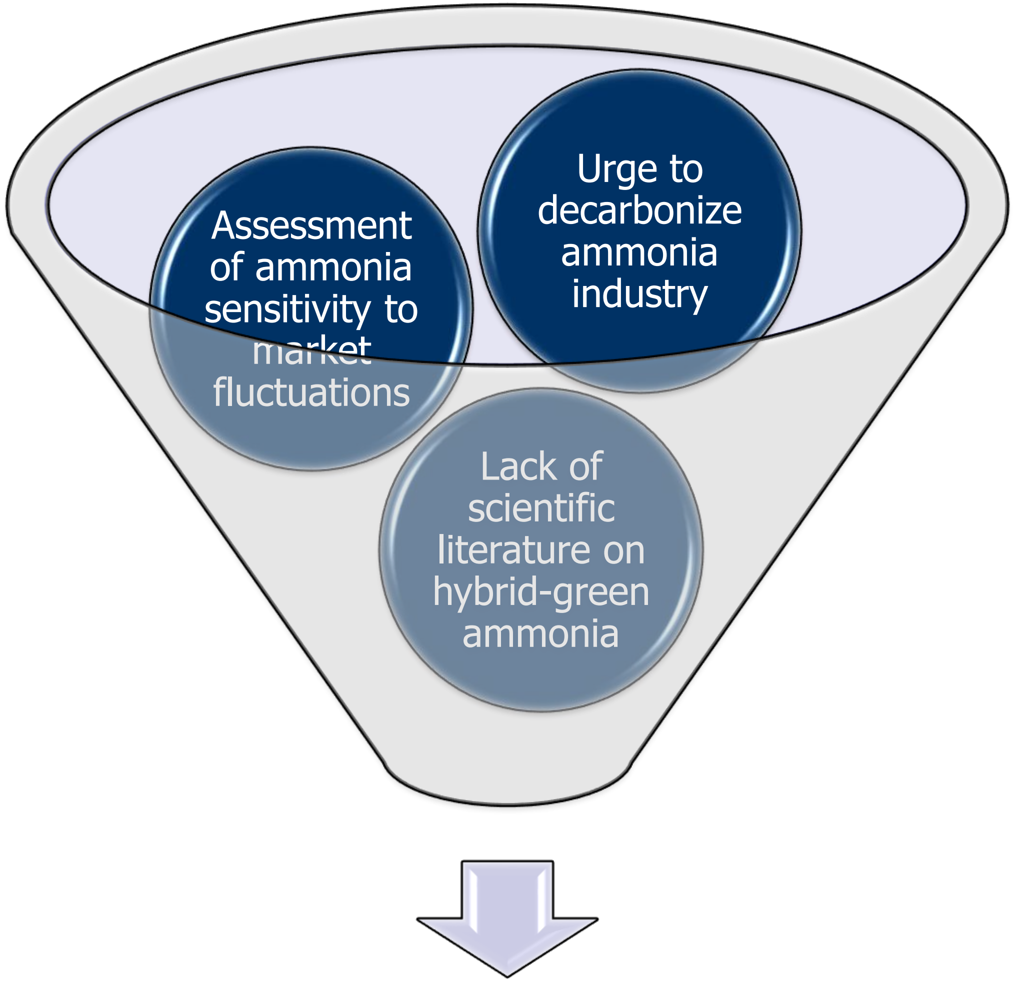
MPP (2022). Making Net-Zero Ammonia Possible: An Industry-Backed, 1.5°C-Aligned Transition Strategy. Mission Possible Partnership.

Causes of ammonia cost sensitivity to market fluctuations



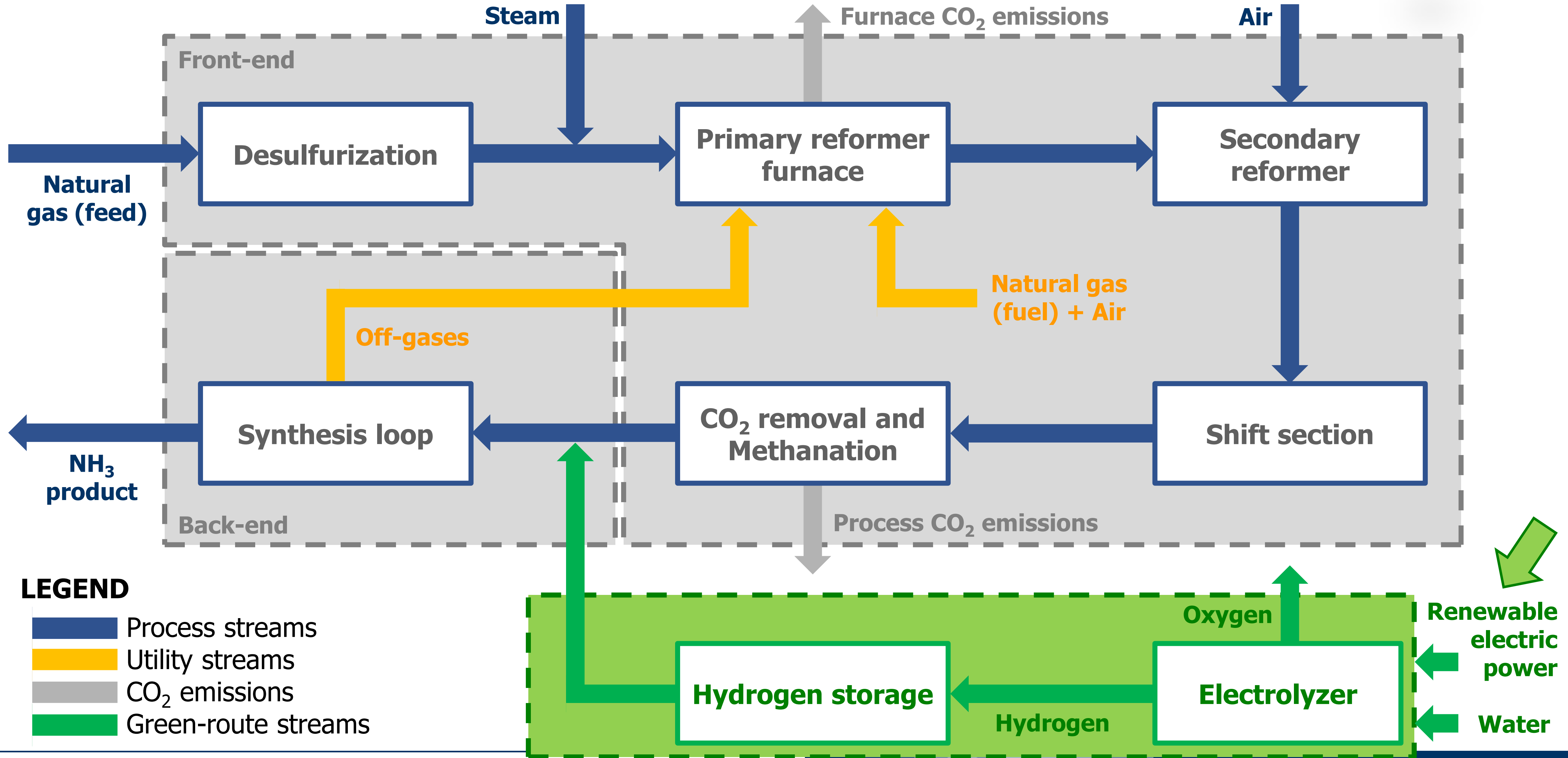
Hybrid green ammonia

Why investigate hybrid-green ammonia synthesis?



Detailed **process simulation** of 2 ammonia synthesis configurations:
1 "**gray**" (*i.e.* fossil) and 2 "**hybrid-green**" (10%- and 20%-green)

Hybrid-green ammonia model plant (2000 t_{NH_3}/d)



Hybridization constraints and model assumptions

HYBRIDIZATION CONSTRAINTS

Availability of renewable power

Need for "intermittency-mitigating" features

Fluctuating renewable energy profiles converted into hydrogen flows oscillating from a minimum of zero (*i.e.* no power available) to a certain maximum value.

Operating conditions of the ammonia plant

Process flow to the primary reformer

A conventional steam reformer cannot operate properly when its "throughput" decreases too much.

Assumption: 80% of nominal capacity at minimum

Temperature at the secondary reformer

A conventional secondary reformer cannot operate properly when its temperature increases too much.

Assumption: +100 °C temperature rise at maximum

Fuel gas fed to the reformer furnace burners

Natural gas (as fuel) input to the burners is needed to maintain a safe temperature for reforming tubes.

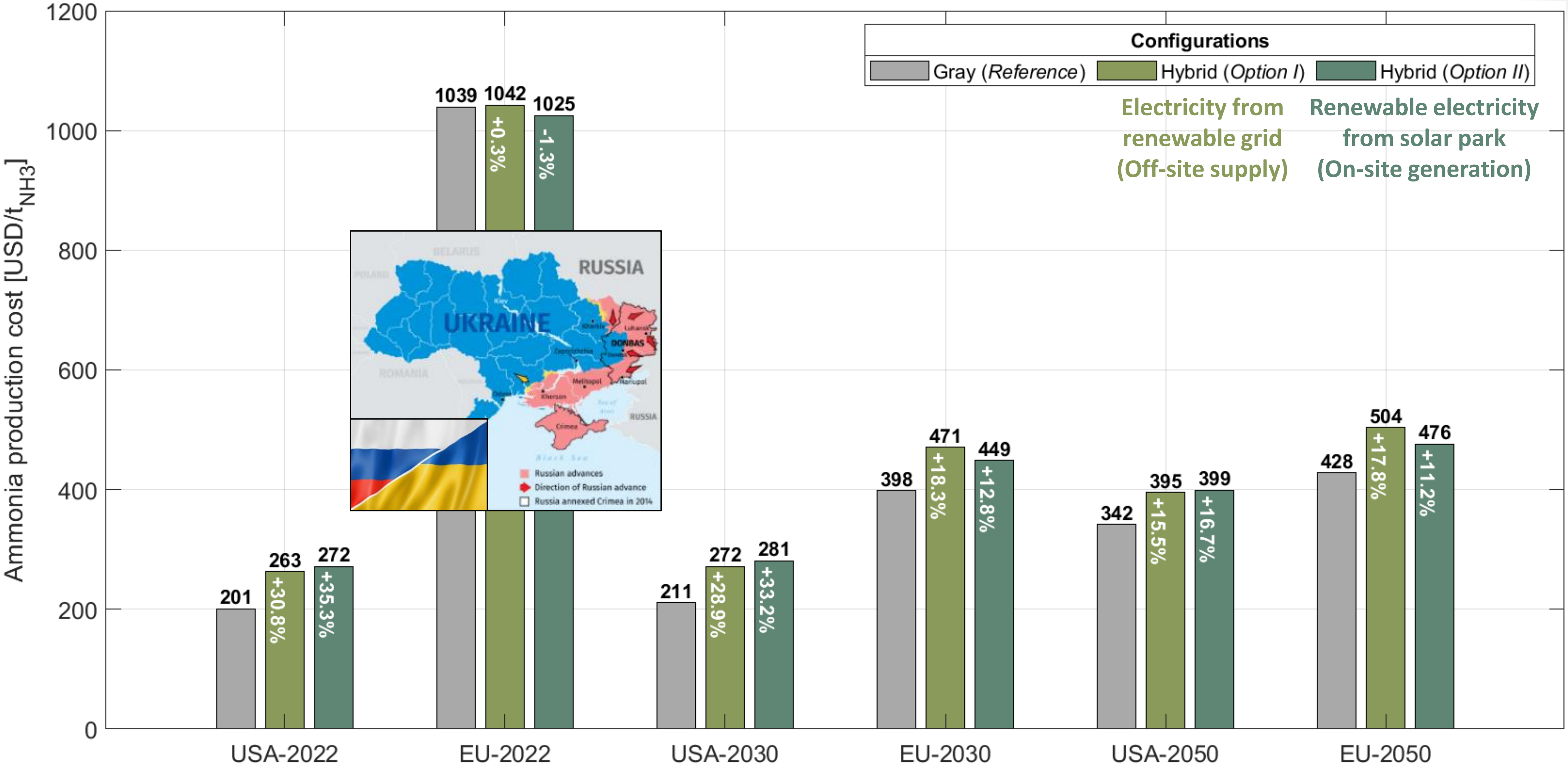
Assumption: fuel gas to the furnace cannot be null

How much "green" can hybrid-green ammonia be?

Process variables of the model plant (2000 t_{NH_3}/d)

Process variable [unit]		Gray ammonia ($deCO_2$ = 0%)		Mean hybrid-green ($deCO_2$ = 10%)		High hybrid-green ($deCO_2$ = 20%)	
Average green H_2 to the synloop	[t/h]	0		1.74		3.55	
Primary reformer throughput	[t/h]	163	**100%**	146	**89.3%**	129	**78.8%**
Secondary reformer temperature	[°C]	996	**100%**	1043	**104.7%**	1104	**+108 °C**
Natural gas feed to the front-end	[t/h]	38.0	100%	33.9	89.3%	29.9	78.8%
Natural gas fuel to the furnace	[t/h]	12.9	**100%**	11.9	**92.3%**	10.7	**82.8%**
Furnace CO_2 emissions	[t/h]	38.9	100%	34.8	89.5%	30.7	78.8%
	[t_{CO2}/t_{NH3}]	0.467		0.418		0.368	
Process CO_2 emissions	[t/h]	97.4	100%	87.9	90.3%	78.1	80.1%
	[t_{CO2}/t_{NH3}]	1.17		1.06		0.937	
Total CO_2 emissions	[t/h]	136.3	**100%**	122.7	**90%**	108.8	**80%**
	[t_{CO2}/t_{NH3}]	1.64		1.48		1.31	

Gray vs. Hybrid-green production costs



Isella *et al.* (2024). **Chemical Engineering Journal**, 486, 150132

Take-away messages

In summary:

- This study shows how hybrid-green ammonia is an **up-to-date** retrofitting strategy to **partially decarbonize** (up to **−20%** of t_{CO_2}/t_{NH_3}) the ammonia production industry.
- Depending less on natural gas inputs, hybrid-green ammonia is **cheaper** than gray ammonia as the natural gas quotations rise (*e.g.*, **Russia-Ukraine war**) by the results of the simulated case.
- By gradually entering a "**green economy**" (*e.g.*, by introducing increasing carbon taxes, decreasing renewable energy costs, fossil fuel limitations, *etc.*), hybrid-green ammonia is expected to reach **progressively higher competitiveness** in the modeled market scenarios.

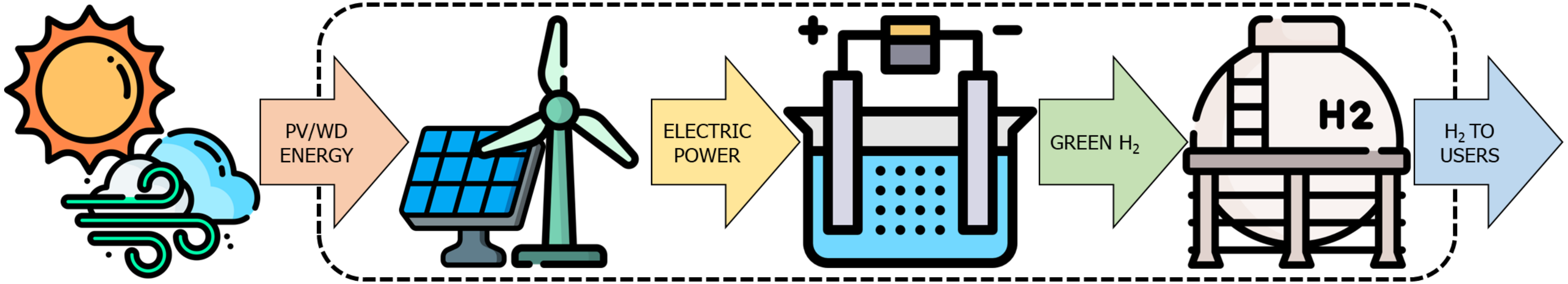
Based on the present analysis, a higher decarbonization extent and a lower retrofit cost may allow the industry to deliver early emissions reductions.

Hydrogen storage in green processes

Hydrogen storage role in green H_2 production systems

Levelized Cost of Hydrogen (LCOH) assessment:

- Solar+Wind power plant + Electrolyzer + Hydrogen storage



Specifications and Techno-economic data

TARGET H_2 PRODUCTIVITY: 1 [t_{H2}/h] → *e.g.*, to produce ≈136 [t_{NH3}/d] or ≈192 [t_{CH3OH}/d]

ASSESSED TIMESPAN: 1 [y] = 8760 [h] → *i.e.*, assuming no maintenance breaks or emergency shutdowns occur

TECHNO-ECONOMIC DATA: Discount rate = 5%

Unit	Life [y]	CapEx [USD/kW]	OpEx [CapEx/y]
Solar PV	25	1119	1.7%
Wind Onshore	25	1285	2%
Electrolyzer	10	700	2%

Unit	Life [y]	CapEx [USD/kg_{H2}]	OpEx [CapEx/y]
H_2 storage	20	1900	1%

California, USA

→ CF=27.41%

≈

→ CF=26.64%

CAISO (2024)

USA, 2022 values

IRENA (2023). Renewable power generation costs in 2022. International Renewable Energy Agency.

Solar/Wind park + Electrolyzer + H_2 storage

$$\min_{P_{PV}^{inst},\,P_{WD}^{inst}} \Phi_{OBJ} = LCOH = \frac{\sum_{j=PV,WD,EL,ST} (CapEx_y + OpEx)_j}{8760 \cdot \dot{m}_{H_2}^{target}} \quad (2a)$$

s.t.

$$\int_0^{8760} P_{EL}(t)\, dt = 8760 \cdot P_{EL}^{target} \quad (2b)$$

$$P_{EL}(t) = \min\left(P_{EL}^{inst},\, P_{PV}(t) + P_{WD}(t)\right) \quad (2c)$$

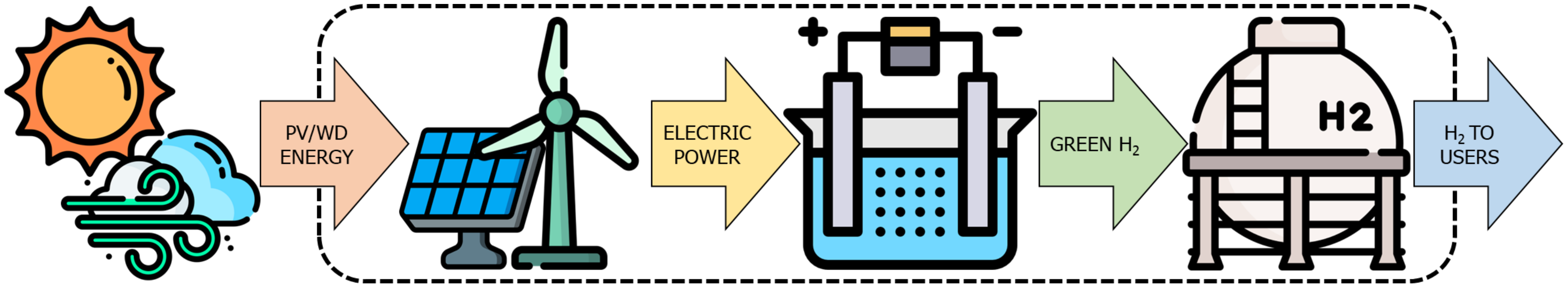
$$\int_0^{8760} \dot{m}_{H_2}^{ST,out}(t)\, dt = 8760 \cdot \dot{m}_{H_2}^{target} \quad (2d)$$

Hydrogen storage

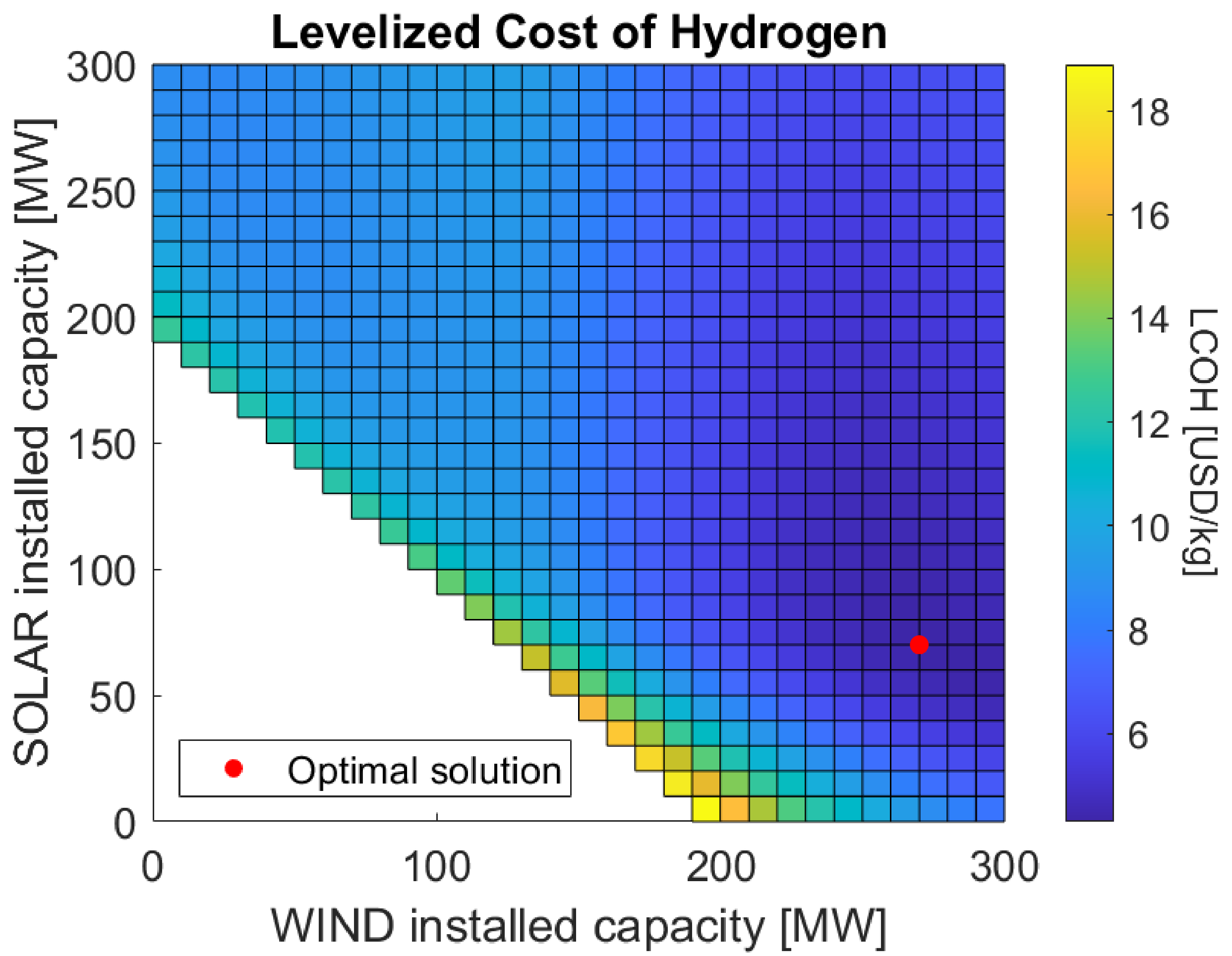
California (CAISO) solar profiles in 2022

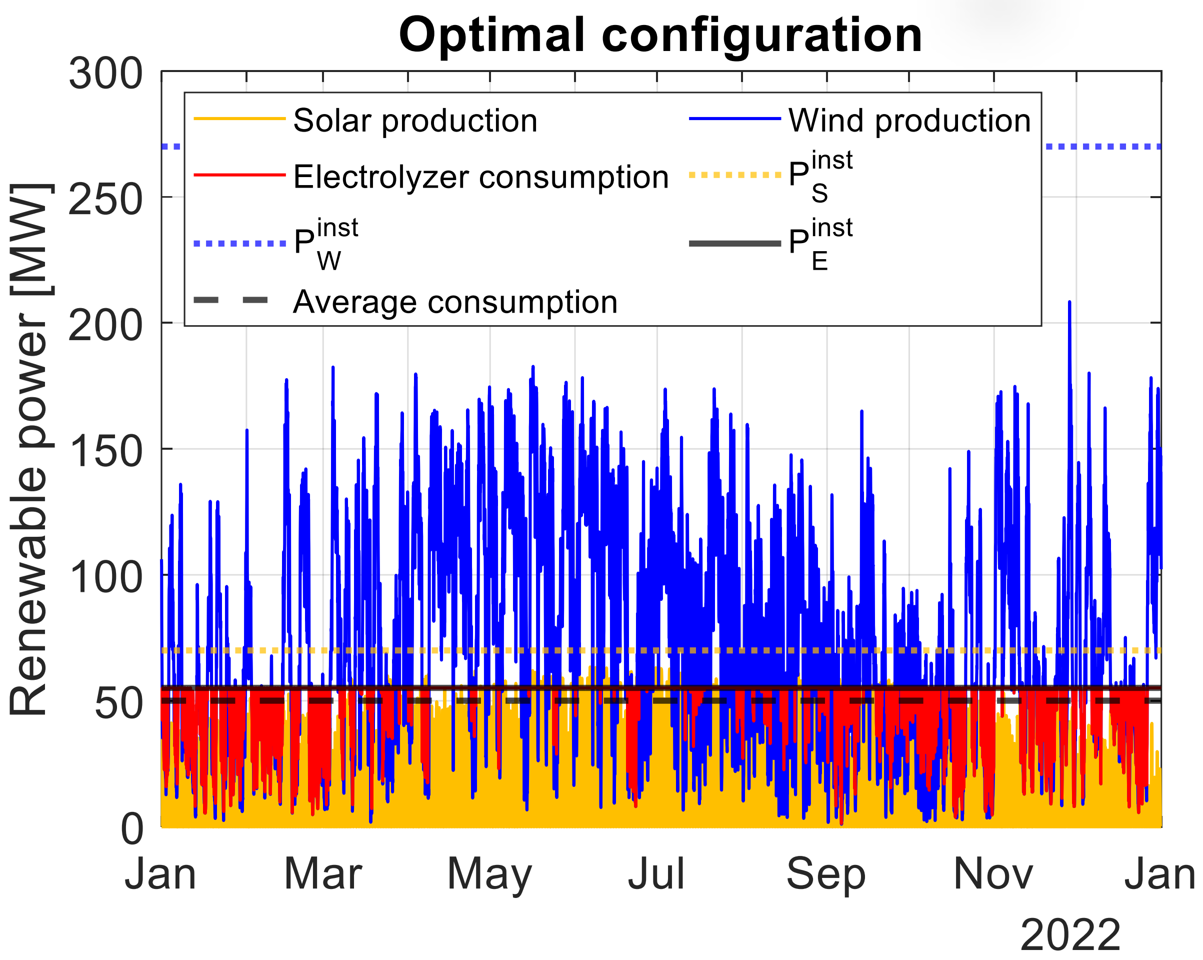
California (CAISO) wind profiles in 2022

Hp. Flexible operation	
MAX	+10%
MIN	−30%
(w.r.t. TARGET)	



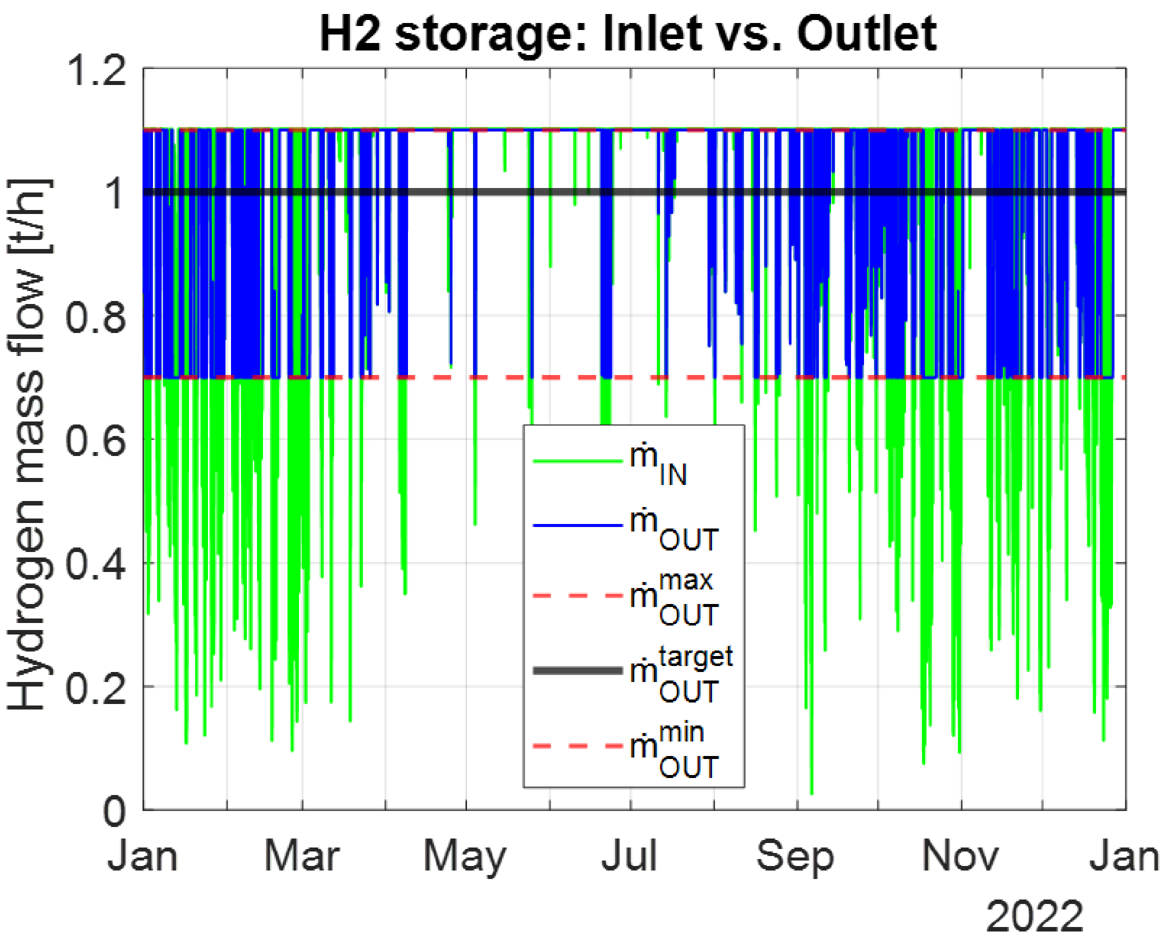
Solar/Wind park + Electrolyzer + H_2 storage



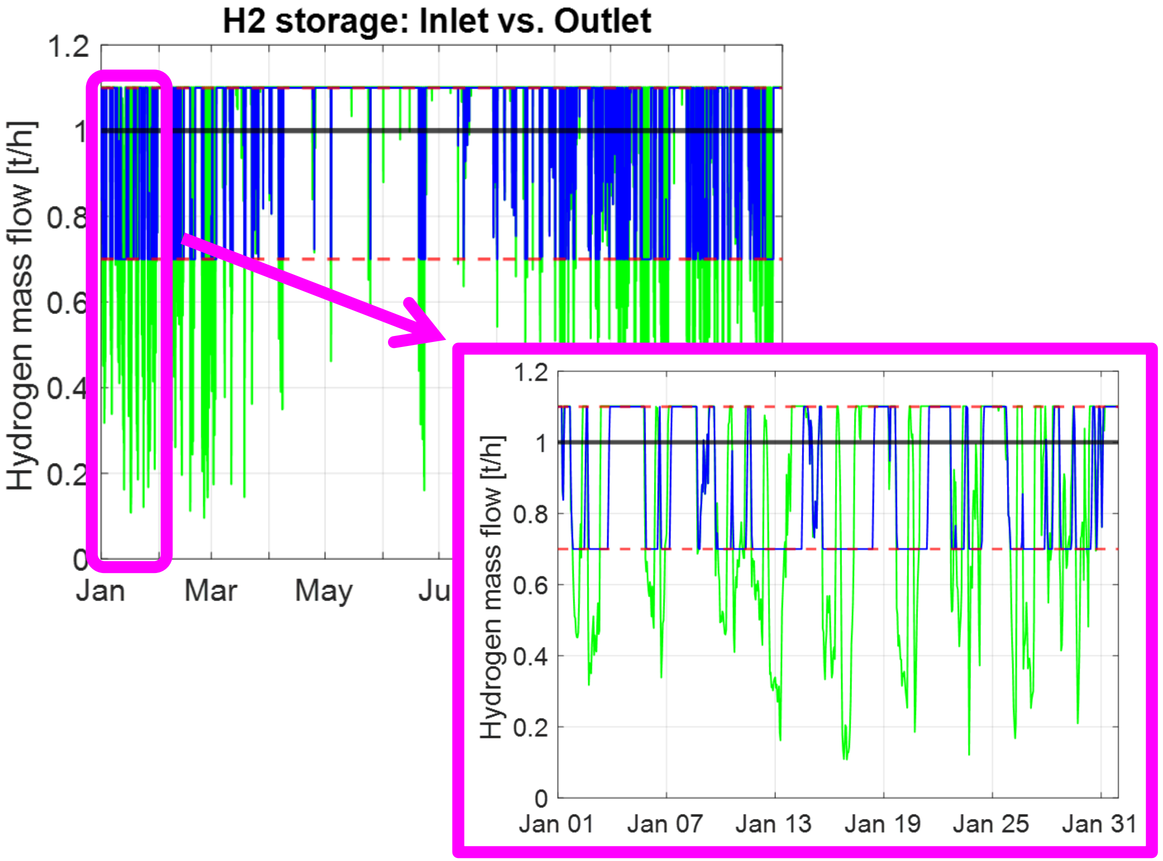


Solar [MW]	Wind [MW]	Electrolyzer [MW]	LCOH [USD/kg]
70	270	55	**4.31**

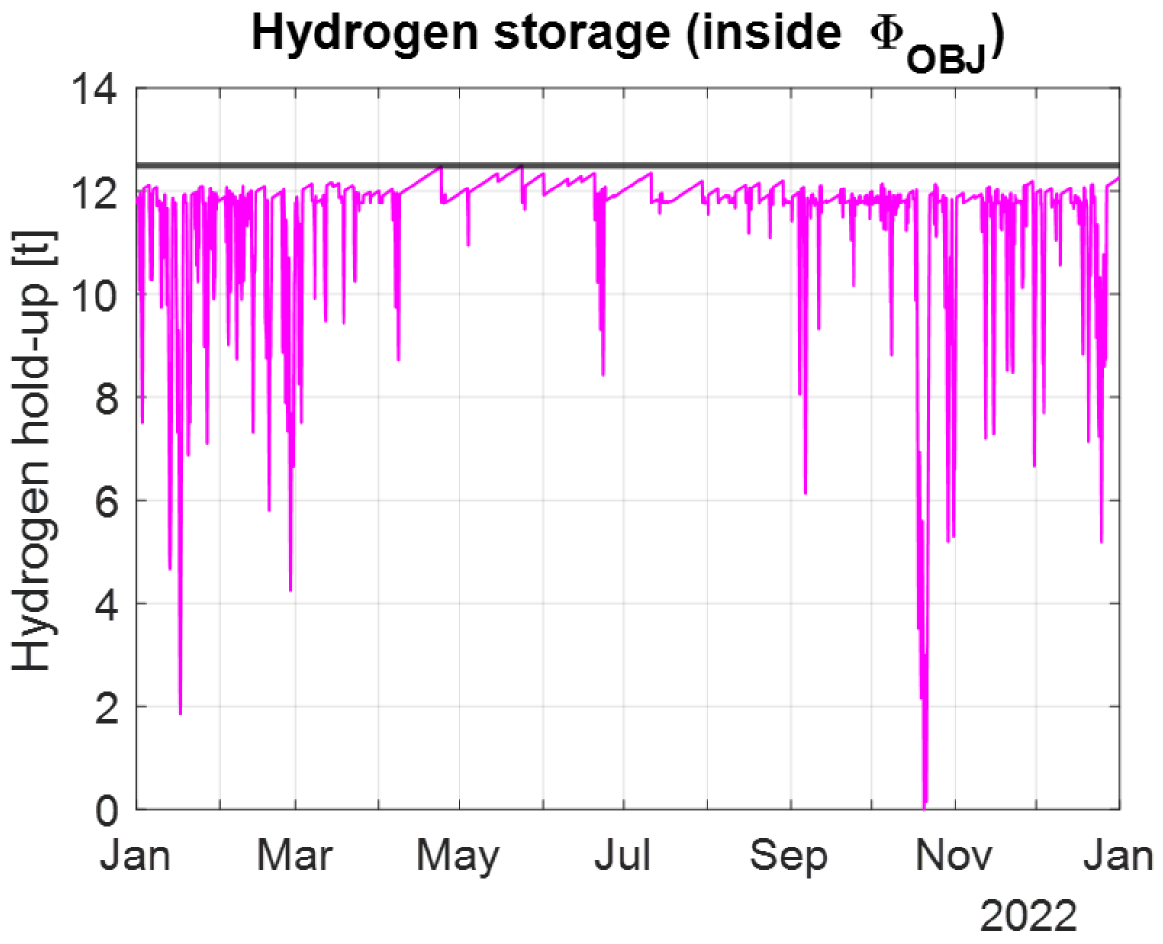
H_2 storage



Storage capacity [t]
12.5



H_2 storage



Storage capacity [t]
12.5

Take-away messages

In summary:

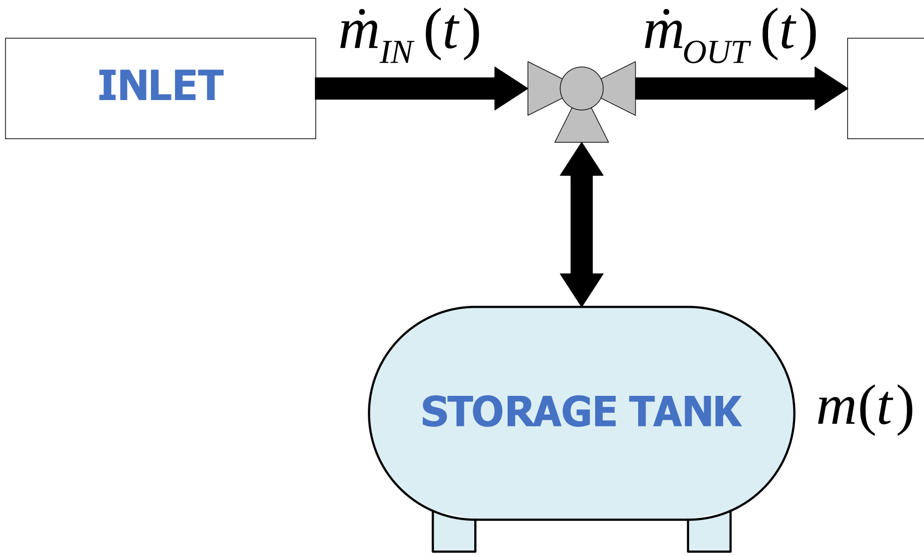
- The **control volume of the optimization problem** shows a **crucial** impact on the results.
- When addressing the **H_2 storage** (*e.g.*, in case of downstream conversion processes), the optimal configurations typically show **wind power oversizing** as its higher daily/seasonal availability allows for smaller storage (→ higher amounts of renewable energy to be **curtailed**).

We developed a flexible tool that determines the optimal design (*i.e.*, renewable park, electrolyzer, and electricity/hydrogen storage sizes) of green H_2 production facilities.

Optimal hydrogen storage

Optimally-flexible mass storage

Isella & Manca (Under Review). **International Journal of Hydrogen Energy**.



Given the mass balance of the storage node:

$$\frac{d}{dt}m(t) = \dot{m}_{IN}(t) - \dot{m}_{OUT}(t)$$

How should this term behave to minimize the accumulation instantaneously? (hence the storage capacity)

By applying the following operating schedule…

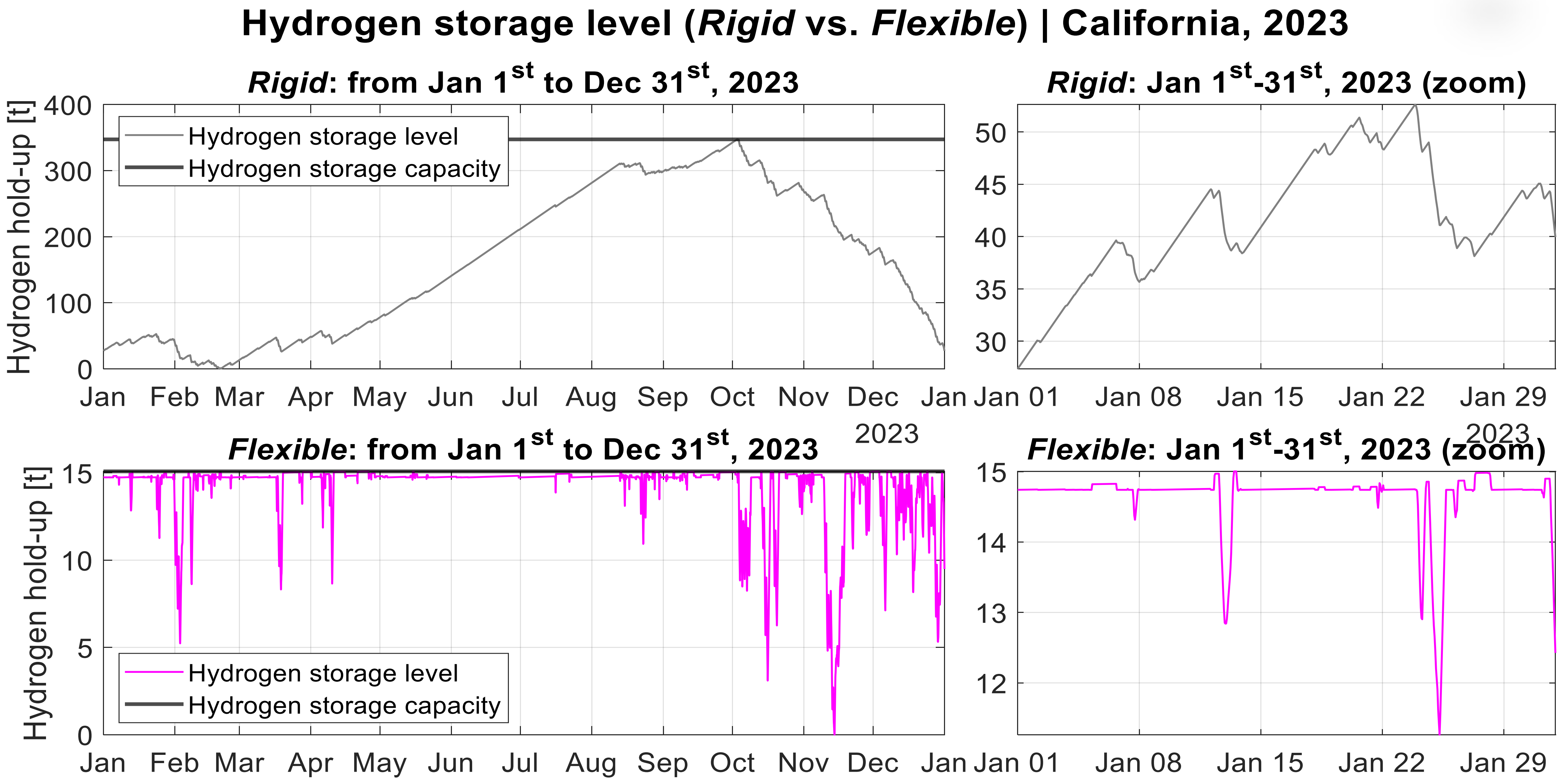
$$\dot{m}_{OUT}(t) = \dot{m}_{IN}(t) + \frac{1}{\Delta t} \cdot \int_{1}^{t-1} \left[\dot{m}_{IN}(\tau) - \dot{m}_{OUT}(\tau) \right] d\tau$$

+ Filtering for compliance with the upper and lower limits and allowable ramping rates of the downstream process

… the storage size is:

$$m_{tot} = \max\left(\sum_{\tau=1}^{t} \left[\dot{m}_{IN}(\tau) - \dot{m}_{OUT}(\tau) \right] \Delta t \right) - \min\left(\sum_{\tau=1}^{t} \left[\dot{m}_{IN}(\tau) - \dot{m}_{OUT}(\tau) \right] \Delta t \right)$$

An example: the same case study with Rigid vs. Flex storage

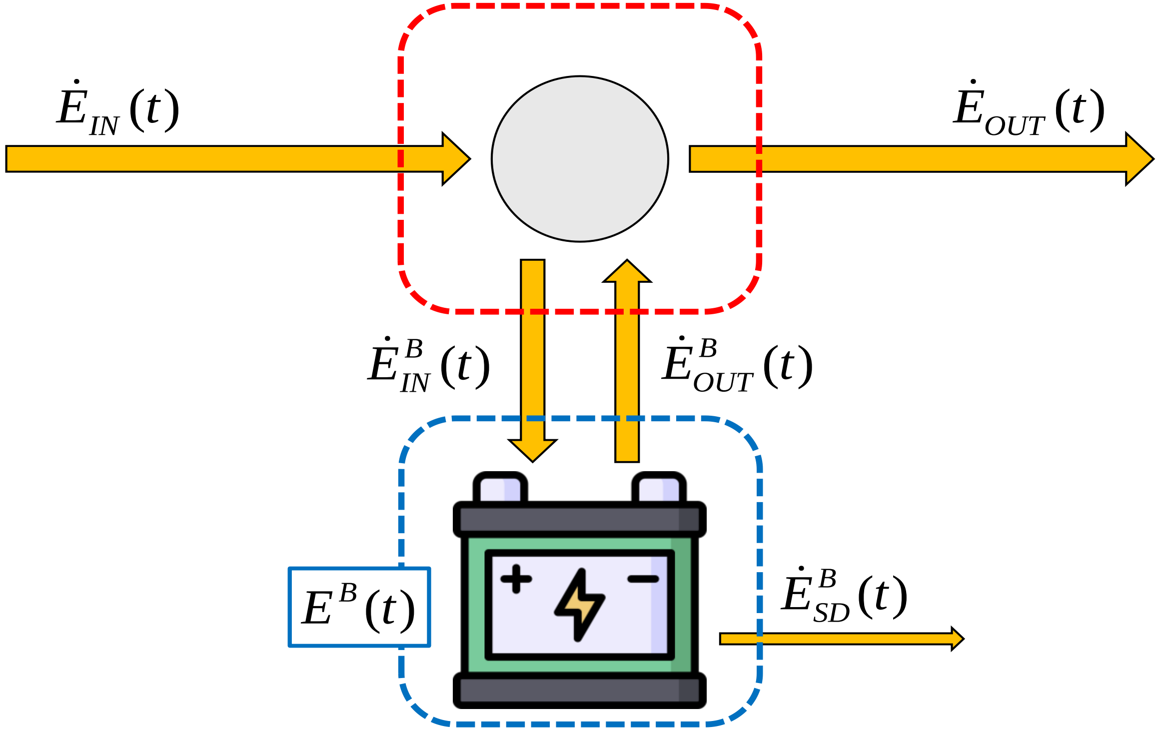


Isella & Manca (Under Review). **International Journal of Hydrogen Energy**.

Optimal electricity storage

Optimally-flexible electricity storage

Isella & Manca (Submitted). **Journal of Energy Storage**.



Given the energy balance of the battery:

$$\frac{d}{dt}E^{B}(t)=\eta_{C}\cdot\dot{E}_{IN}^{B}(t)-\frac{1}{\eta_{D}}\cdot\dot{E}_{OUT}^{B}(t)-\dot{E}_{SD}^{B}(t)$$

Case (i) : charging

if $\dot{E}_{IN}(t)-\dot{E}_{OUT}(t)\geq 0$

$$\begin{cases}\dot{E}_{IN}^{B}(t)=\left|\dot{E}_{IN}(t)-\dot{E}_{OUT}(t)\right| \\ \dot{E}_{OUT}^{B}(t)=0 \\ \frac{d}{dt}E^{B}(t)=\eta_{C}\cdot\left|\dot{E}_{IN}(t)-\dot{E}_{OUT}(t)\right|\end{cases}$$

Case (ii) : discharging

if $\dot{E}_{IN}(t)-\dot{E}_{OUT}(t)<0$

$$\begin{cases}\dot{E}_{IN}^{B}(t)=0 \\ \dot{E}_{OUT}^{B}(t)=\left|\dot{E}_{IN}(t)-\dot{E}_{OUT}(t)\right| \\ \frac{d}{dt}E^{B}(t)=-\frac{1}{\eta_{D}}\cdot\left|\dot{E}_{IN}(t)-\dot{E}_{OUT}(t)\right|\end{cases}$$

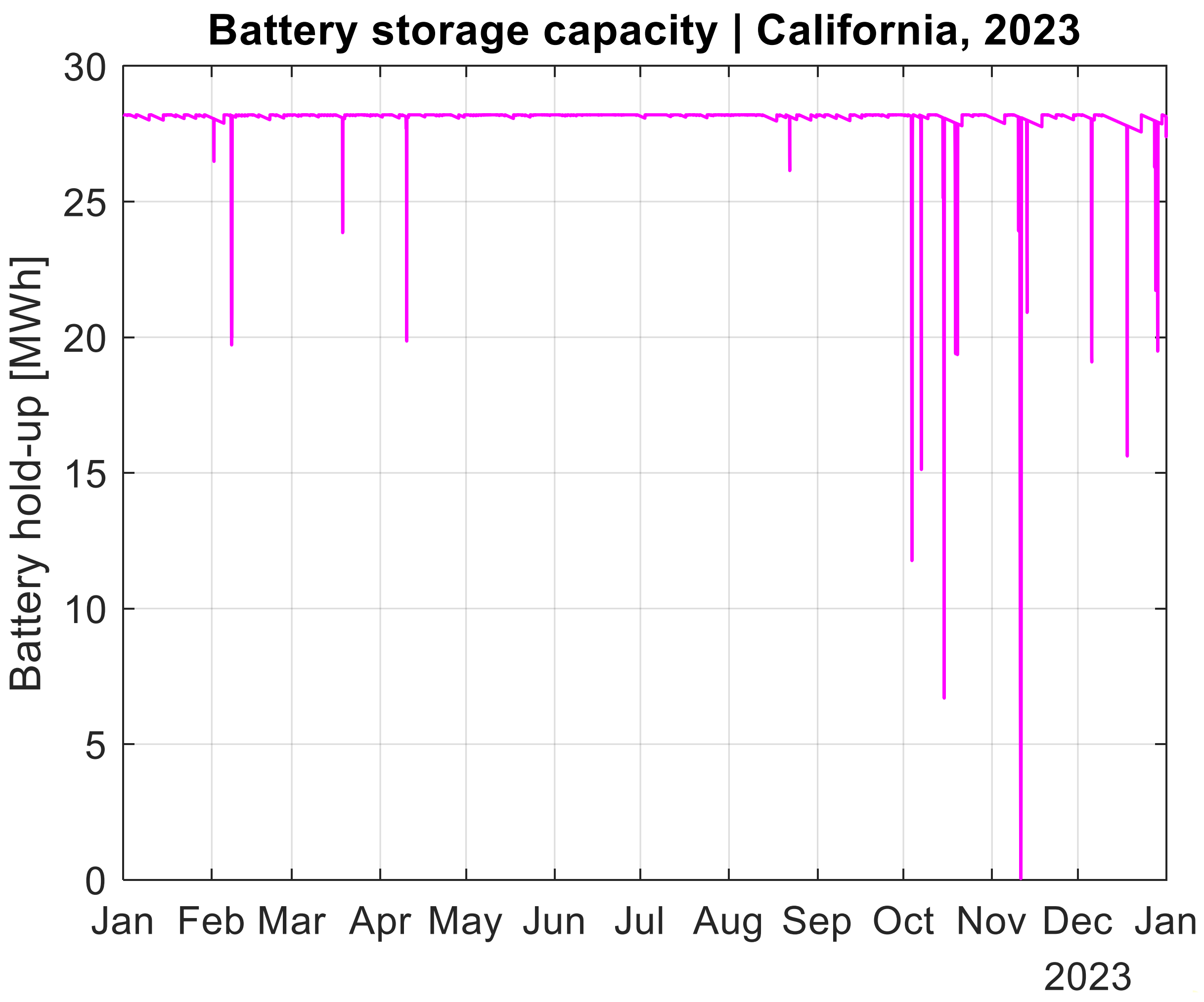
The operating schedule minimizing the storage capacity is:

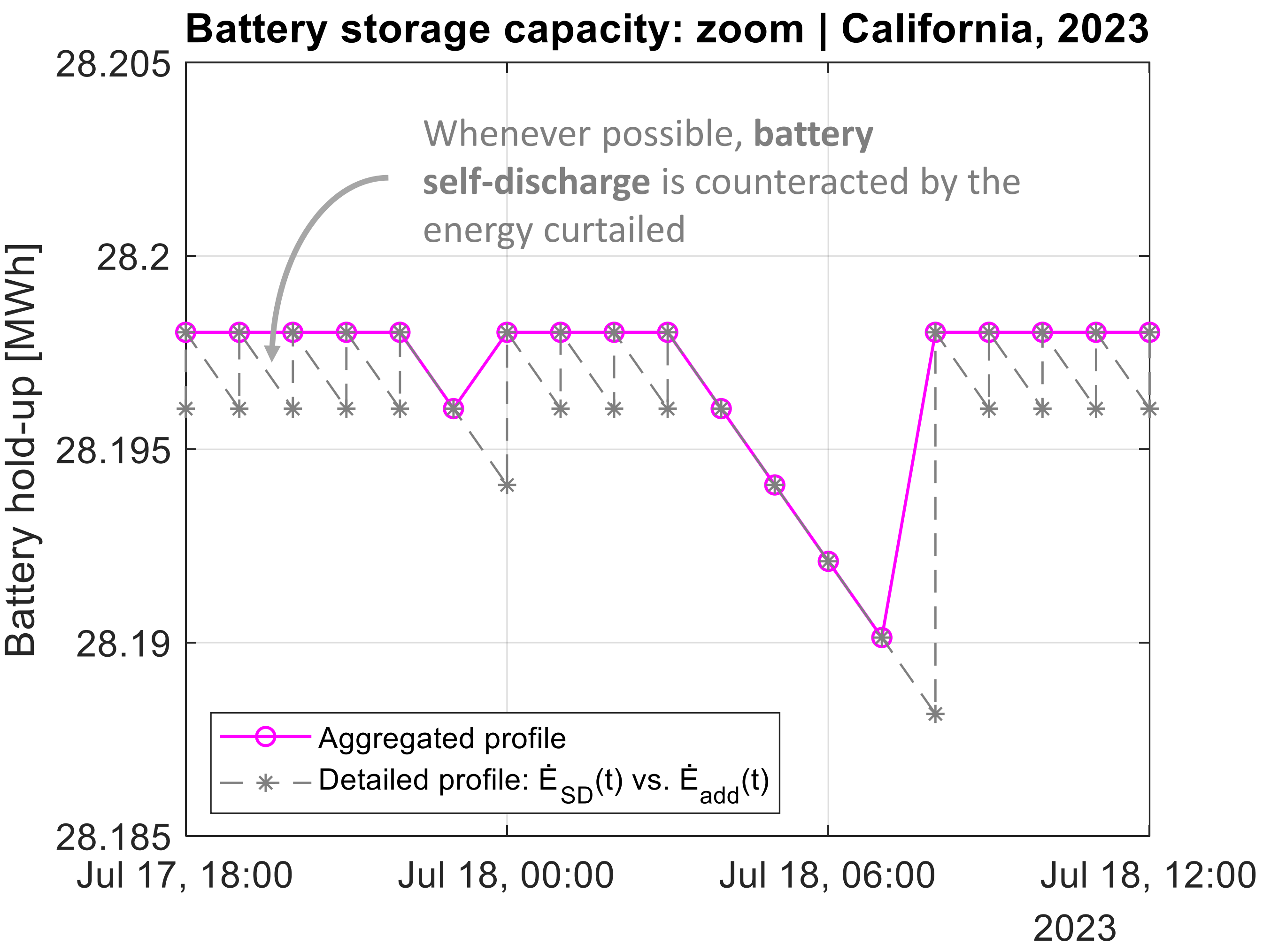
$$\dot{E}_{OUT}(t)=\begin{cases}\dot{E}_{IN}(t)+\left[\eta_{D}\cdot\sum_{\tau=1}^{t-1}\left(\frac{d}{dt}E^{B}(\tau)\right)\right] & \text{if } \sum_{\tau=1}^{t-1}\left(\frac{d}{dt}E^{B}(\tau)\right)\geq 0 \\ \dot{E}_{IN}(t)+\left[\frac{1}{\eta_{C}}\cdot\sum_{\tau=1}^{t-1}\left(\frac{d}{dt}E^{B}(\tau)\right)\right] & \text{if } \sum_{\tau=1}^{t-1}\left(\frac{d}{dt}E^{B}(\tau)\right)<0\end{cases}$$

✚ Filtering for compliance with the upper and lower limits and allowable ramping rates of the downstream process

Optimally-flexible electricity storage: an application

Isella & Manca (Submitted). **Journal of Energy Storage**.



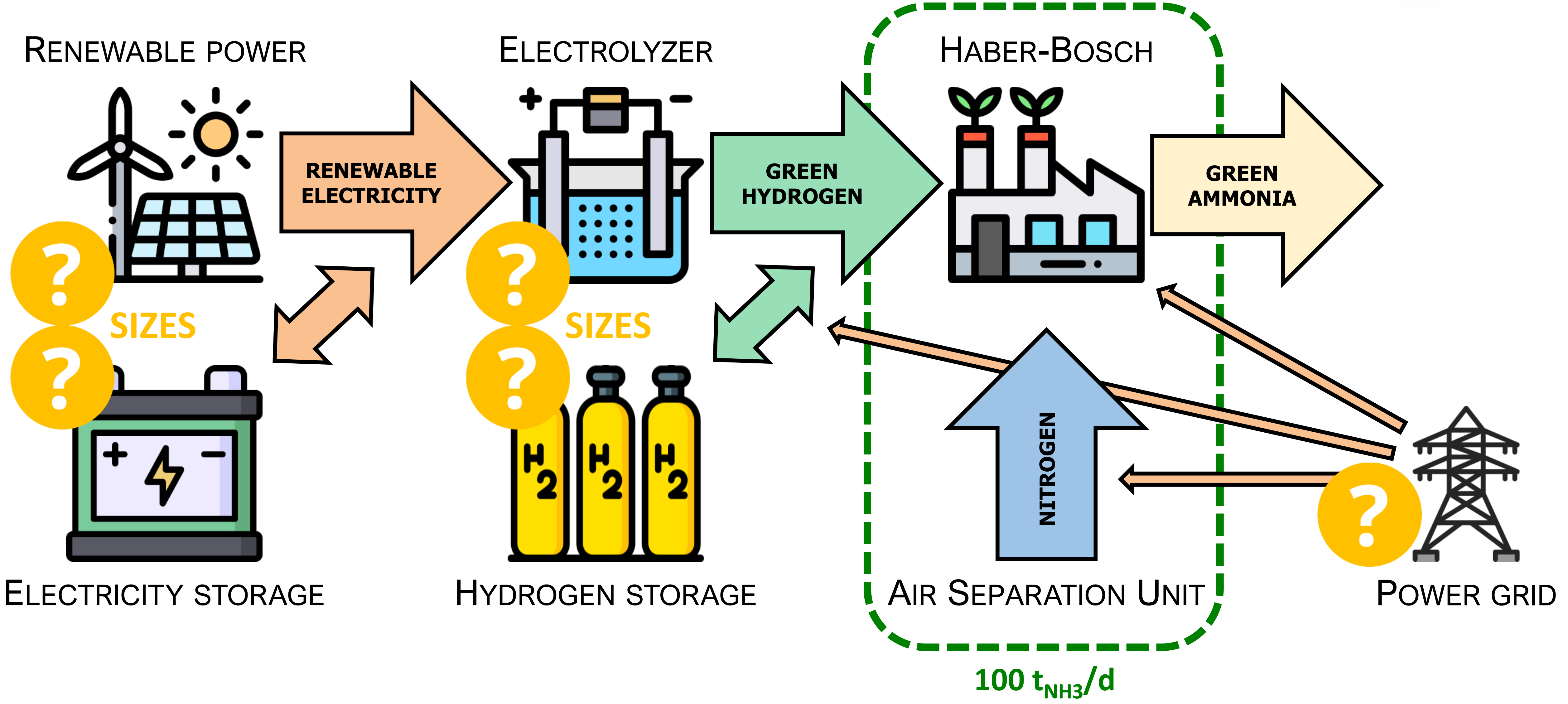


Sustainability of a green ammonia plant

Power-to-Ammonia (P2A) plant

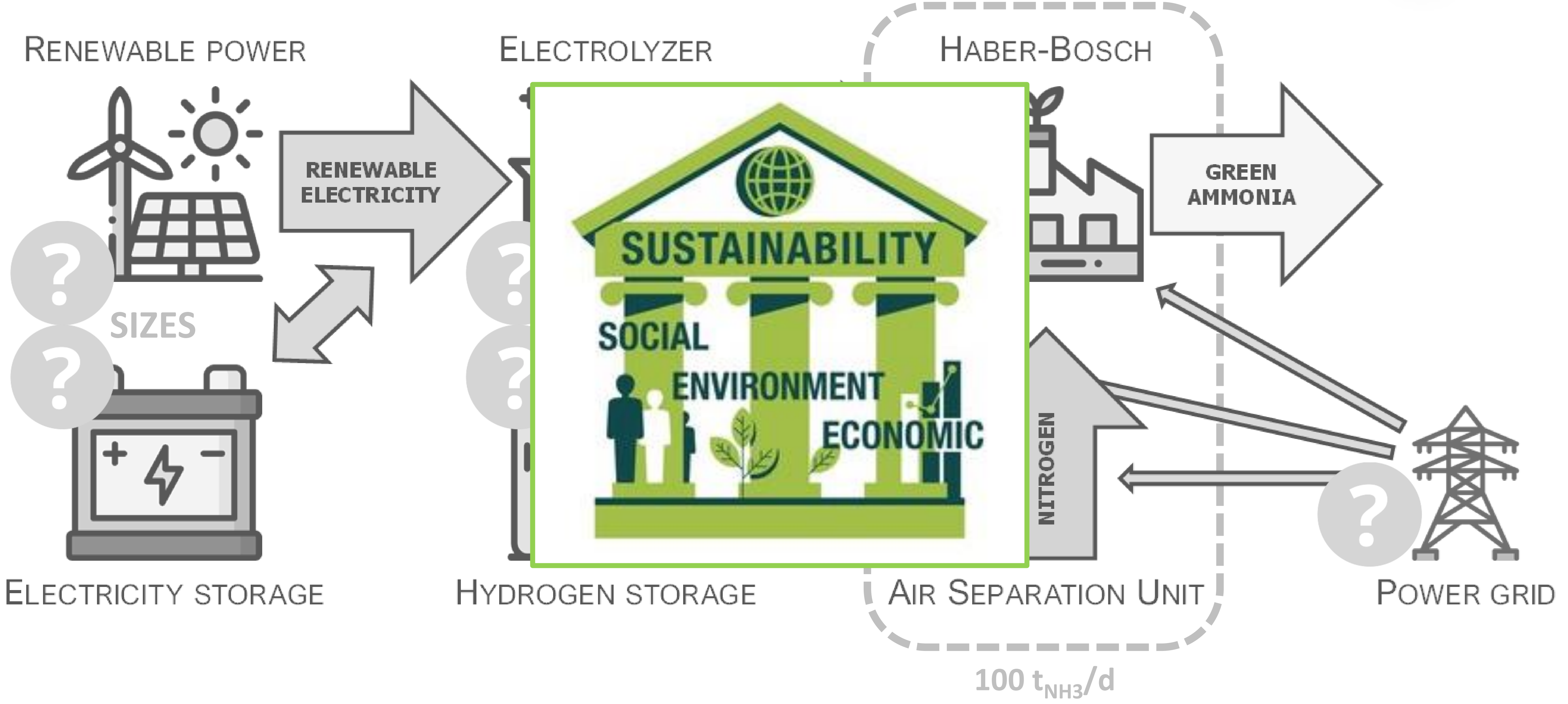
i.e., green ammonia production from renewable power

Isella & Manca (Submitted). **Computers & Chemical Engineering.**



Power-to-Ammonia (P2A) plant
i.e., green ammonia production from renewable power

Isella & Manca (Submitted). **Computers & Chemical Engineering**.



The single-objective optimization (SOO) problem

Isella & Manca (Submitted). **Computers & Chemical Engineering**.

MATLAB

$$\min_{P^S_{\text{inst}},\,P^W_{\text{inst}}} \left[\Phi^{X}_{\text{OBJ}}\right] \quad \text{with X = ECO, ENV, or SOC}$$

s.t.:

$$\dot{E}_{IN}(t) = \min\left(\dot{E}^S(t) + \dot{E}^W(t), P^E_{\text{inst}}\right) \qquad \text{(a)}$$

MATLAB

$$\dot{E}_{OUT}(t) = \begin{cases} \dot{E}_{IN}(t) + \left[\eta_D \cdot \sum_{\tau=1}^{t-1}\left(\frac{d}{dt}E^B(\tau)\right)\right] & \text{if } \sum_{\tau=1}^{t-1}\left(\frac{d}{dt}E^B(\tau)\right) \geq 0 \quad \text{(i)} \\ \dot{E}_{IN}(t) + \left[\frac{1}{\eta_C} \cdot \sum_{\tau=1}^{t-1}\left(\frac{d}{dt}E^B(\tau)\right)\right] & \text{if } \sum_{\tau=1}^{t-1}\left(\frac{d}{dt}E^B(\tau)\right) < 0 \quad \text{(ii)} \end{cases} \qquad \text{(b)}$$

$$\sum_{\tau=1}^{8760} \dot{E}_{OUT}(\tau) = 8760 \cdot \dot{E}^E_{\text{target}} \qquad \text{(c)}$$

$$\dot{m}^{H_2}_{IN}(t) = \dot{E}_{OUT}(t) \cdot \frac{\rho_{H_2}}{\eta_E} \qquad \text{(d)}$$

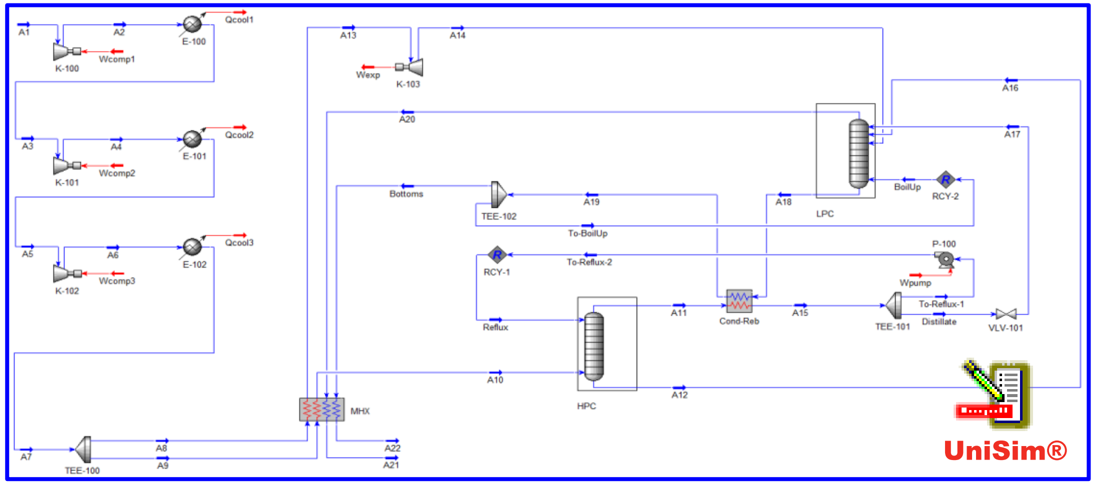
MATLAB

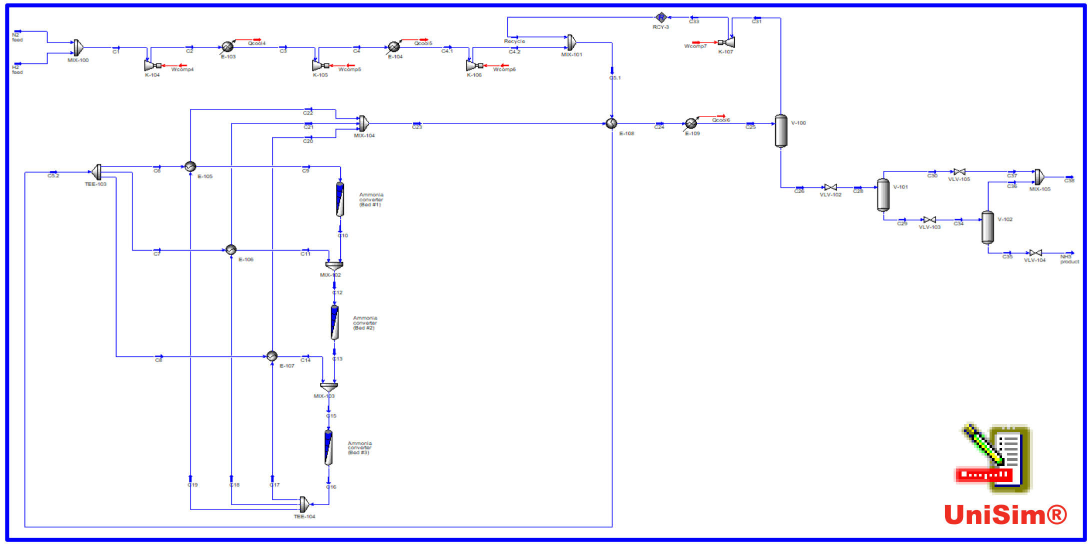
$$\dot{m}^{H_2}_{OUT}(t) = \dot{m}^{H_2}_{IN}(t) + \sum_{\tau=1}^{t-1}\left[\dot{m}^{H_2}_{IN}(\tau) - \dot{m}^{H_2}_{OUT}(\tau)\right] \qquad \text{(e)}$$

HC process simulation (Mass and Energy balances) (f)

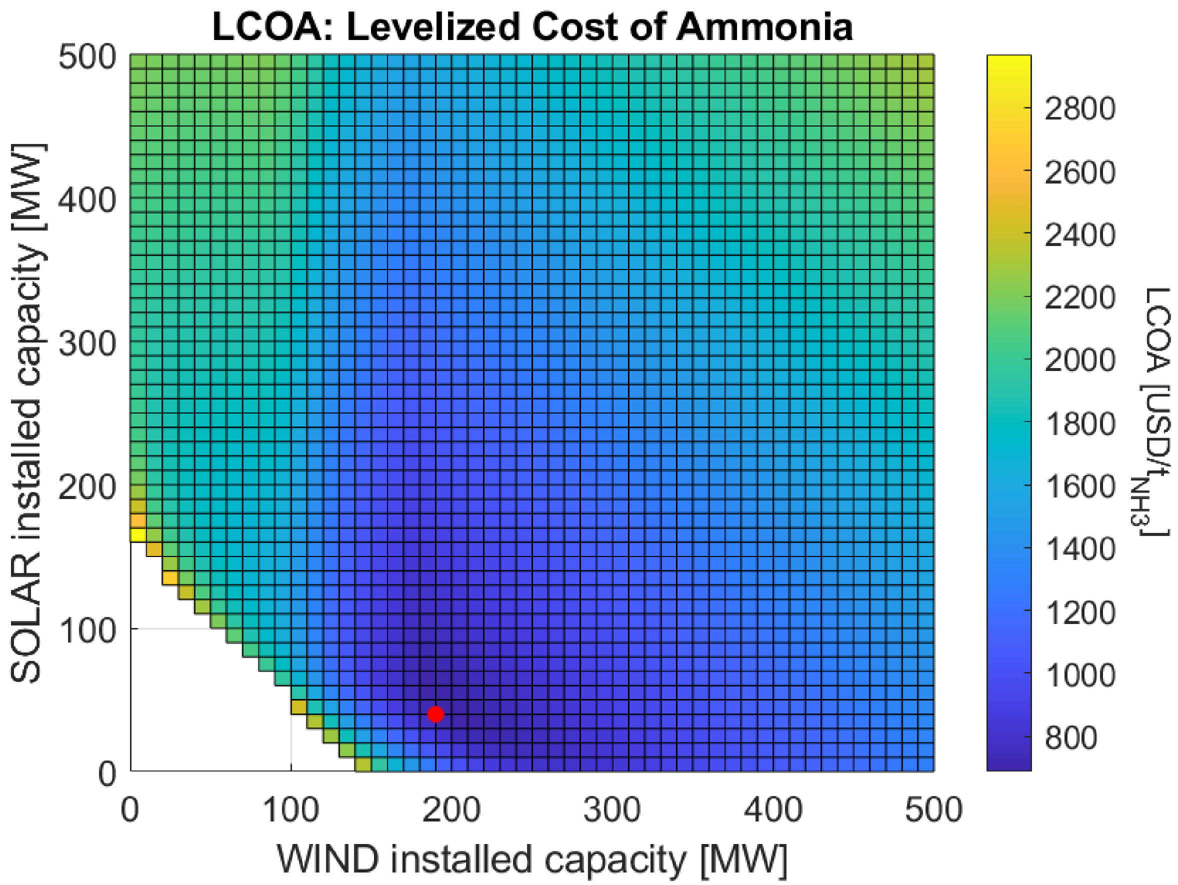
ASU process simulation (Mass and Energy balances) (g)

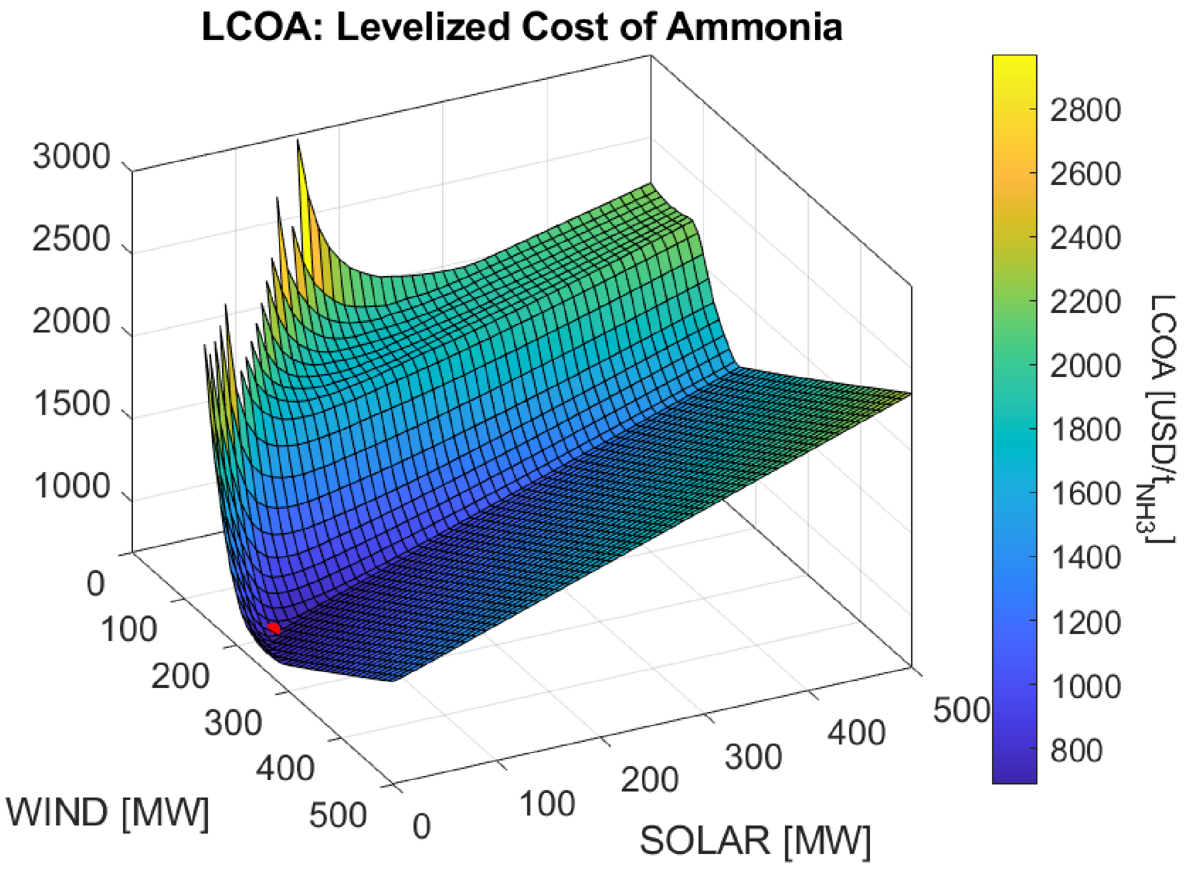
HB process simulation (Mass and Energy balances) (h)





Economic optimization: LCOA





$$\Phi_{OBJ}^{ECO} = LCOA = \frac{\sum_{j=S,W,B,E,H,G} \left(\frac{CAPEX_j}{\sum_{n=1}^{NY_j} (1+r)^{-n}} + OPEX_j \right)}{8760 \cdot \dot{m}_{target}^{NH_3}}$$

The **ECONOMIC** sustainability objective function is the **Levelized Cost of Ammonia** (**LCOA**)

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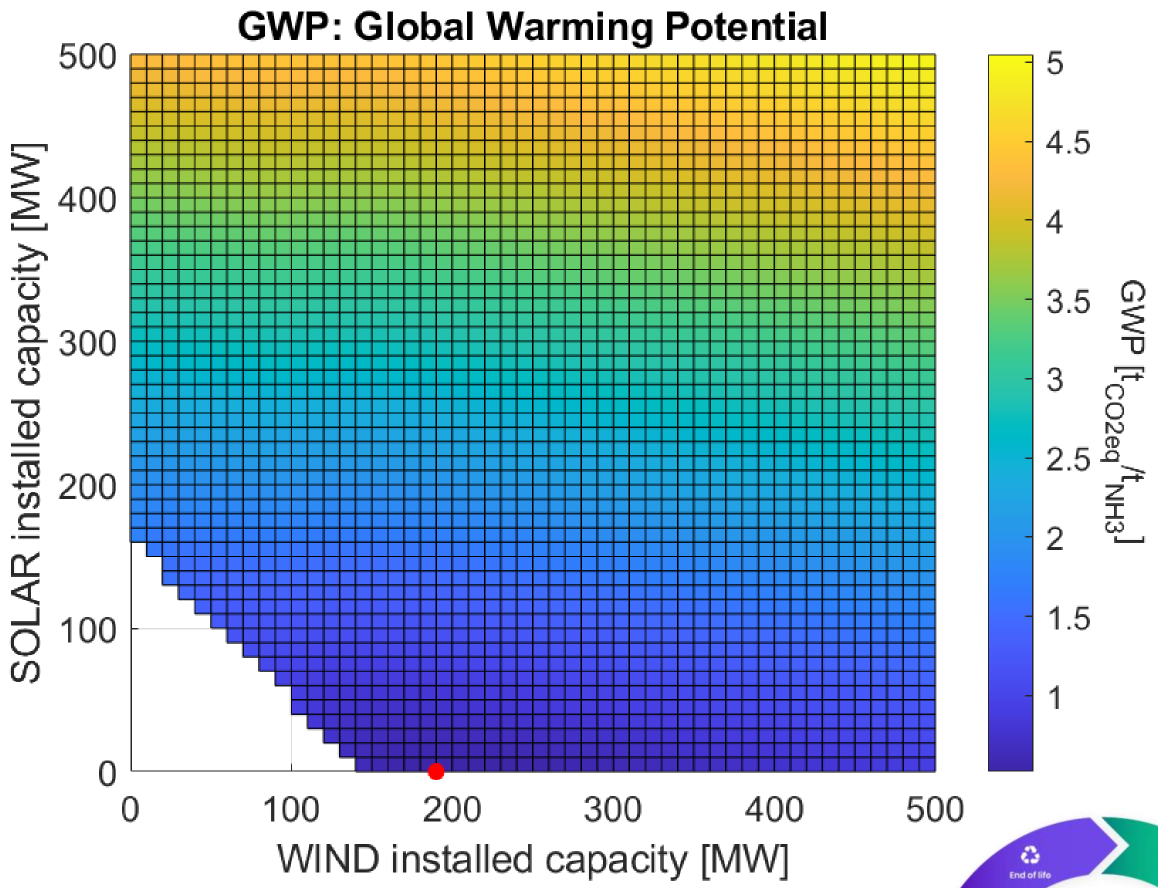
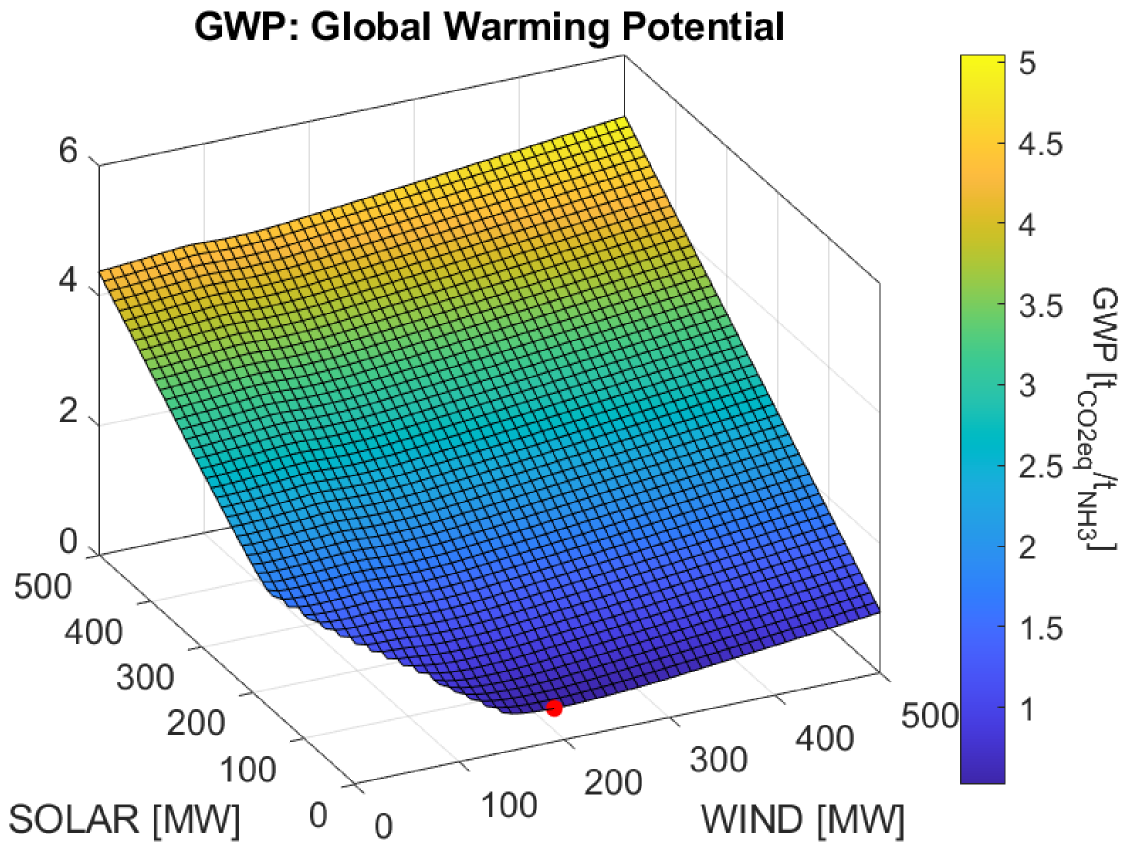
Environmental optimization: GWP



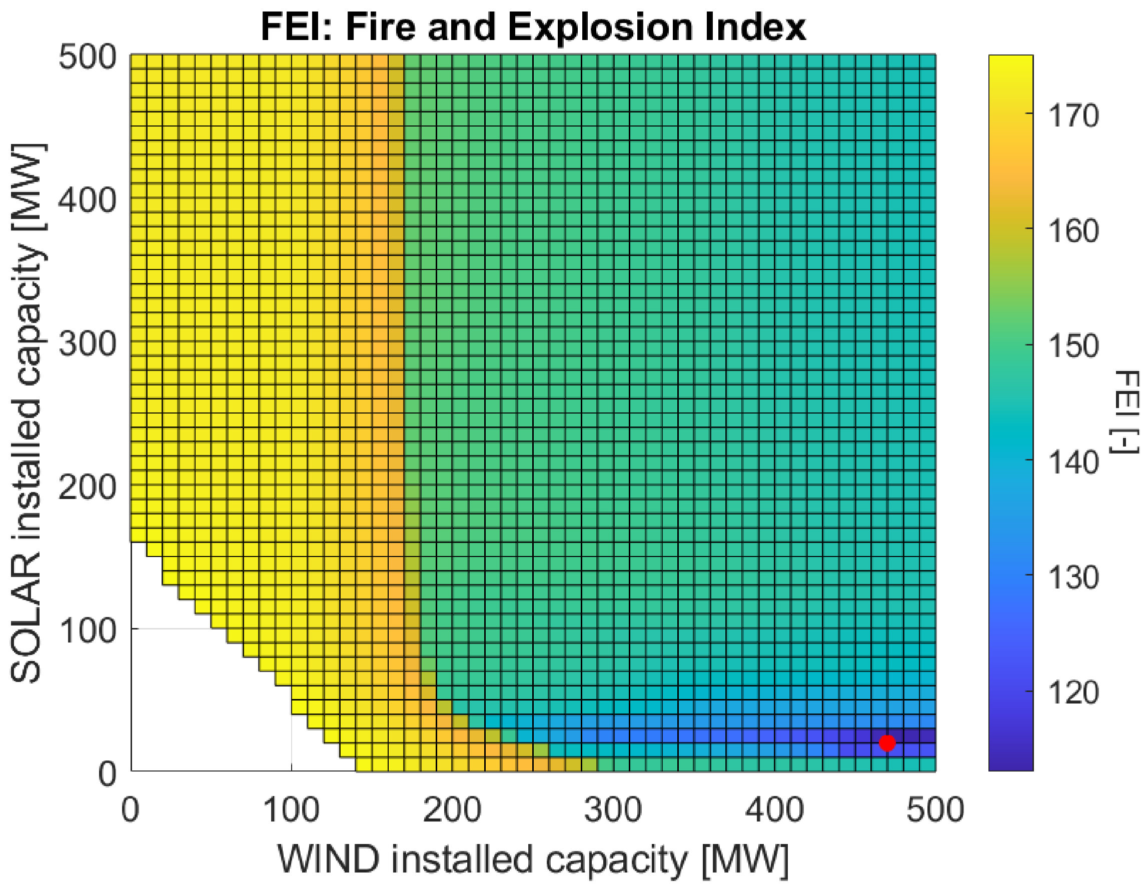


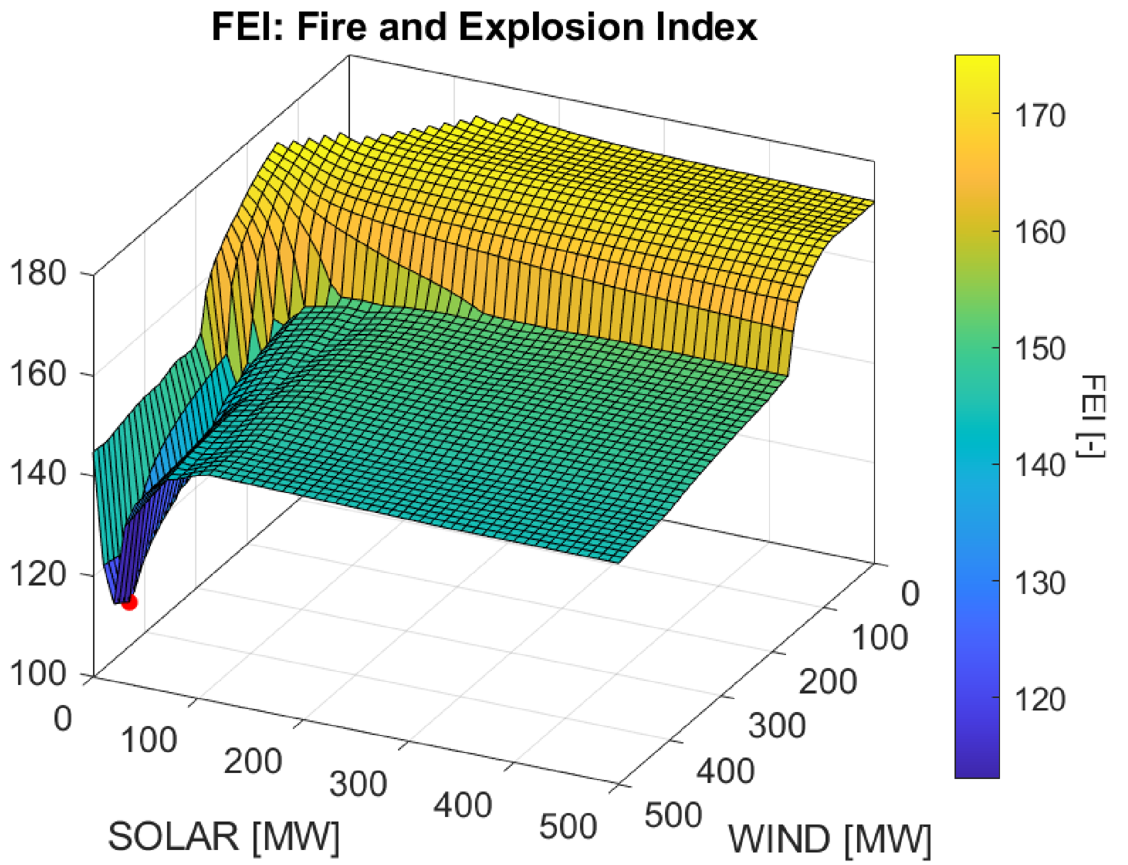
$$\Phi_{\text{OBJ}}^{\text{ENV}} = GWP_{\text{tot}} = \frac{\sum_{j=S,W,B,E,H,G} \left(GWP_j^y \right)}{8760 \cdot \dot{m}_{\text{target}}^{NH_3}}$$

The **ENVIRONMENTAL** sustainability objective function is the **Global Warming Potential** (**GWP**) by the plant

Isella & Manca (Submitted). **Computers & Chemical Engineering**.

Social optimization: FEI





$$\Phi_{\mathrm{OBJ}}^{\mathrm{SOC}} = FEI_{tot} = \sum_{j=E,H} \left(FEI_j \right)$$

Electrolyzer
and **H_2 storage**
Both handle
hydrogen
(hazards)

The **SOCIAL** sustainability objective function is the **Fire and Explosion Index** (**FEI**) by the plant

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The multi-objective optimization (MOO) problem

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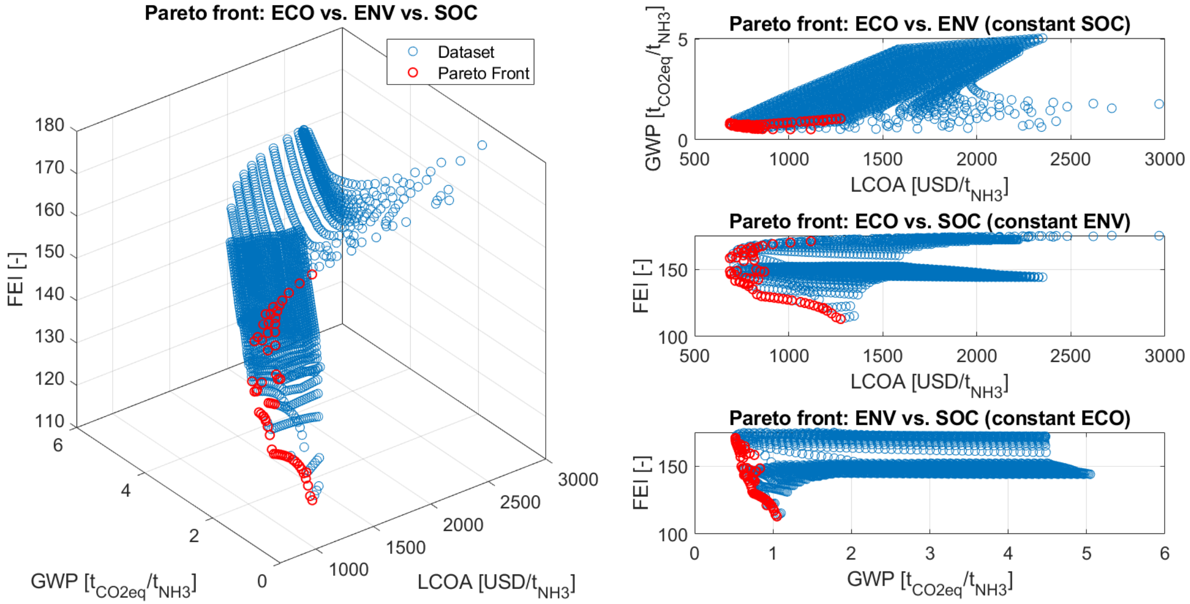
Solving MOO problems always requires some human decision-making

a posteriori

Pareto front analysis



Postponing the decision process after the searching phase, evaluating those points within the decision space whose corresponding objective functions cannot be all simultaneously improved

a priori

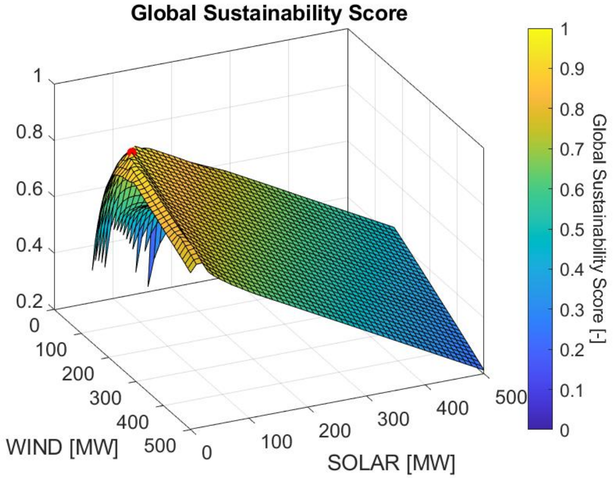
Scalarization

$$GSS = \left\{ w_{ECO} \cdot EcoSI + w_{ENV} \cdot EnvSI + w_{SOC} \cdot SocSI \right\}$$

$$EcoSI_i = \frac{\max(LCOA) - LCOA_i}{\max(LCOA) - \min(LCOA)}$$

$$EnvSI_i = \frac{\max(GWP) - GWP_i}{\max(GWP) - \min(GWP)}$$

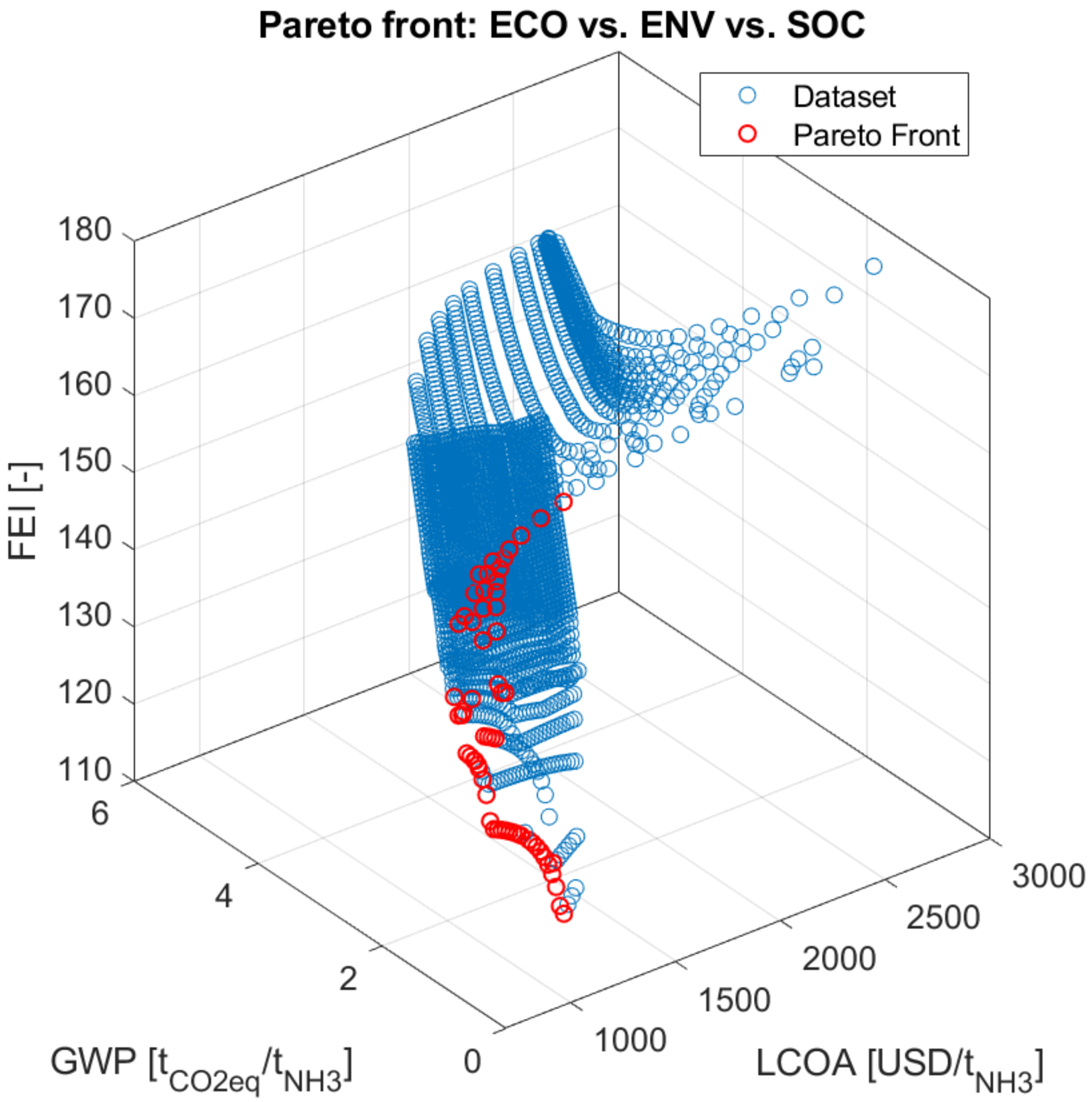
$$SocSI_i = \frac{\max(FEI) - FEI_i}{\max(FEI) - \min(FEI)}$$

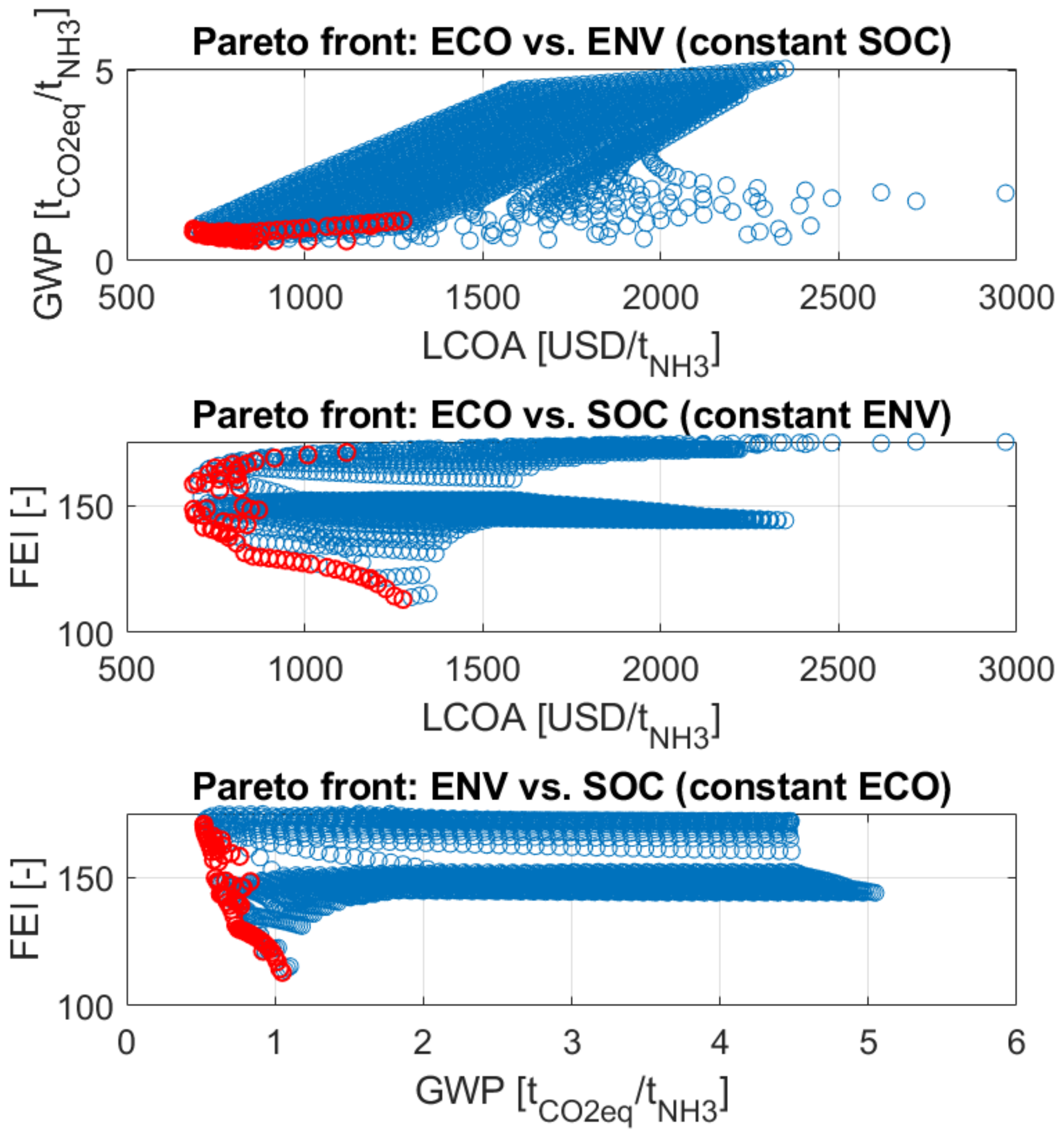


Combining more objective functions into one through an appropriate scalarization function (*e.g.*, linear combination)

→ **weight values** = core of the decision-making process

MOO problem → Pareto front analysis





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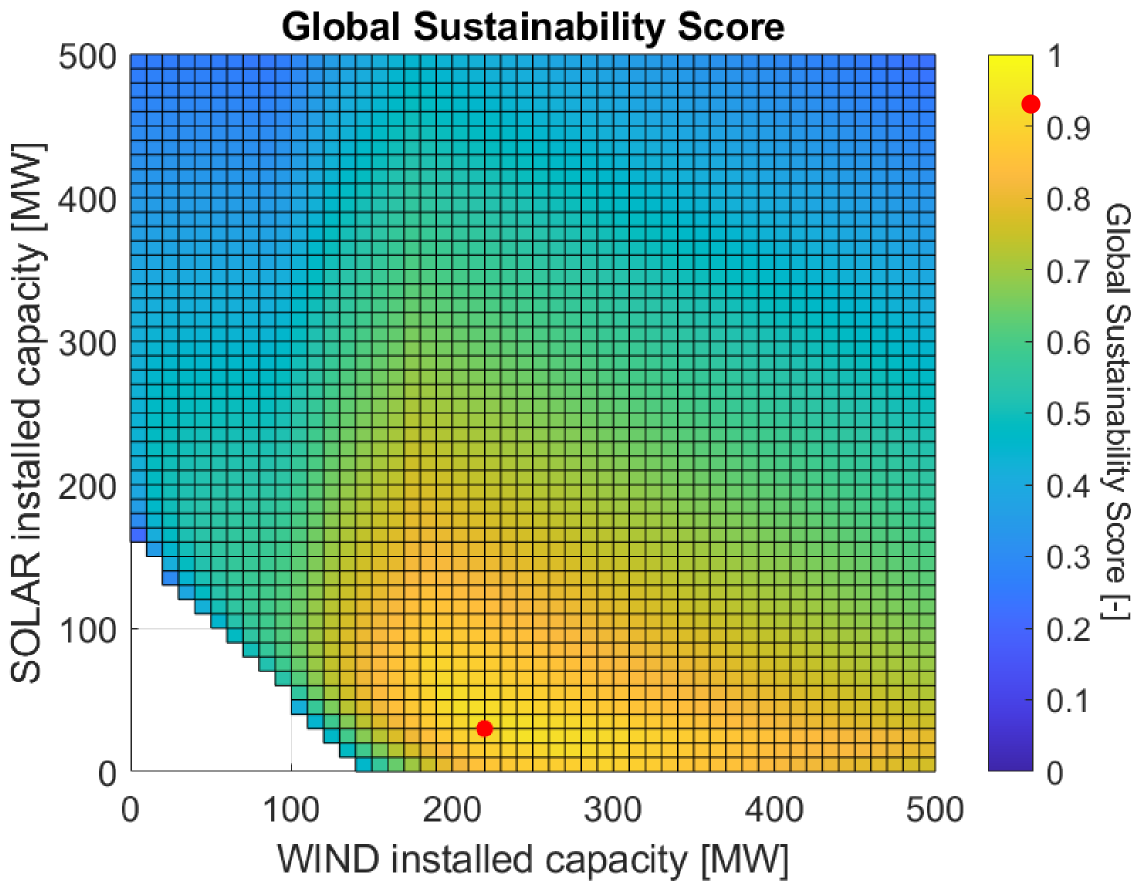
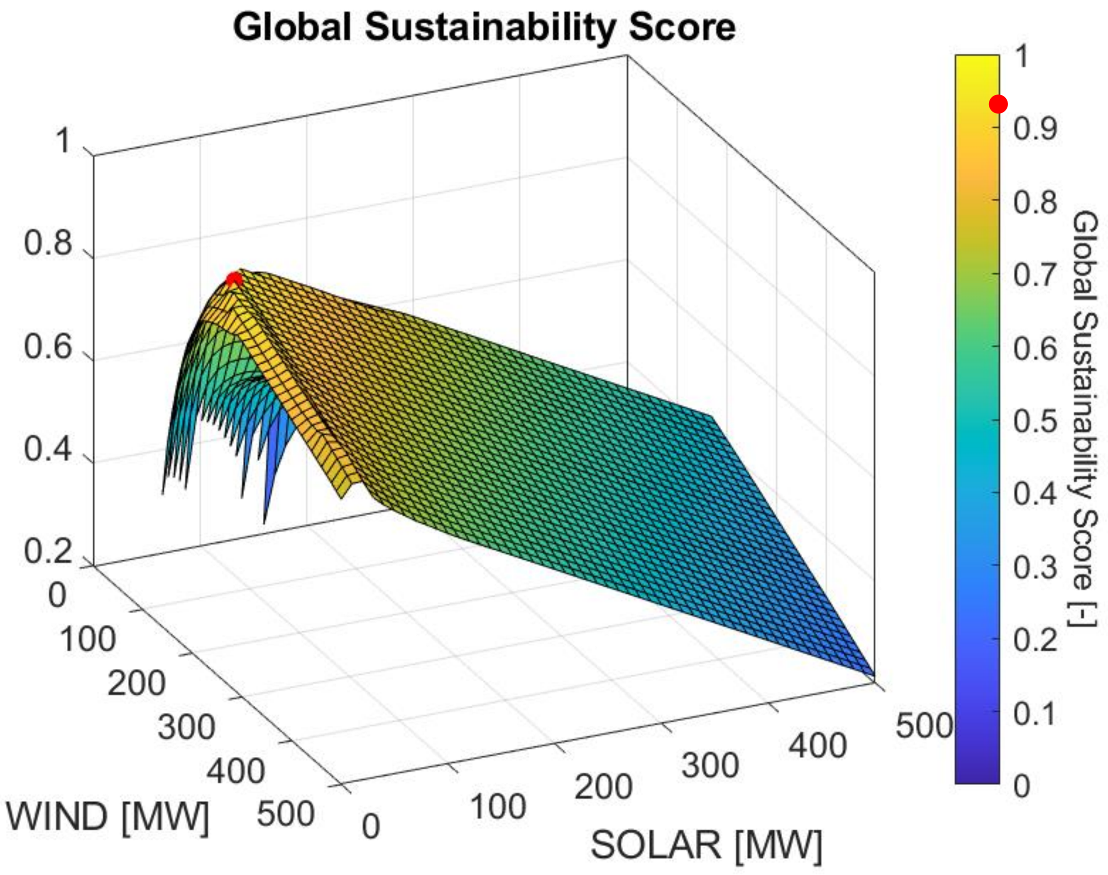
MOO problem → Scalarization





$$\textbf{Max}\{GSS\} = \left(w_{\text{ECO}} \cdot EcoSI + w_{\text{ENV}} \cdot EnvSI + w_{\text{SOC}} \cdot SocSI\right)$$

$$\text{with} \quad w_{\text{ECO}} + w_{\text{ENV}} + w_{\text{SOC}} = 1$$

The Global Sustainability Score (**GSS**) is the linear combination of the **ECO**, **ENV**, and **SOC** indexes, those coefficients act as user-defined weighting factors for each sustainability pillar (*e.g.*, **60%**+**30%**+**10%**)

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Conclusions

Conclusions

- The chemical industry is undergoing a **paradigm shift from steady-state to discontinuous processes**, driven by the adoption of **renewable energy sources** and the need for more **sustainable, flexible, and resilient operations**.

- **Renewable energy sources**, such as solar and wind, introduce significant **variability and intermittency** to chemical processes, necessitating **new approaches** to process design, control, and optimization.

- **Hybrid-green ammonia** production, which combines conventional and **renewable hydrogen sources**, offers a promising **pathway for decarbonizing** the ammonia industry while **maintaining economic viability**.

- **Optimal sizing** and integration of **hydrogen storage systems** are crucial for managing the variability of renewable energy inputs and ensuring stable downstream process operations.

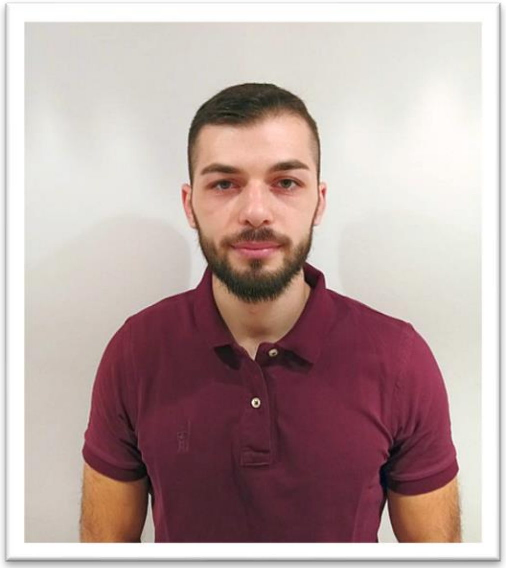
- Advanced optimization techniques, such as **multi-objective optimization** considering **economic, environmental, and social factors**, are essential for designing sustainable and efficient green chemical processes.

Future Developments

- Further research is needed to develop **robust control strategies** and **process intensification techniques** that enable chemical plants to operate flexibly and efficiently under variable renewable energy inputs.
- The integration of **advanced data analytics, machine learning, and digital twin technologies** will be crucial for real-time monitoring, optimization, and decision-making in the context of **discontinuous green chemical processes**.
- Investigating the potential **synergies between green chemical processes and other sectors**, such as **transportation**, **energy storage**, and **waste management**, will open up new opportunities for industrial symbiosis and **circular economy solutions**.
- Developing **innovative business models** and **policy frameworks** that incentivize **adopting green chemical technologies** and support the transition towards a more sustainable and resilient chemical industry will be essential for driving progress in this field.

A Sincere Thank You

I want to take a moment to thank two key members of our research team at PSE-Lab:



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Green Chemical Engineering: Tackling Discontinuities for a More Sustainable Future

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