Linking Cluster-Level and National-Level Models

to assess chemical industry transition pathways

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Why?

- Chemical industry is a critical part of the transition to net-zero emissions
- Even greater climate impact when considering embedded carbon in chemical products

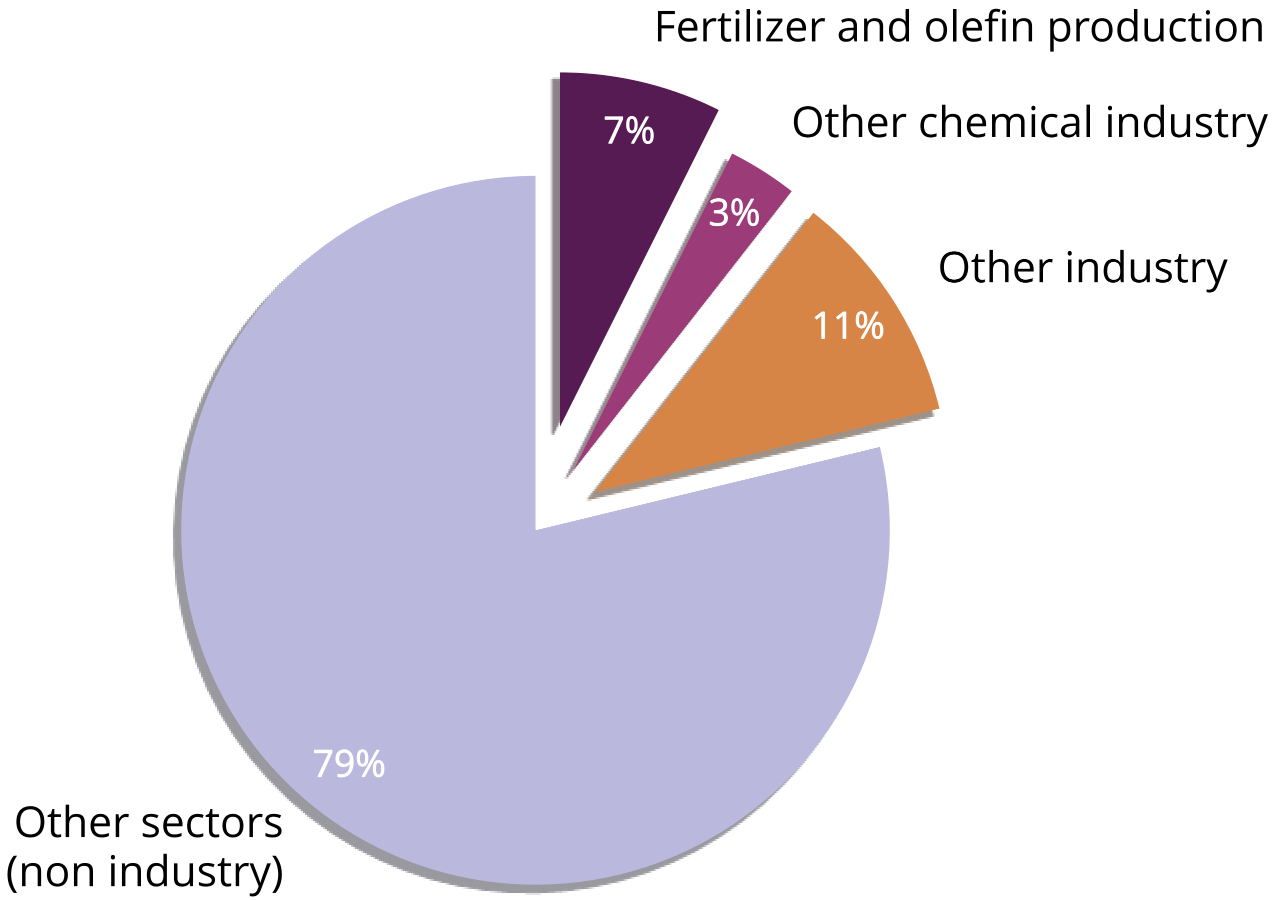


Figure 1: Global GHG emissions by sector in 2023 [1-3].

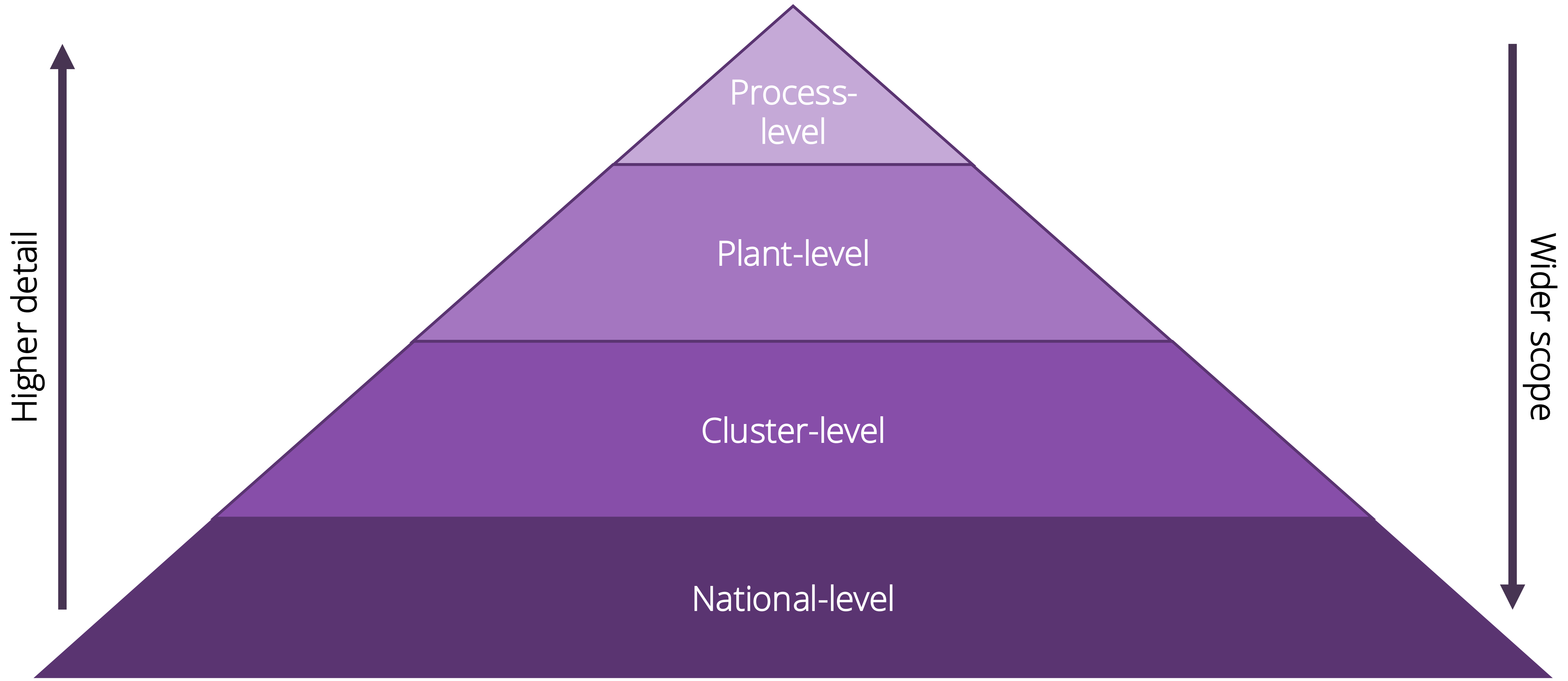
(1) Crippa, M. et al. *GHG emissions of all world countries*; European Commission and Joint Research Centre, 2024.
(2) Bauer, F.; Tilsted, J. P.; Pfister, S.; Oberschelp, C.; Kulionis, V. *Curr. Opin. Chem. Eng.* **2023**, *39*, 100881
(3) IEA *Tracking Clean Energy Progress*; International Energy Agency (IEA), Paris, 2023.

Challenges of chemical industry transformation

- Complex processes
- Plants co-located in industrial clusters
- Central role in global economy
- Need to redesign production routes at the Mt/year scale

Aim:
To **develop analytical tools** that can support **long-term decision-making** by capturing the economic and technical complexity **at different scales**.

Modeling the transition at different scales



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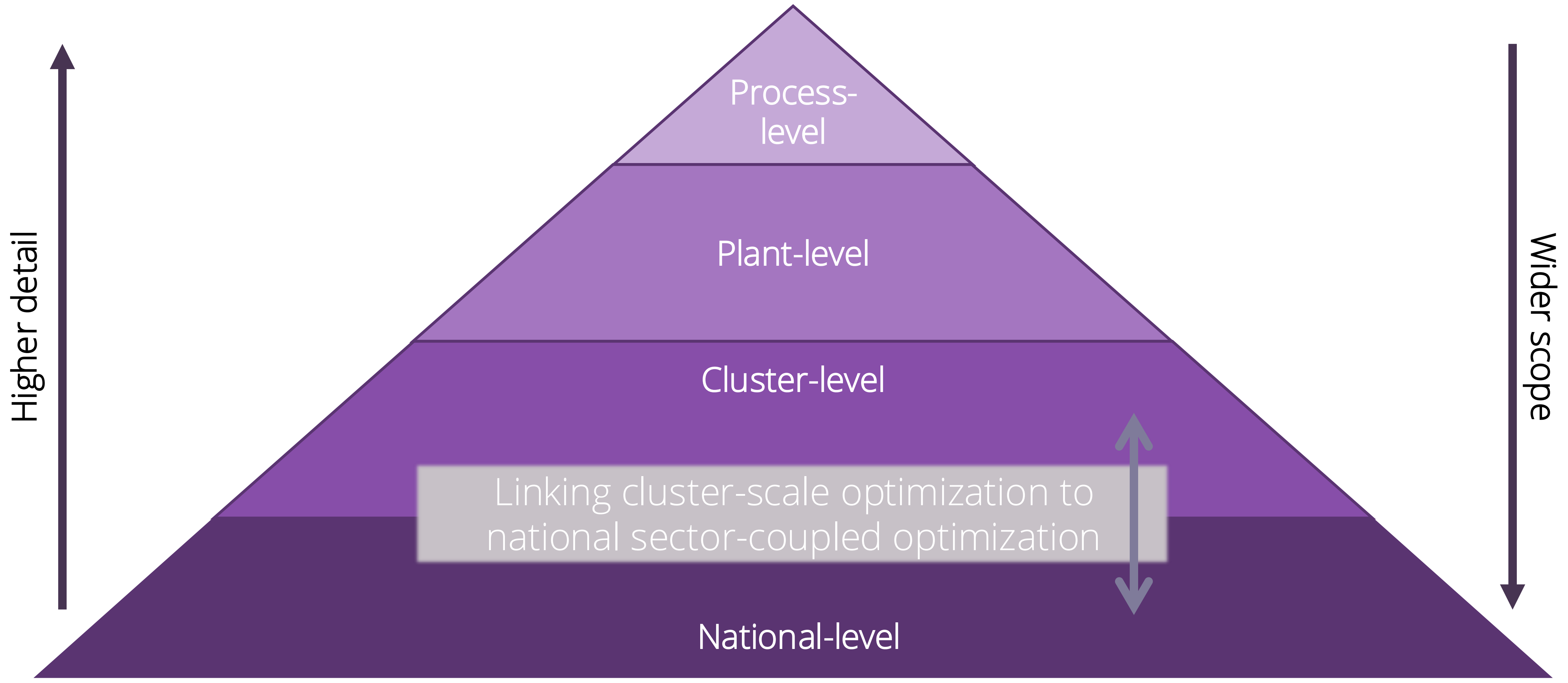
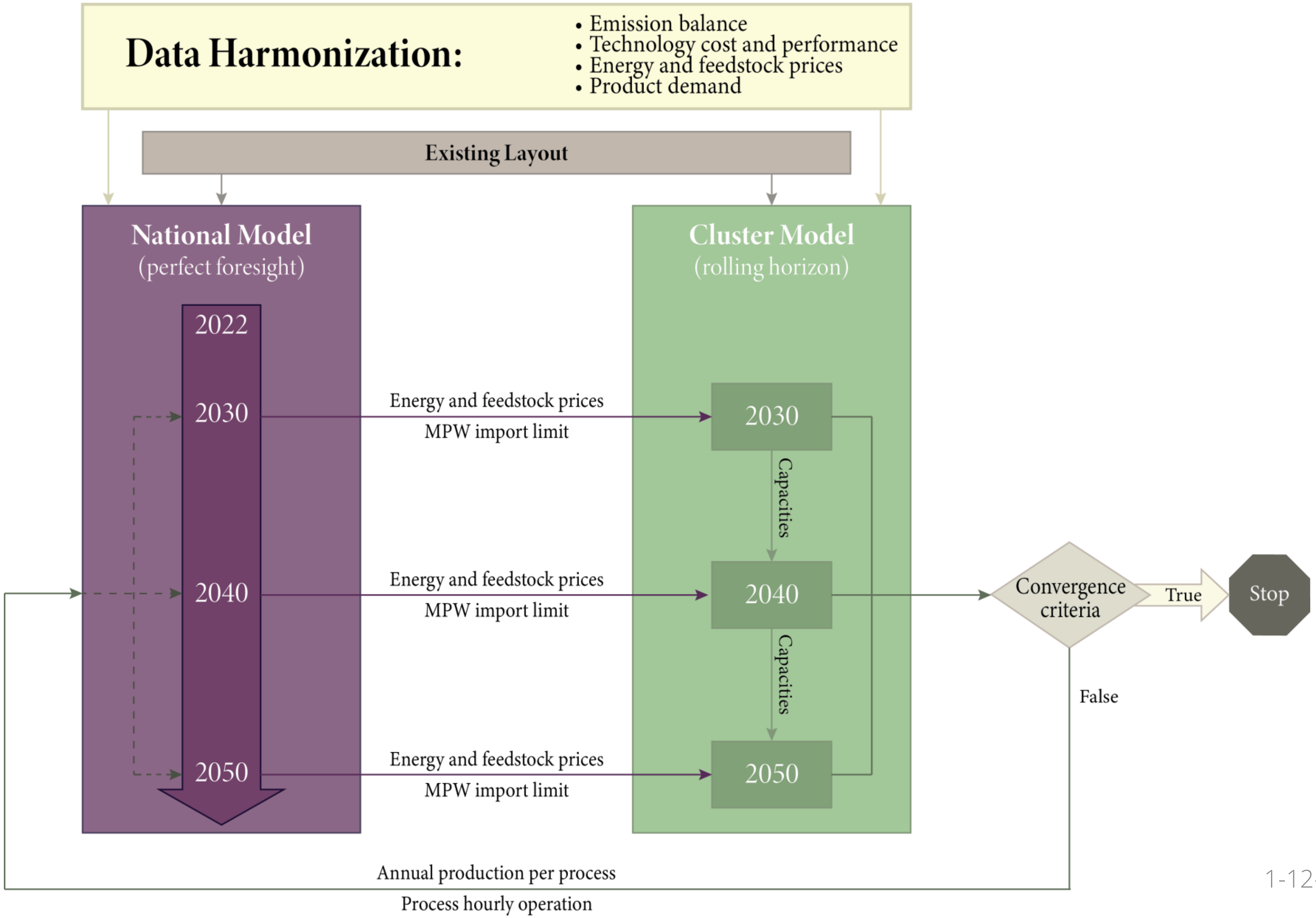


Agenda

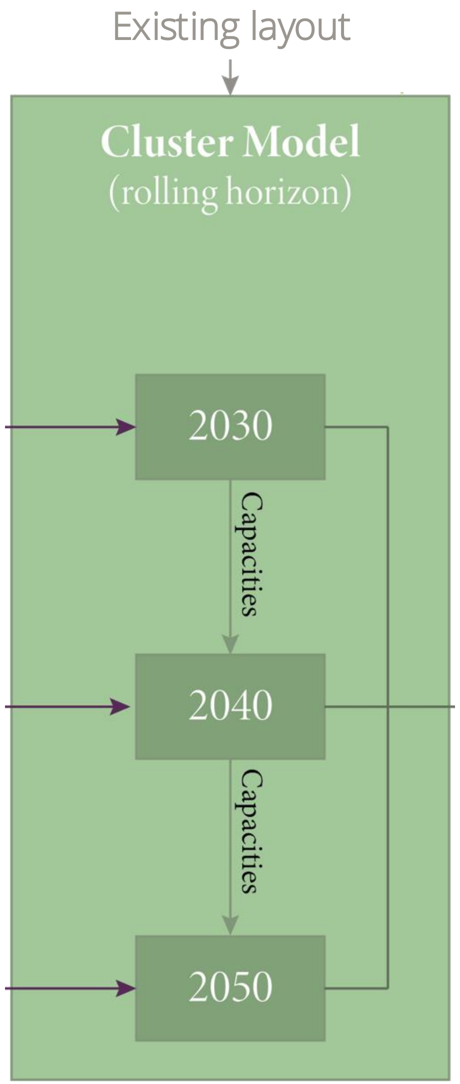
1. Models and case study
2. Standalone results
3. Hard-linking framework
4. Cluster ambitions within national strategies
5. Conclusion

Hard-linking framework



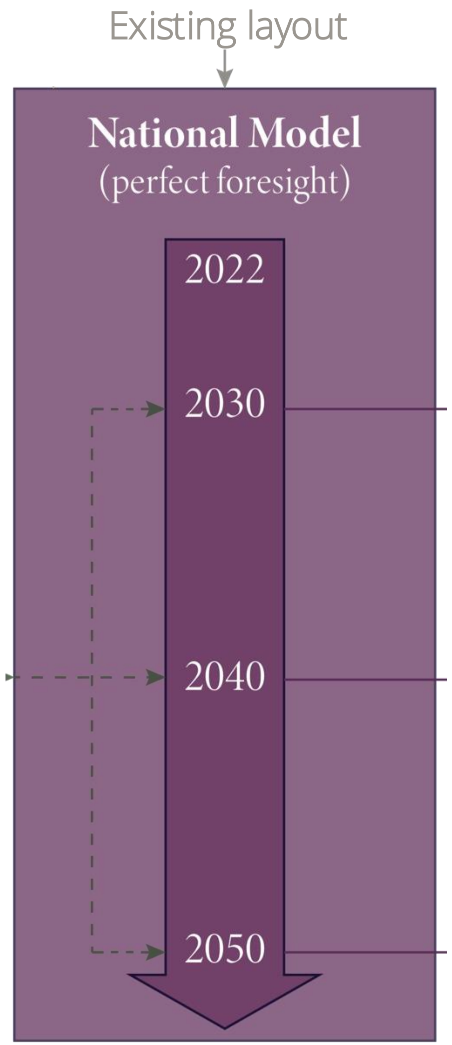
Cluster-level model

- MILP optimization framework
- Include both design and operational variables in optimization problem
- Full-year and hourly resolution (with design days)
- Sequential optimization of investment intervals

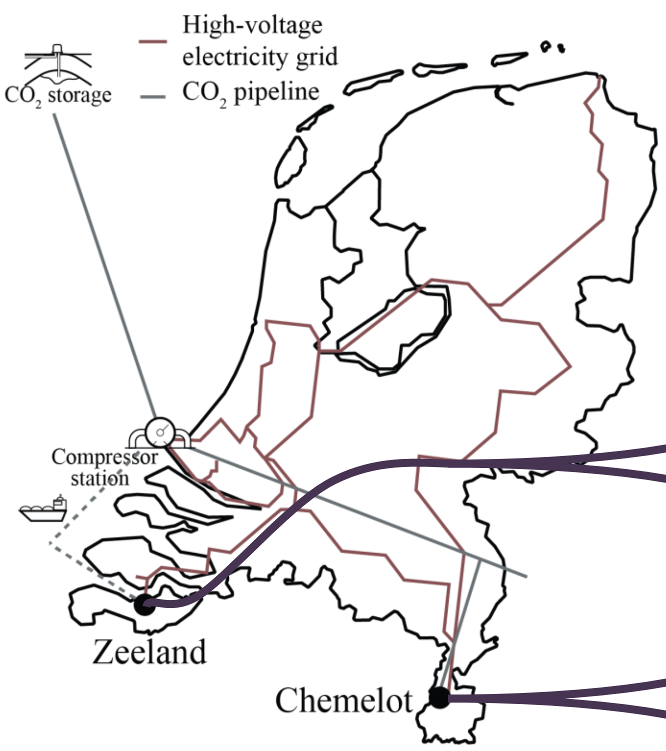


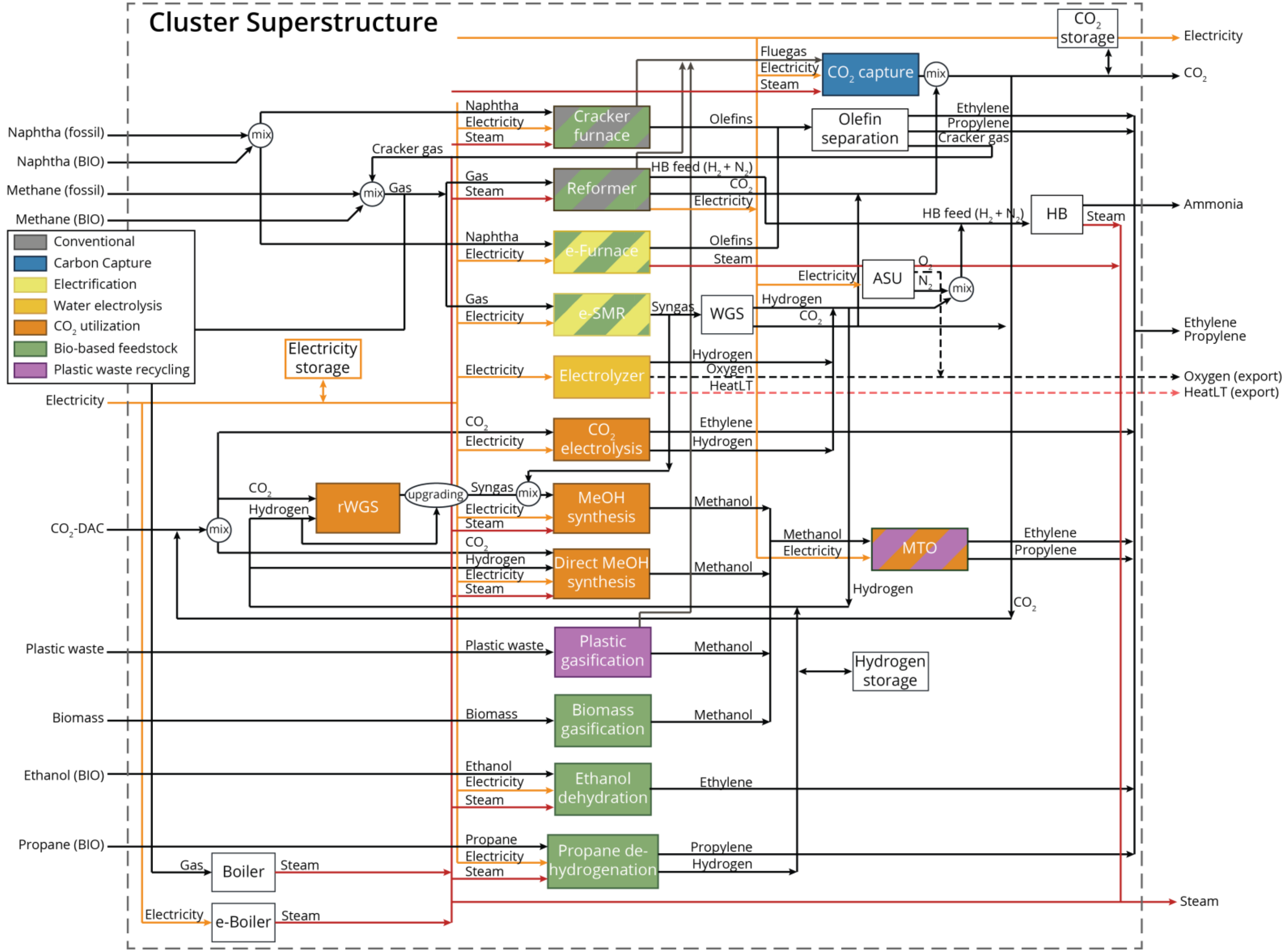
National model

- LP formulation in AIMMS
- Fully sector-coupled model of the Netherlands
- Hourly resolution with perfect foresight until 2050



Case study at cluster-level

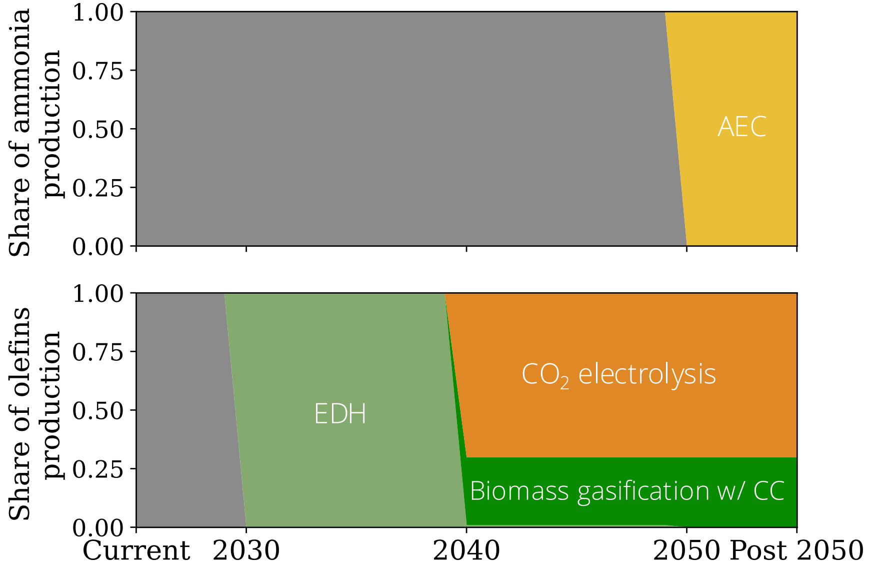




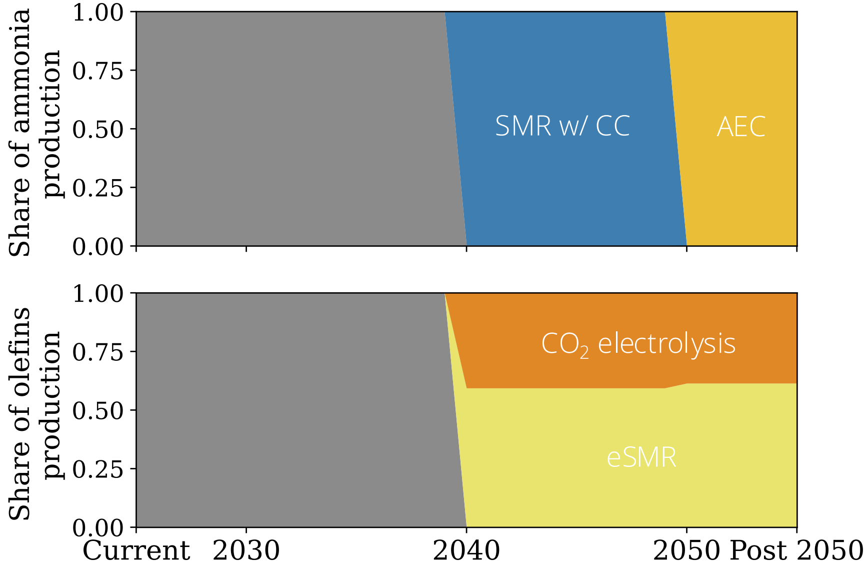
Cluster emission reductions

- Three ambition levels for the cluster to reduce emissions
  - High ambition: direct, energy-related and end-of-life emissions
  - Medium ambition: direct and energy-related emissions
  - Low ambition: cost-minimization
- All have a CO_2 price of 150 €/t from 2030 onwards

Cluster emission reduction pathways – standalone results

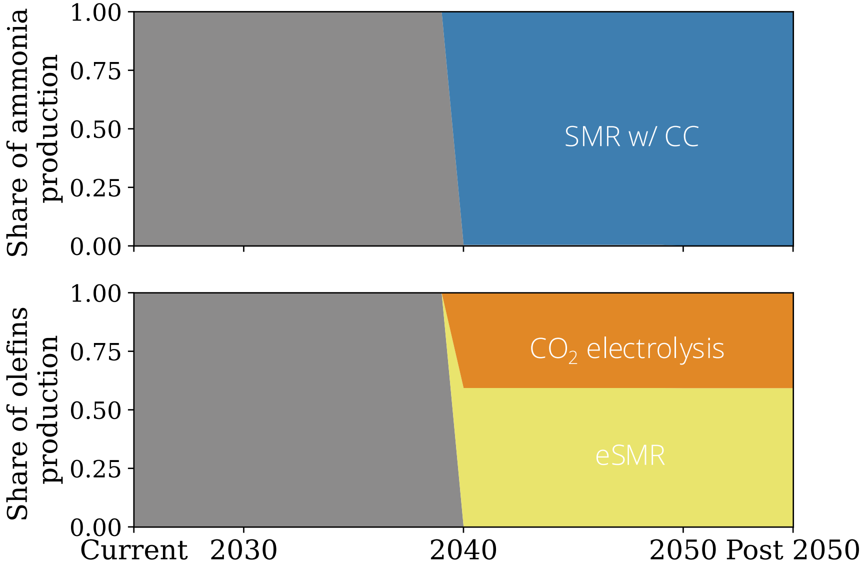


High ambition (scope 1-3)



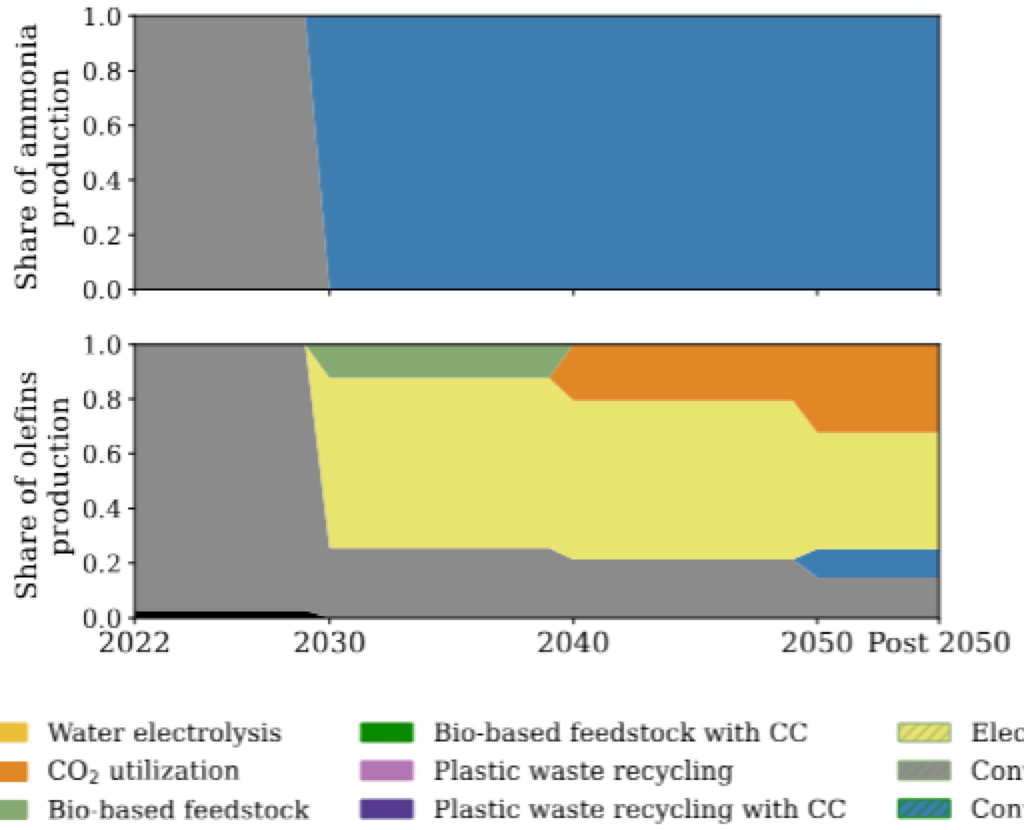
Medium ambition (scope 1-2)

- Conventional
- Carbon Capture
- Electrification
- Water electrolysis
- CO_2 utilization
- Bio-based feedstock
- Plastic waste recycling

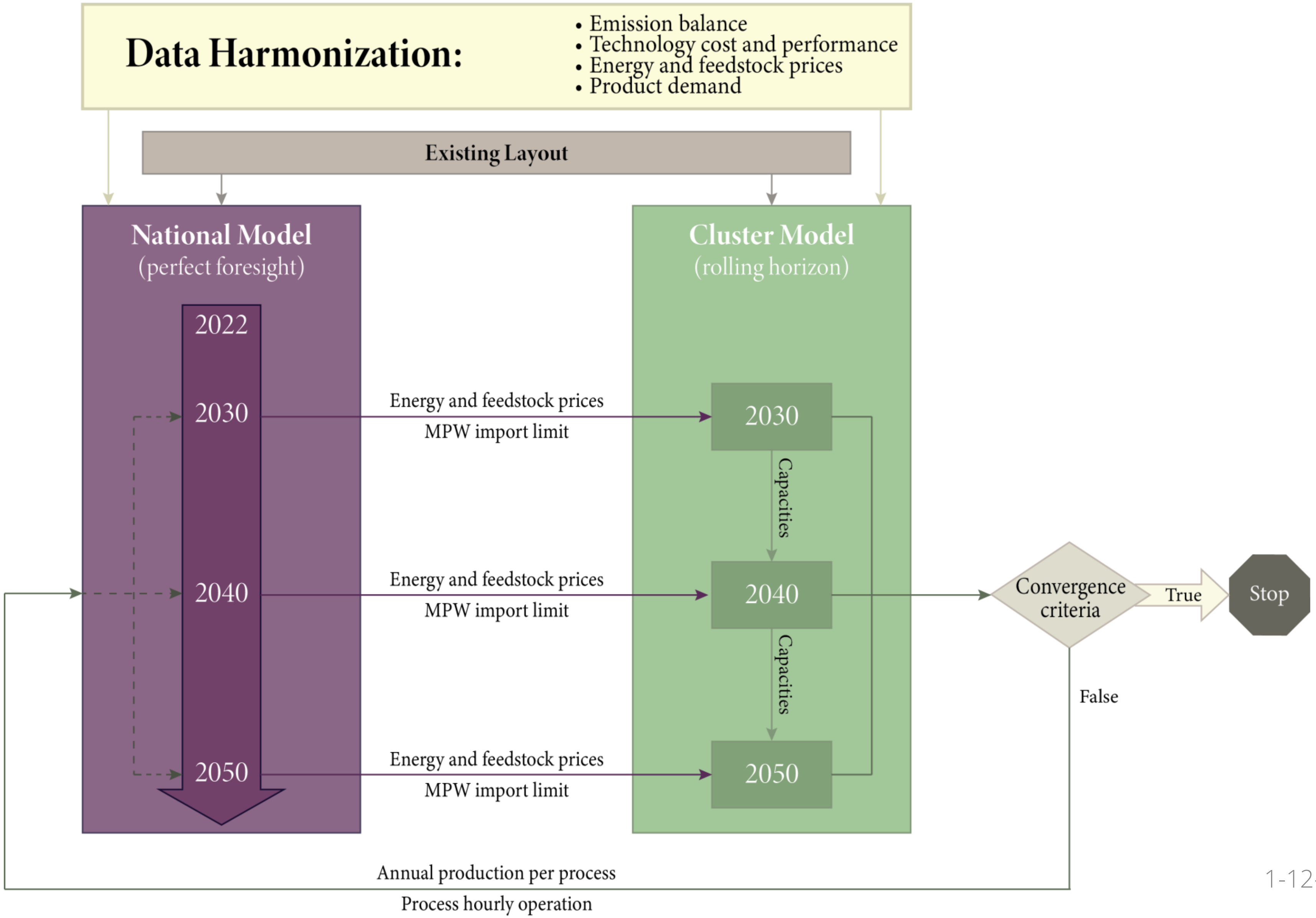


Low ambition (minimum costs)

National strategy – standalone results

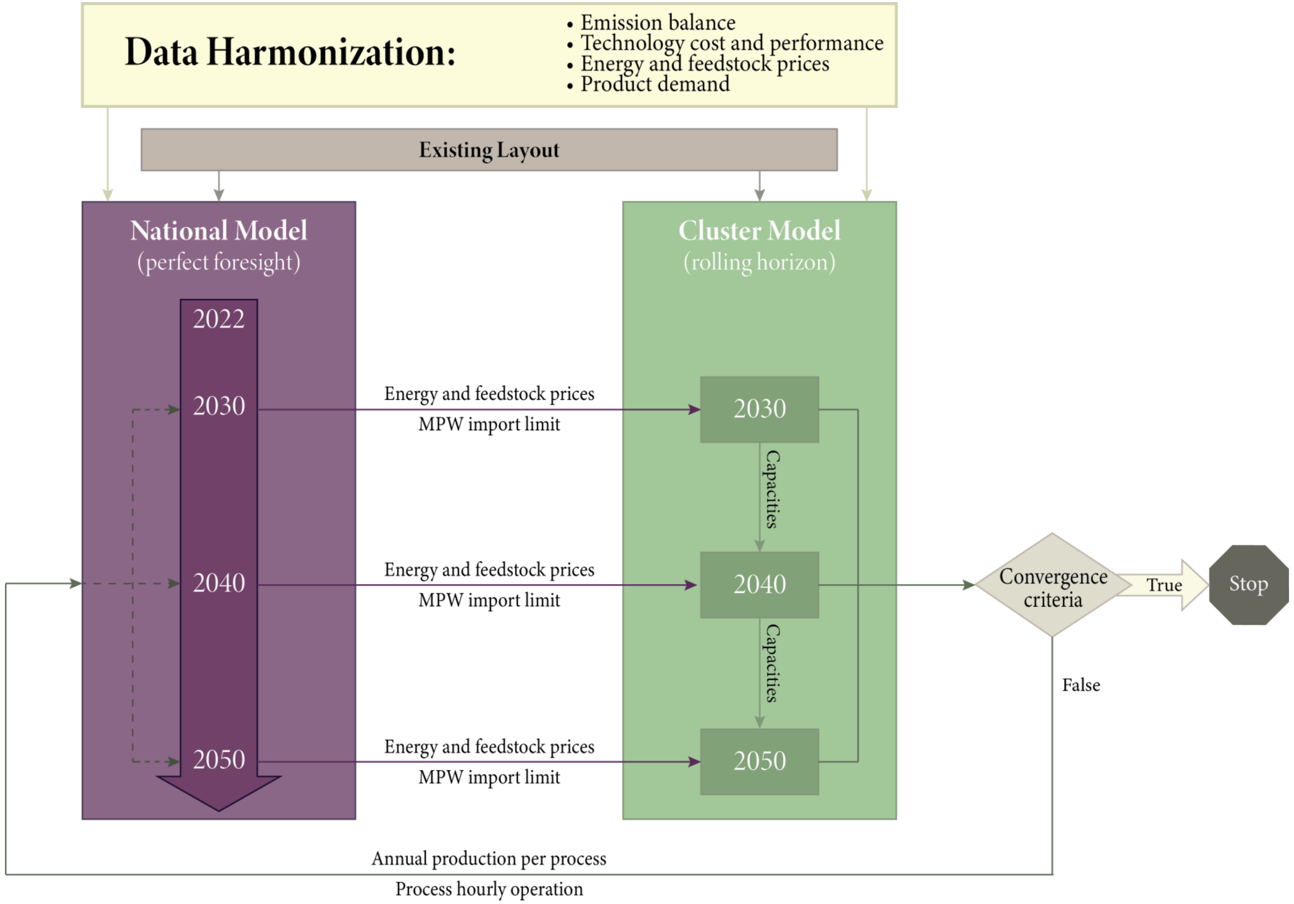


Hard-linking framework



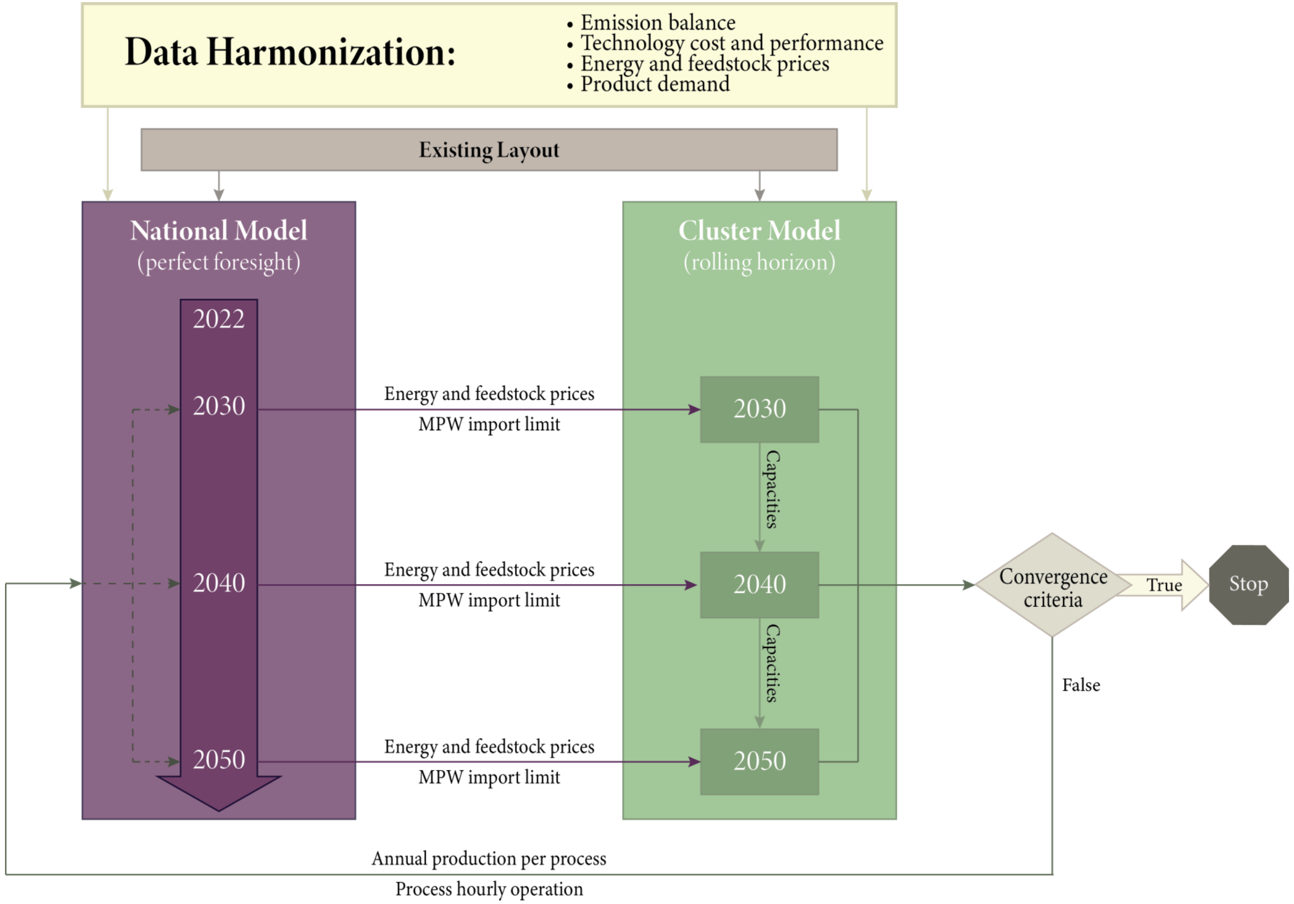
Linking variables
National to cluster

- Endogenous variables from the national model:
  1. Marginal costs of energy and feedstocks
  2. Availability of plastic waste for gasification



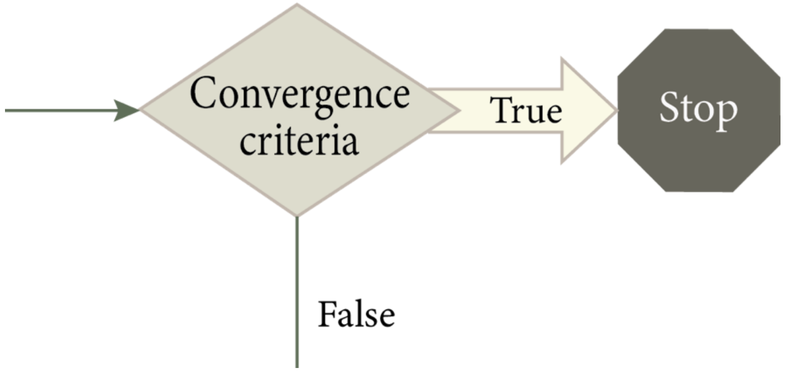
Linking variables
Cluster to national

- Endogenous variables from the cluster model:
  1. Annual production of installed technologies
  2. Hourly operating profiles of electrified technologies



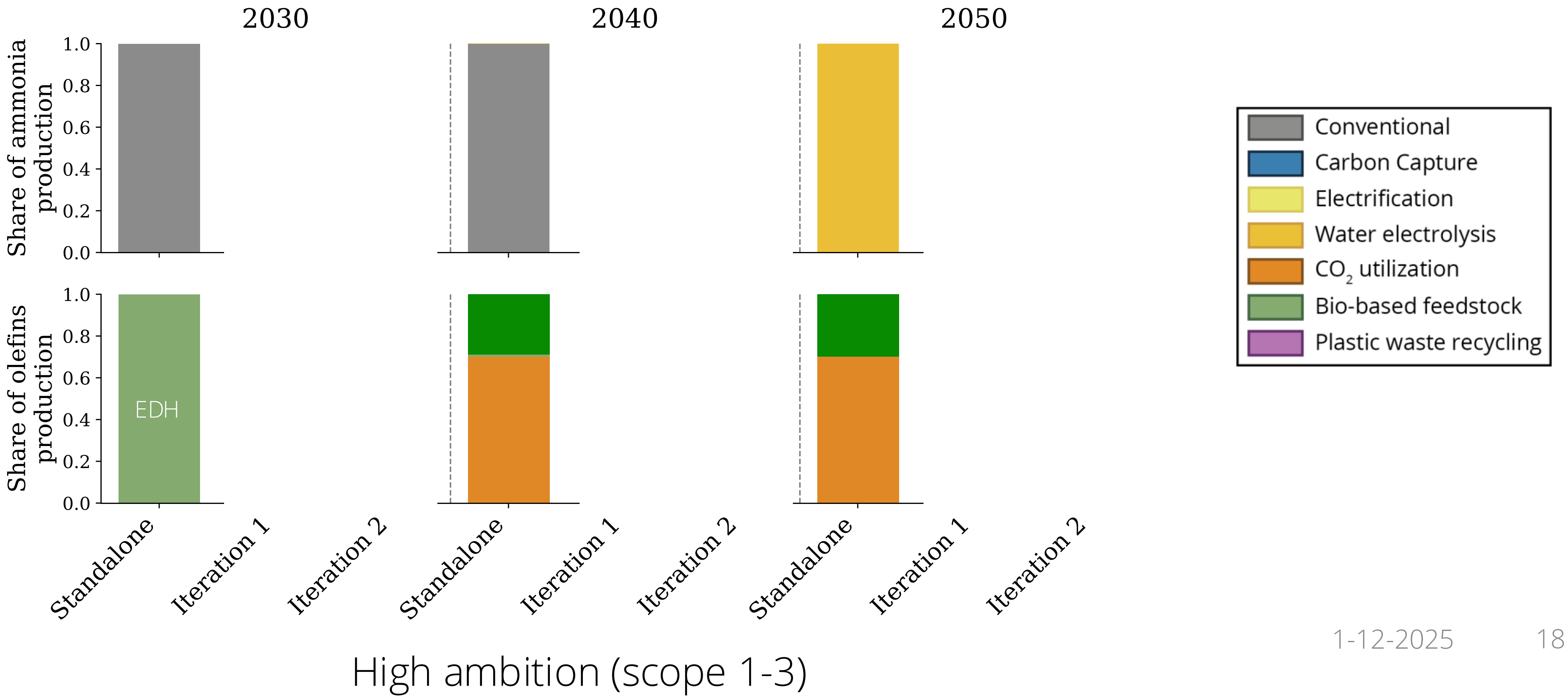
Convergence criteria

- Convergence assessment based on cluster variables
- Calculate the relative change in annual production between iterations for each process
- Required to meet both criteria:
  1. Average relative change of all processes: <1%
  2. Max relative change of all processes: <10%



Cluster ambitions and national policy alignment

- Mismatch of supply and demand at national level leads to alternative least-cost olefin pathway in 2030
- Path-dependent consequences: eSMR is used for ammonia production in 2040



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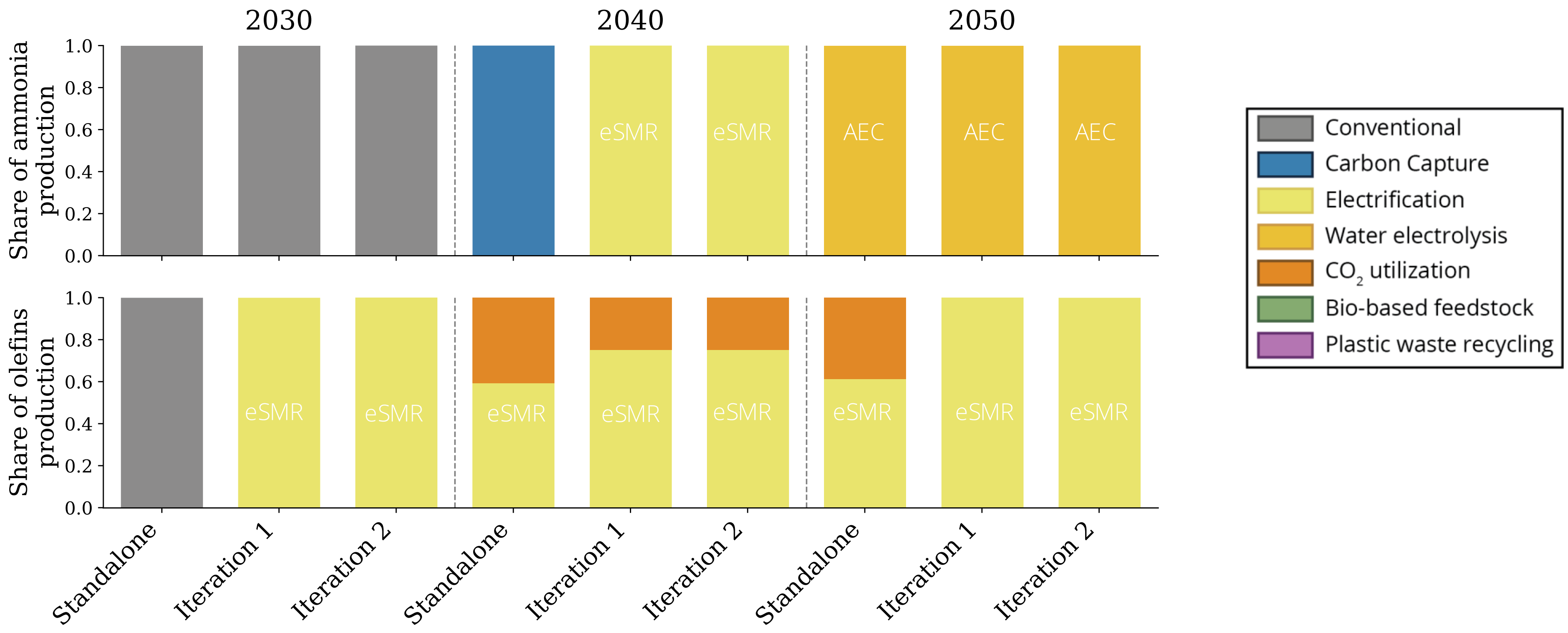
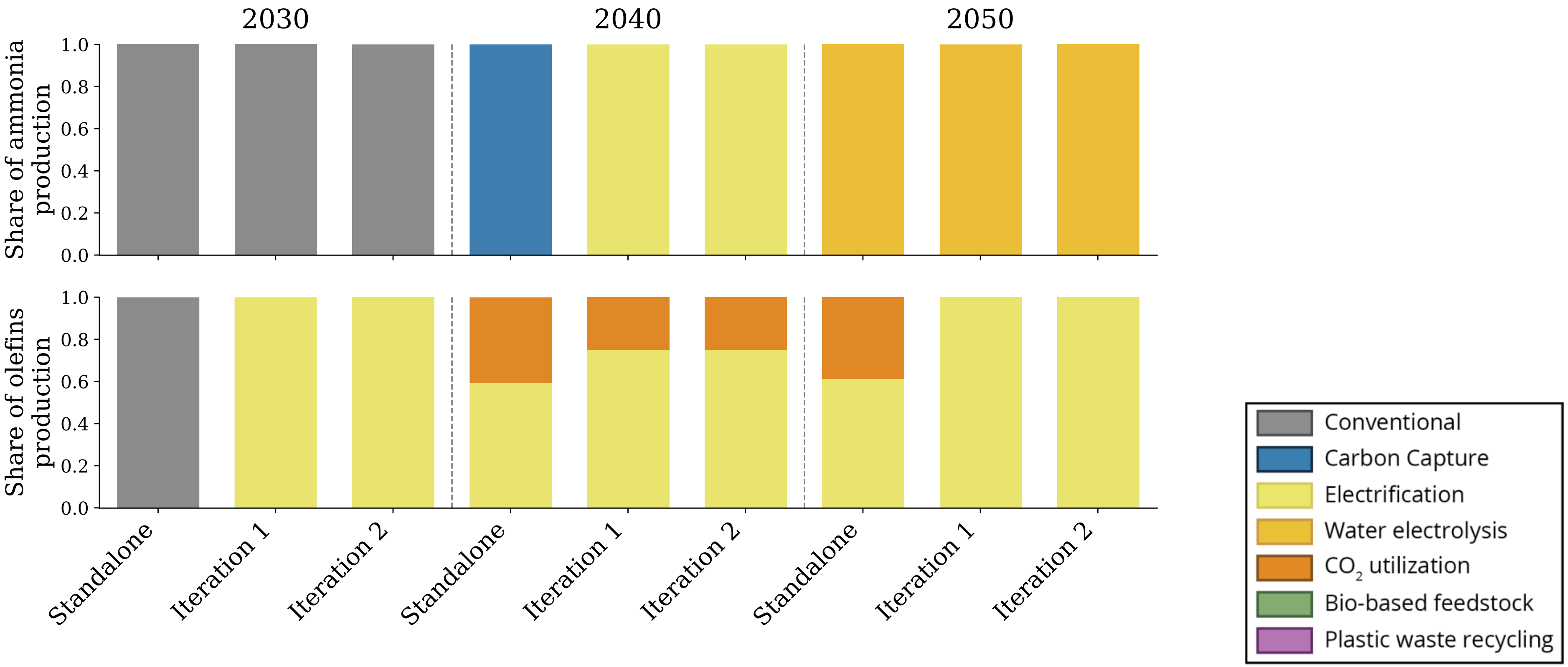


Medium ambition (scope 1-2)

Costs of misaligned emission reduction ambitions



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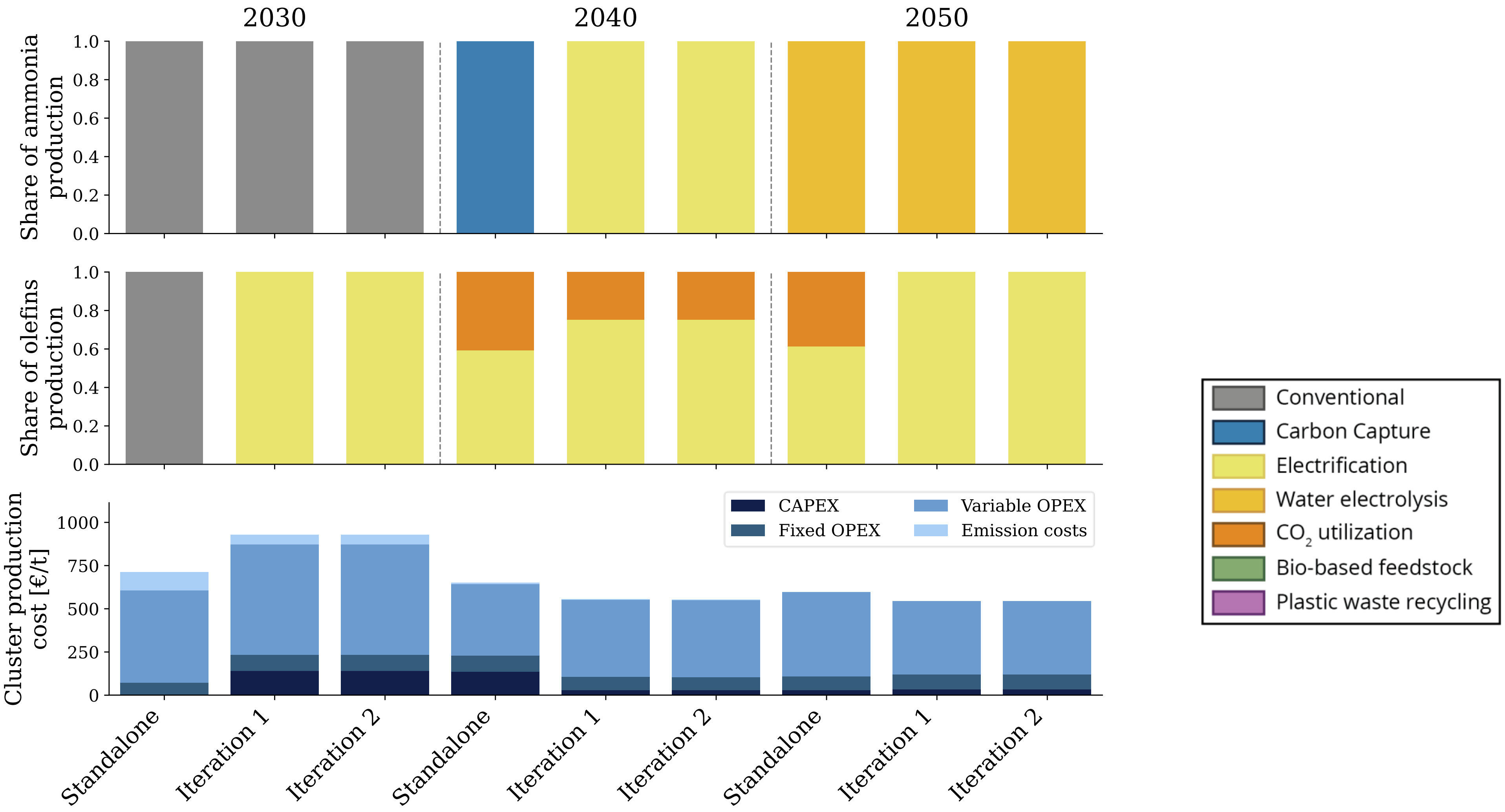

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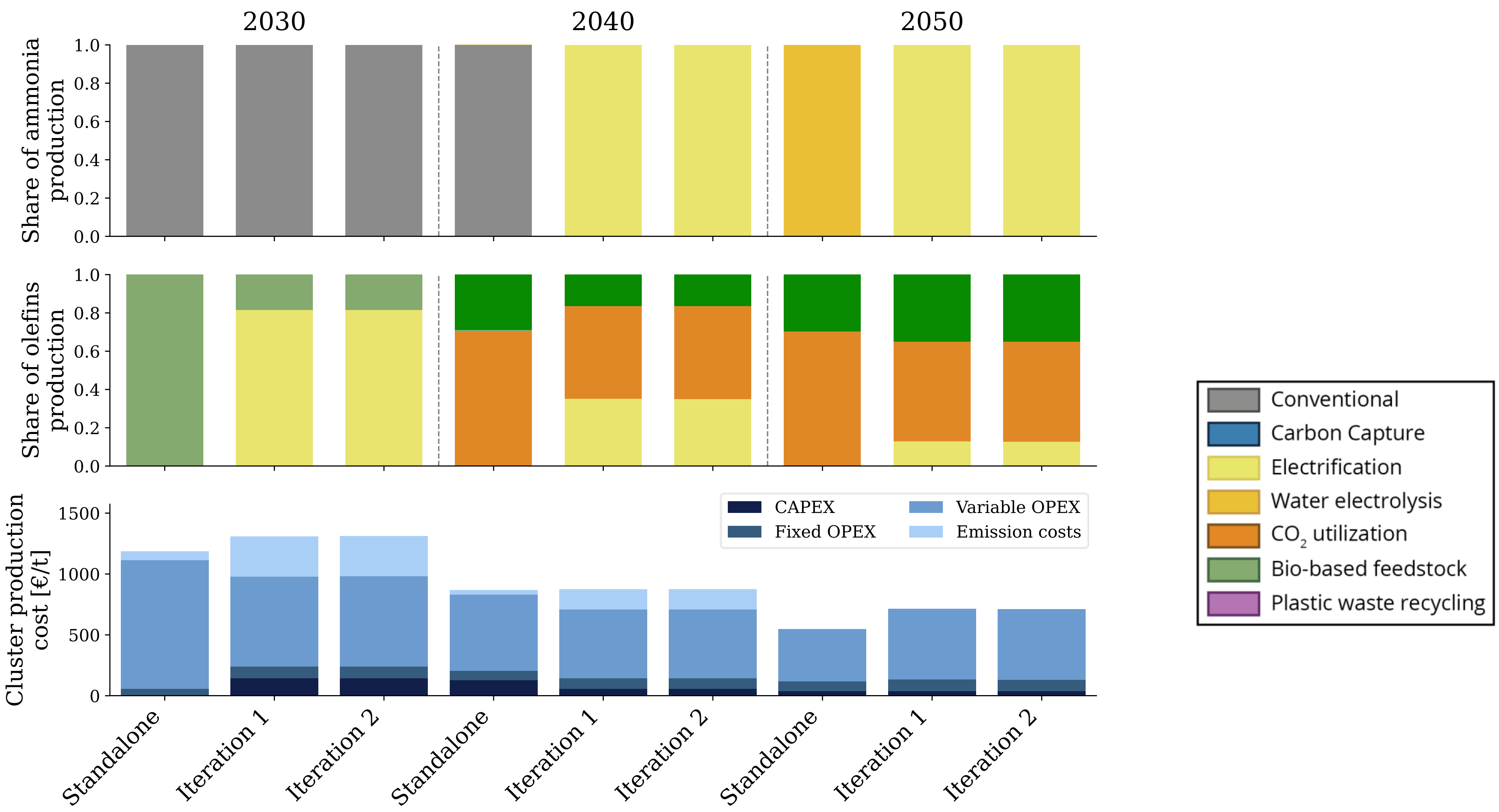

High ambition (scope 1-3)

Conclusions

1. Several near-term investments consistently emerge as “low-regret” technologies
2. Alternative feedstocks need end-of-life carbon pricing to compete with fossil
3. Data harmonization and model-linking can identify trade-offs between different scales of the transition
4. Misaligned ambitions between clusters and the national system can lead to alternative least-cost pathways and higher costs

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References, data and code availability

Tiggeloven, J. L., Faaij, A. P. C., Kramer, G. J., & Gazzani, M. (2023). *Optimization of Electric Ethylene Production: Exploring the Role of Cracker Flexibility, Batteries, and Renewable Energy Integration. Industrial & Engineering Chemistry Research*, 62(40), 16360–16382.

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Tiggeloven, J. L., Faaij, A. P. C., Kramer, G. J., & Gazzani, M. (submitted). *Rethinking Chemical Clusters: Greenfield and Brownfield Transition to Net-Zero by 2050.*

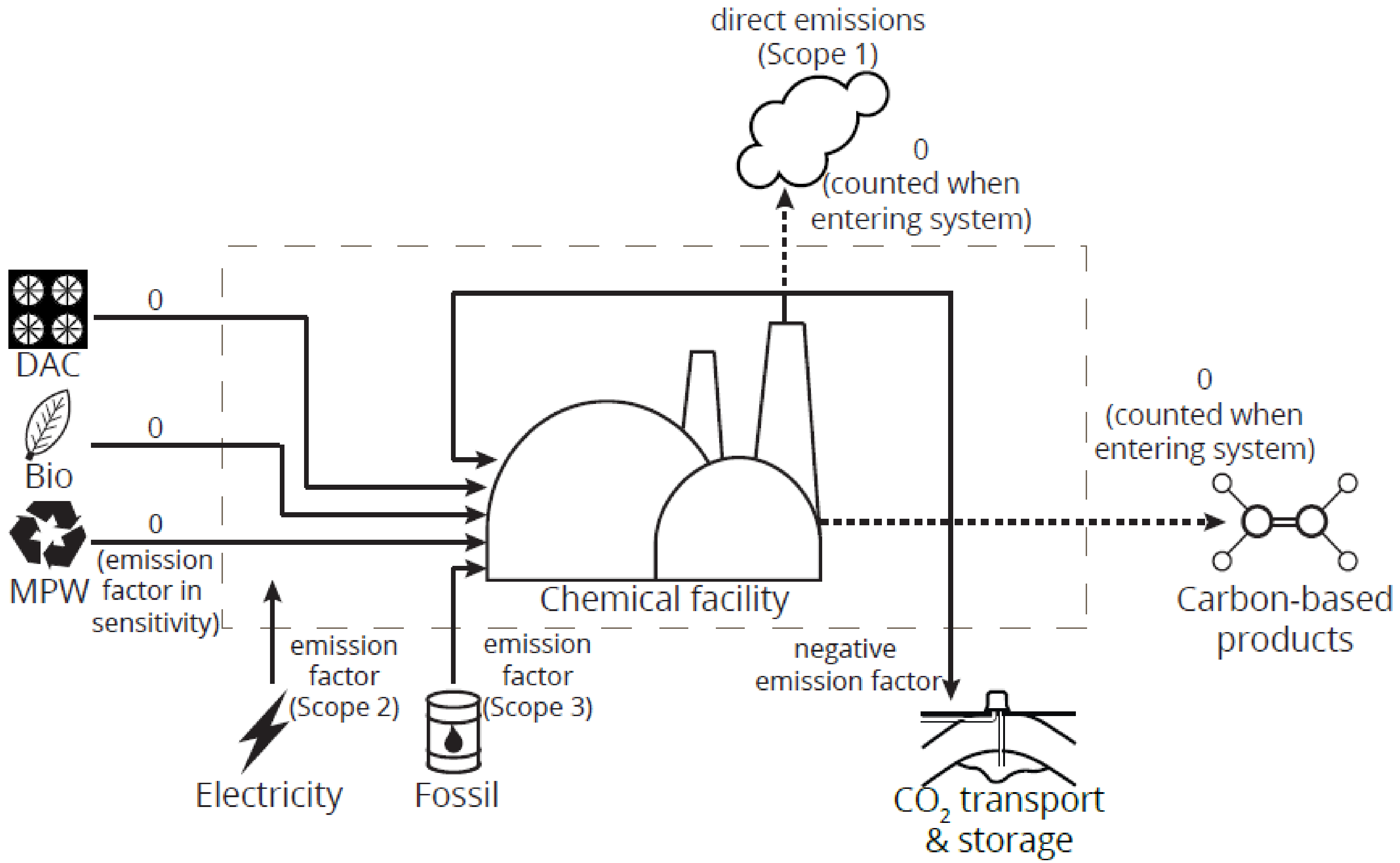
Tiggeloven, J. L., West, K., Mulder, A.J., Faaij, A. P. C., Kramer, G. J., Koning, V., & Gazzani, M. (in preparation). *Supporting the transition to a net-zero chemical industry by coupling national and cluster-level models.*

Data and code availability:

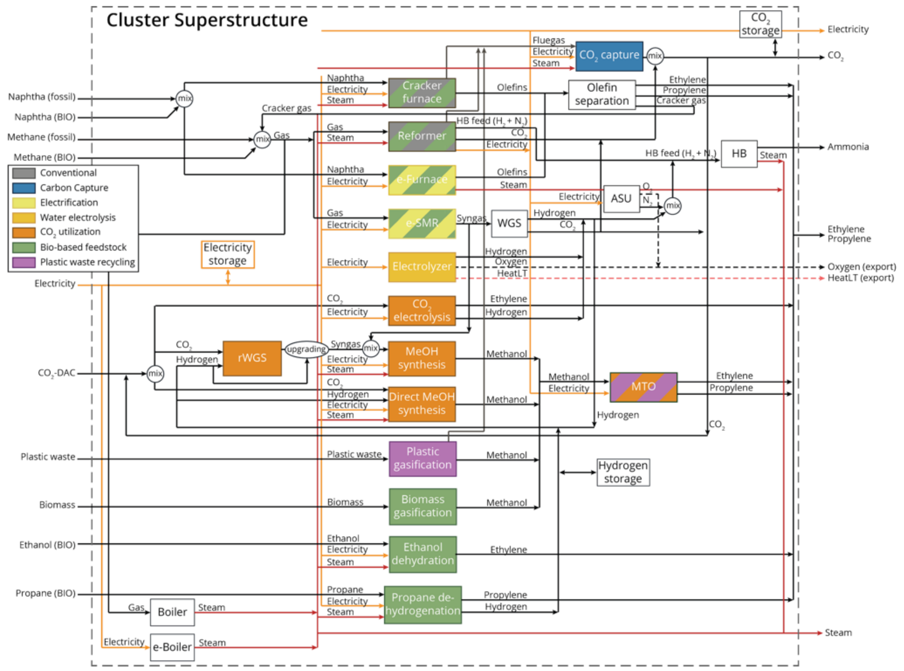
The AdOpT-NET0 optimization framework and all data supporting the research are open source.

- https://github.com/julia1071
- Wiegner, J. F., Tiggeloven, J. L., Bertoni, L., Ossentjuk, I. M., & Gazzani, M. (2025). AdOpT-NET0: A technology-focused Python package for the optimization of multi-energy systems. Journal of Open Source Software, 10(106), 7402

Emission scope



Optimization framework



- MILP optimization framework
- Include both design and operational variables in optimization problem
- Full-year and hourly resolution (with design days)

$$\min_{x,y} \left(c^T x + d^T y \right)$$

subject to

$$Ax + By = b$$

$$x \geq 0 \in \mathbb{R}^N, y \in \mathbb{N}^M$$

Decision var.	Constraints
• Plant capacity • Tech. selection & size • Plant operation (production level)	• Technology performance • Energy balances • Material balances

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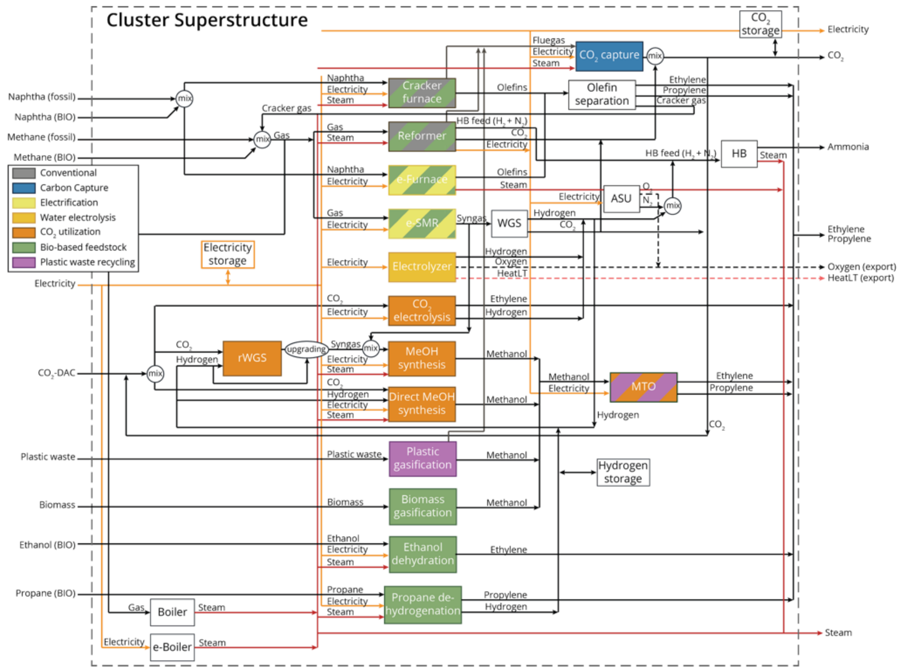
Optimization framework



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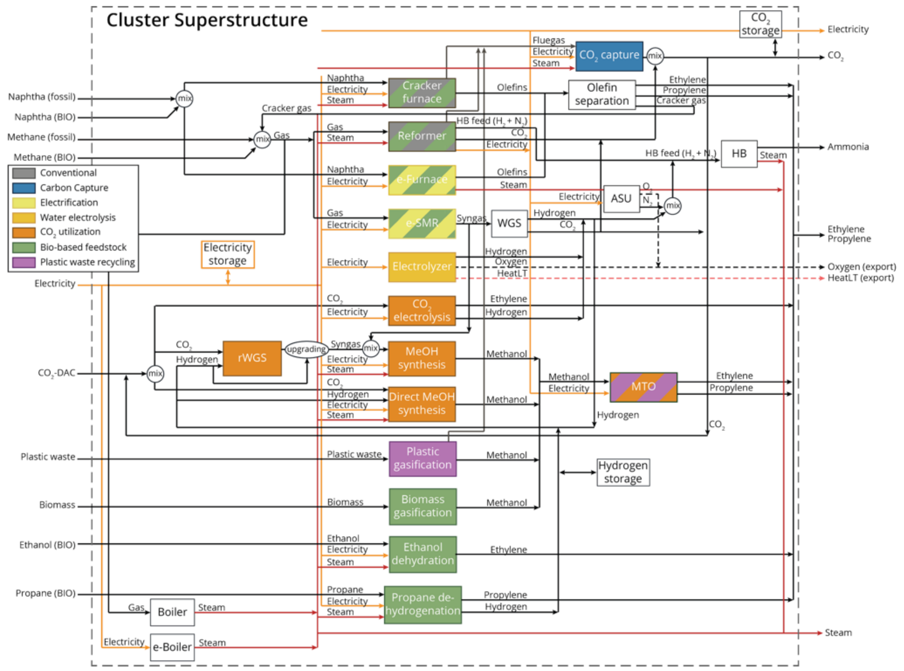

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Objective funct.

- Total annual cost
- Total annual emissions

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