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Modeling and Statistical Analysis for Low-Carbon Transition Pathways

Hydrogen Storage Optimization and Data-Driven Methane Leak Mitigation Strategies

By

Elena Rozzi

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Supervisor(s):
Prof. Andrea Lanzini, Supervisor
Prof. Massimo Santarelli, Co-Supervisor

Doctoral Examination Committee:
Prof. Emanuele Martelli, *Referee*, Politecnico di Milano
Prof. Bilainu Oboirien, *Referee*, University of Johannesburg
Prof. Pierluigi Leone, Politecnico di Torino
Prof. Alessandro Hugo Monteverde Videla, Politecnico di Torino
Dr. Paola Gislon, ENEA

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Declaration

I hereby declare that the contents and organization of this dissertation constitute my own original work and does not compromise in any way the rights of third parties, including those relating to the security of personal data.

This dissertation was conducted at the Energy Center Lab, Energy Department (DENERG), Politecnico di Torino.

The content of this thesis builds upon the following works, comprising both peer-reviewed publications and manuscripts under review:

- **Section 2.2** is based on material published as:

  Elena Rozzi, Francesco D. Minuto, and Andrea Lanzini. *"Dynamic modeling and thermal management of a power-to-power system with hydrogen storage in microporous adsorbent materials"*. Journal of Energy Storage, vol. 41, 102953, 2021. doi: https://doi.org/10.1016/j.est.2021.102953

- **Section 2.3** is based on the manuscript:

  Elena Rozzi, Alberto Grimaldi, Francesco D. Minuto, and Andrea Lanzini. *"Model complexity and optimization trade-offs in the design and scheduling of hybrid hydrogen-battery systems"*. Energy Conversion and Management, vol. 344, 120306, 2025. doi: https://doi.org/10.1016/j.enconman.2025.120306

- **Section 3** is partially based on the manuscript:

  Elena Rozzi, Francesco D. Minuto, and Andrea Lanzini. *"A nation-wide quantification of methane emissions from the natural gas distribution network"*. Manuscript in preparation.

Elena Rozzi
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Modeling and Statistical Analysis for Low-Carbon Transition Pathways

Elena Rozzi

The urgent need to mitigate climate change and achieve climate neutrality by mid-century has placed the energy sector at the center of global decarbonization strategies. Within this transformation, hydrogen is increasingly recognized as a flexible, zero-carbon energy carrier capable of enabling sector coupling and supporting the decarbonization of hard-to-abate industries. At the same time, the natural gas infrastructure is required to mitigate its environmental impact, particularly by curbing fugitive methane emissions. This thesis investigates both fronts through a dual research effort, combining high-fidelity simulation, advanced optimization techniques, and machine learning to support the design and management of low-emission energy systems.

Hydrogen integration is investigated with detailed models addressing both residential and industrial energy applications. A dynamic simulation model is developed to analyze a power-to-power (P2P) system employing hydrogen storage through physisorption in microporous solid materials. Operating at high temporal resolution, the model captures rapid fluctuations in demand and generation, enabling an accurate assessment of energy, thermal, and storage dynamics. Results demonstrate that sorbent materials reduce tank volume by up to 88% compared to compressed storage and improve system autonomy by a factor of 1.7. Furthermore, 90% of heat losses are recoverable at medium temperature (80°C), opening up opportunities for residential cogeneration. The findings confirm the viability of solid-state hydrogen storage as a compact, efficient, and reversible solution for long-duration storage in distributed applications.

At the industrial scale, a comprehensive techno-economic optimization of a grid-connected power-to-hydrogen system integrating battery and hydrogen storage is implemented. Three optimization strategies are evaluated: mixed-integer linear programming (MILP), particle swarm optimization (PSO), and hybrid MILP-PSO. A rolling horizon framework is proposed to improve dispatch under dynamic pricing and renewable generation. Results show that the rule-based model minimizes emissions but raises LCOH (+26%), while MILP models are cost-optimal but exceed EU carbon intensity limits. Hybrid approaches strike a favorable balance, with

competitive costs, moderate emissions, and lower computational burden. The study also underscores the role of energy management strategies, storage utilization, and electrolyzer operation in determining system sustainability.

Methane emission mitigation in natural gas distribution networks is investigated through predictive models based on real-world operational data. A unique dataset from a European distribution system operator which covers multi-year mobile leak detection, GIS pipeline data, and maintenance logs is used to build predictive models for leak identification and emission quantification. Emission and activity factors are estimated through a Bayesian regression framework, whereas machine learning classifiers rank pipeline segments according to their likelihood of leakage, thereby supporting decisions on maintenance and replacement. Spatial regression extends the analysis to above-ground pipelines and supports the development of dual-index GIS maps combining regulatory benchmarks with model-derived scores indicating whether a given area is exhibiting improving or worsening emission trends. These tools provide DSOs with actionable insights to enhance operational efficiency and prioritize interventions in line with methane reduction policies.

The two research strands converge around a common methodological foundation: the use of computational modeling and data analytics to support energy system decarbonization. Through the combined application of optimization, simulation, and predictive algorithms, the work delivers validated tools and methodological advancements that enable data-informed energy planning and infrastructure management. This thesis supports the development of flexible, resilient, and low-emission energy systems aligned with long-term climate neutrality targets by integrating engineering models with environmental objectives.