

Modeling Approaches and Decarbonization Pathways in Multi-Sector Integrated Energy Systems

by

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Achieving deep decarbonization requires planning frameworks that capture interactions across electricity, hydrogen, low-carbon fuels, and carbon management sectors. As decarbonization extends beyond the power sector, system outcomes increasingly depend on cross-sector coordination, infrastructure availability, operational flexibility, and resource constraints. Capturing these interactions requires multi-sector energy system models with high spatial and temporal resolution, which in turn pose computational challenges. This thesis examines low-carbon hydrogen and liquid fuel pathways under net-zero emissions scenarios, as well as clustering-enhanced Benders decomposition methods for large scale energy systems.

Using a multi-sector integrated energy system modeling framework, the first part focuses on how grid coupling and technology flexibility shape low-carbon hydrogen production pathways. The results show that grid connection and hydrogen storage enable low-cost electrolysis while providing demand-side flexibility to the power sector, thereby improving renewable electricity integration and reducing battery deployment. In contrast, natural gas-based hydrogen dominates when hydrogen storage is unavailable, while operational flexibility affects system outcomes to a lesser extent than assumptions about hydrogen storage and grid connection.

The second part of the thesis examines how biomass availability, CO₂ sequestration capacity, and fuel production flexibility shape competition among low-carbon liquid fuel pathways. The results show that biofuels provide a substantial share of liquid fuel supply, while synthetic fuels deploy only when biomass or CO₂ sequestration is more limited. In all scenarios, the continued use of fossil liquid fuels depends largely on the extent to which their emissions can be offset with removals. Limiting biomass increases biogenic CO₂ capture within biofuel pathways, while limiting sequestration availability increases the share of captured carbon directed toward synthetic fuel production. Although assumptions about liquid fuel demand distributions and fuel product supply flexibility affect competition among individual fuel production technologies, broader energy system outcomes remain relatively robust. Biomass and CO₂ sequestration availability emerge as key drivers of system outcomes in deeply decarbonized energy systems.

Finally, this thesis addresses the computational challenge of solving large-scale energy system models by developing clustering-enhanced Benders decomposition methods that group similar subproblems for Benders cut construction, thereby reducing master-problem growth and computational burden. These include adaptive grouped-cut formulations based on realized subproblem information, a fixed-grouping formulation based on clustering exogenous time-series inputs, and a representative-subproblem strategy for limited parallelization settings. The results show that adaptive grouped cuts consistently outperform fixed grouping and often provide an advantage over a benchmark multi-cut Benders formulation, especially in settings where the master problem dominates overall runtime and inter-temporal coupling is limited. However, the multi-cut formulation

performs best when subproblems are strongly coupled through inter-temporal emission budgeting variables. In contrast, the representative-subproblem method is most effective when subproblem solutions dominate runtime under limited parallelization. Overall, the preferred Benders decomposition strategy depends on inter-temporal coupling strength and whether the computational burden lies in the master problem or the subproblems.

Overall, this thesis advances both the analysis of deep decarbonization pathways and the computational tractability of large-scale multi-sector energy system planning models.

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