Abstract

Achieving deep decarbonization of fuels while preserving energy security demands pathways that convert renewable electricity and biogenic carbon into drop-in energy carriers with credible efficiency, cost, and environmental performance. Hydrogen is central to this challenge: as a clean intermediate and design variable, it can couple electrolysis, heat recovery, oxygen and carbon management, and fuel synthesis into polygeneration systems that co-produce gaseous and liquid fuels. This dissertation tests the hypothesis that electrolyzer-centric integration of hydrogen with targeted separations and thermal–power coupling can systematically raise conversion efficiency, reduce levelized costs, and lower cradle-to-gate impacts. Using Aspen Plus, EES, and SimaPro software, a unified framework links detailed thermodynamic modeling with techno-economic assessment and both attributional and consequential life-cycle analysis (LCA) across eight configurations: biogas-to-methanol (baseline and with LNG cold-energy recovery and oxy-fuel gas turbine), biomass-to-methanol via gasification (with and without compressed-air/thermal energy storage), three green-ammonia plants using electrolysis or gasification and water gas-shift (WGS) reactions, and a Fischer–Tropsch sustainable aviation fuel (SAF) route. Key performance indicators include overall energy efficiency, levelized cost of fuel, global warming potential (GWP), and fossil resource depletion (FDP).

Across routes, integration around the solid-oxide electrolysis cell (SOEC) is the dominant lever. The biomass-to-methanol system augmented with compressed-air and thermal energy storage converts transient waste heat into steady biomethanol and delivers approximately 95% efficiency, a levelized cost near 602 $/tonne, and a GWP around 0.135 kgCO2eq/kgFuel. In a gasification-based polygeneration case that co-produces natural gas and biomethanol with utilized oxygen and CO2 management, the plant attains about 82% efficiency, a levelized cost near 961 $/tonne, a GWP around 0.167 kgCO2eq/kgFuel, and an FDP around 0.0345 kgoileq/kgFuel. capital expenditure is concentrated in the electrolyzer and synthesis loop. A wind-powered biogas-to-methanol configuration with LNG cold-energy recovery and an oxy-fuel turbine achieves a GWP near 0.206 kgCO2eq/kgFuel and an FDP near 0.042 kgoileq/kgFuel.

For ammonia, outcomes hinge on the WGS design and the electrolyzer operating window. The biomass-to-ammonia plant with a counter-current membrane WGS reactor is preferred, reaching roughly 54.6% efficiency, a levelized cost near 513 $/tonne, and a GWP around 0.175 kgCO2eq/kgFuel due to superior hydrogen recovery and integrated management of hydrogen, oxygen, and nitrogen.

The sustainable aviation fuel pathway clarifies trade-offs for highly electrified fuels: electrical efficiency is about 56.2%, and a representative cost around 1893 $/tonne with a GWP near 0.464 kgCO2eq/kgFuel.

The electrolyzer and fuel-synthesis sections dominate investment. Electricity sourcing is decisive: wind power markedly improves environmental indicators, reducing GWP and FDP significantly relative to Poland's grid, while current grid prices remain more economical.

Collectively, for optimizing the design rules: prefer high-temperature SOEC where thermal integration is feasible. adopt counter-current membrane water-gas-shift for ammonia. recover LNG cold energy and use oxy-fuel gas turbines where grid relief and flue-gas recycling are priorities. co-produce gaseous and liquid fuels to hedge electricity-price volatility. and prioritize renewable electricity when environmental performance dominates.

Keywords:

Optimization, Hydrogen energy, LCA, Techno-economic analysis, Biofuels, CCUS