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Modeling the energy transition: Multiobjective optimization of green hydrogen deployment strategies

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Abstract. The energy transition is a complex concept that requires progressively addressing various technical, environmental, social, and political issues. Green hydrogen is recognized as a clean fuel to support the energy transition worldwide. This study presents a modeling framework for green hydrogen deployment strategies in the transport and fertilizer sectors on a long-term basis. The mathematical model includes decision variables to account for the amount of hydrogen produced from different energy sources and the importation of fossil-based commodities. Additionally, it incorporates demand-supply and production capacity restrictions in 5-year intervals from the year 2020 to 2050. The case study focuses on the Ecuadorian context, and two deployment strategies are proposed: (i) utilizing surplus renewable energy and (ii) developing local PV capacity. Both strategies positively contributed to adopting more sustainable alternatives; however, Strategy II exhibited superior performance in terms of costs and GHG emissions. Thus, this work provides a framework for designing energy transition strategies and their evaluation to achieve specific renewable and green hydrogen adoption targets over time.

Keywords: Green hydrogen, Energy transition, Optimization, Sector coupling.

1 Introduction

Sustainable strategies focusing on decarbonizing energy-intensive sectors (i.e., transport, fertilizer) are crucial for the energy transition. Finding renewable substitutes to cover the

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ever-growing demands of raw materials and energy is a critical area of ongoing research and study. In this regard, one of the major discussions nowadays is whether green hydrogen and its derivatives (e.g., ammonia, methanol, urea) are suitable candidates for energy transition since renewable-based production systems present techno-economic limitations [1]. For instance, the volatility in renewable energy sources (RES) can lead to variations in the production of green hydrogen, with both low and peak production periods. Alternatively, green hydrogen systems using electrolyzers can load additional energy from the grid, increasing the carbon footprint of hydrogen [2].

Hydrogen deployment strategies must be undertaken with comprehensive planning and evaluation to achieve specific decarbonization goals in accordance with the Paris Agreement, which aims for carbon neutrality by 2050. For example, Zhao et al. [3] performed a multi-supply-demand 3E-optimization (energy, economic, environmental) to assess the viability of hydrogen production from various sources, including chloralkali, steam-methane reforming, and electrolysis. Their investigation specifically targeted energy decarbonization within the transportation sector in Shanxi, China. Similarly, Welder et al.[4] conducted a spatio-temporal optimization study focusing on Power-to-Gas scenarios in Germany. Their study aimed to determine the cost-optimal design and operation of sector coupling in mobility and industry.

This work presents a methodology for modeling hydrogen deployment strategies in Ecuador, serving as a case study representative of a developing country abundant in renewable energy resources. This novel approach allows for the optimization and evaluation of strategies for their potential to reduce CO_2 emissions and minimize expenditure on subsidies. This study serves as a valuable framework for forecasting and evaluating green hydrogen deployment strategies, especially for policy decision-makers. Furthermore, the methodology encompasses substituting fossil-based imports in the transportation and fertilizer sectors with locally produced green alternatives. This dual impact promotes local production and facilitates sector coupling for a faster transition towards a carbon-neutral economy and industrialization.

2 Methodology

2.1 Model description

This section introduces a novel formulation for the energy transition path as a mathematical optimization program designed to identify the fittest *hydrogen deployment strategy* for substituting fossil-based commodities with green hydrogen and its derivatives. A set of decision variables is integrated to accurately represent the import and generation dynamics of green hydrogen from diverse energy sources. Furthermore, a comprehensive array of constraints is incorporated to account for the availability of renewable energy sources, thereby enhancing the realism of the model. Through the systematic integration of these variables into the optimization framework, the model endeavors to ascertain the optimal solution that not only maximizes the adoption of green hydrogen but also addresses the intricate complexities and interdependencies inherent within the energy system. Additionally, the energy transition period is delineated up to the year 2050, with intervals of five years, starting from 2020. This structured temporal framework facilitates a gradual substitution of fossil commodities, enabling the attainment of specific market adoption rates at each interval.

The proposed model was examined within the Ecuadorian context focused on the following sectors:

- **Mobility:** Substitution of imported diesel by locally produced green hydrogen for heavy and urban transport vehicles.
- **Fertilizers:** Substitution of imported urea by locally produced green urea (derivate of green hydrogen) for agroindustry.

Diesel and urea are commodities of particular interest in the local context as they require a substantial subsidy from the Government, covering approximately 50% of their selling price [5], [6]. Additionally, diesel and urea contribute to GHG emissions associated with their production, transport, and use. The demand for these commodities was predicted by analyzing historical data using a time series forecasting technique known as autoregressive integrated moving average (ARIMA). Demand data for diesel was obtained from [7], covering the period from 1972 to 2020. For urea, data was collected from [8], [9] covering 1970 to 2020.

This study will allocate the renewable energy surplus, represented by the difference between supply (generation) and demand (consumption) in Ecuador, to produce green hydrogen for mobility and fertilizer (urea). The RES considered include hydropower (H), wind (W), and solar photovoltaic (PV). The surplus was forecasted with multiple linear regression on demand and supply data for 2001 to 2020 [10]. Furthermore, this work integrates the forthcoming renewable energy facilities, as outlined in the Electricity Master Plan of Ecuador [11] until 2035, which will alter the energy mix share throughout the study period.

Two green hydrogen deployment strategies were considered:

- **Strategy I**: Utilizing energy surplus from existing and upcoming (already planned) RES facilities for green hydrogen production.
- **Strategy II**: Expanding Strategy I by constructing additional PV power plants for green hydrogen production. Ecuador has significant potential in PV, especially in the provinces within the Sierra Central region [12]. The PV plant capacity factor (CF) was calculated (around 25.13%) using GHI specific to this region as described in [13]. Furthermore, the capital (CAPEX) and operational (O&M) costs for these PV plants were obtained from [13].

The comparison of these two strategies will involve analyzing their respective subsidy costs and greenhouse gas emissions throughout the deployment period. This analysis will provide insights into the economic feasibility and environmental implications of each strategy, thereby guiding decision-making processes towards a sustainable energy future for Ecuador.

2.2 Multiobjective optimization

The decision variables considered were green hydrogen for mobility from PV (X_1), Wind (X_2) and Hydro (X_3), green hydrogen for urea production from PV (X_4), Wind (X_5) and Hydro (X_6), and the imported diesel (X_7) and urea (X_8). In the case of Strategy II optimization, another decision variable is added to represent the installed capacity of the additional PV facilities (X_9).

The constraints are based on physical, technical, and market-related restrictions. The demand of commodities for the mobility (D_m) and fertilizer (D_f) sectors at period i must be covered using either conventional utilities or its hydrogen-derived substitute.

$$Q \sum_{j=1}^{3} X_{j,i} + PX_{7,i} = D_{m,i} \tag{1}$$

$$R \sum_{j=4}^{6} X_{j,i} + X_{8,i} = D_{f,i} \tag{2}$$

Equations (1) and (2) represent an equality constraint as the supply must match the demand on the left-hand side of the equation. The parameters Q $(1.576 \text{ x } 10^{-2} \text{ GWh/ton H}_2)$, P $(3.167 \text{ x } 10^{-4}$ GWh/ton diesel) and R (7.35 ton urea/ton H_2) correct the units, efficiency, and form of the hydrogen molecule and fossil commodity to set a fair comparison for the given demand.

The production of green hydrogen and its derivatives depends on the local availability of renewable energy surplus (S). This allocation of energy relies on the energy mix fraction share of available renewable sources, i.e. solar (d_{PV}), Wind (d_W), Hydro (d_H), during each period i. This formulation establishes the constraints detailed in Equations (3), (5) and (6) for Strategy I and (4), (5) and (6) for Strategy II, representing the upper bounds for each energy source. The parameter ε $(0.049 \text{ GWh/ton H}_2)$ standardizes units to account for the specific energy consumption of alkaline water electrolysis in green hydrogen production.

$$d_{PV,i}\, S_i \geq \varepsilon(X_1 + X_4) \tag{3}$$

$$d_{PV,i}\, S_i + X_9 \geq \varepsilon\,(X_1 + X_4) \tag{4}$$

$$d_{W,i}\, S_i \geq \varepsilon(X_2 + X_5) \tag{5}$$

$$d_{H,i} S_i \geq \varepsilon(X_3 + X_6) \tag{6}$$

In planning an energy transition strategy, it is crucial to consider both environmental and economic aspects. This study utilizes the annual expenditure on subsidies as an economic performance indicator and the yearly amount of CO_2 emissions as an environmental performance indicator. Together, these indicators offer a comprehensive framework for evaluating the proposed energy transition strategies. The objective functions corresponding to these indicators are presented in Table 1.

Table 1. Objective functions.

Strategy	Annual Carbon Emissions (ton CO_2-eq)	Annual Subsidy Expenditure ($)
I	$\min_{x_i} \sum_{j=1}^{8} e_j X_{j,i}$	$\min_{x_i} s_d X_{7,i} + s_u X_{8,i} + s_h \sum_{j=1}^{6} X_{j,i}$
II		$\min_{x_i} s_d X_{7,i} + s_u X_{8,i} + s_h \sum_{j=1}^{6} X_{j,i} + s_{PV} X_{9,i}$

To calculate the CO_2 emissions associated with each decision variable, the emission factors e were acquired from [3], [14], [15]. Meanwhile, subsidies for diesel s_d [5] and urea s_u [6] were sourced from national reports. A proposed subsidy for green hydrogen production s_h is introduced in this study. To ensure the competitiveness of green hydrogen production [1], a fixed electricity rate of 5 cUSD/kWh is proposed. Given that the current average electricity price is 8.58 cUSD/kWh [16], this subsidy would cover the difference. Moreover, the objective function for the annual subsidy expenditure in Strategy II contemplates an additional subsidy s_{PV}, which was based on the levelized cost of energy for PV plants, considering their CAPEX, O&M, and CF.

The solution for each period i is derived by applying the energy transition model to each deployment strategy within the Python multiobjective optimization library Pymoo [17]. The chosen solver algorithm was NSGA-II, which follows the approach of an evolutionary optimization algorithm. Once the optimization algorithm converges to the Pareto-front, the *optimal* solution was determined using a multi-criteria decision technique known as compromise programming, in which equal weights were assigned to the objective functions.

3 Results

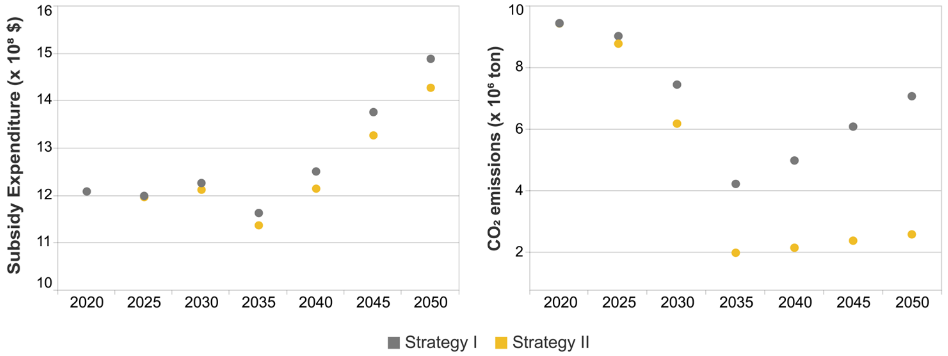

Fig. 1. Comparison of objective functions results for each green hydrogen deployment strategy.

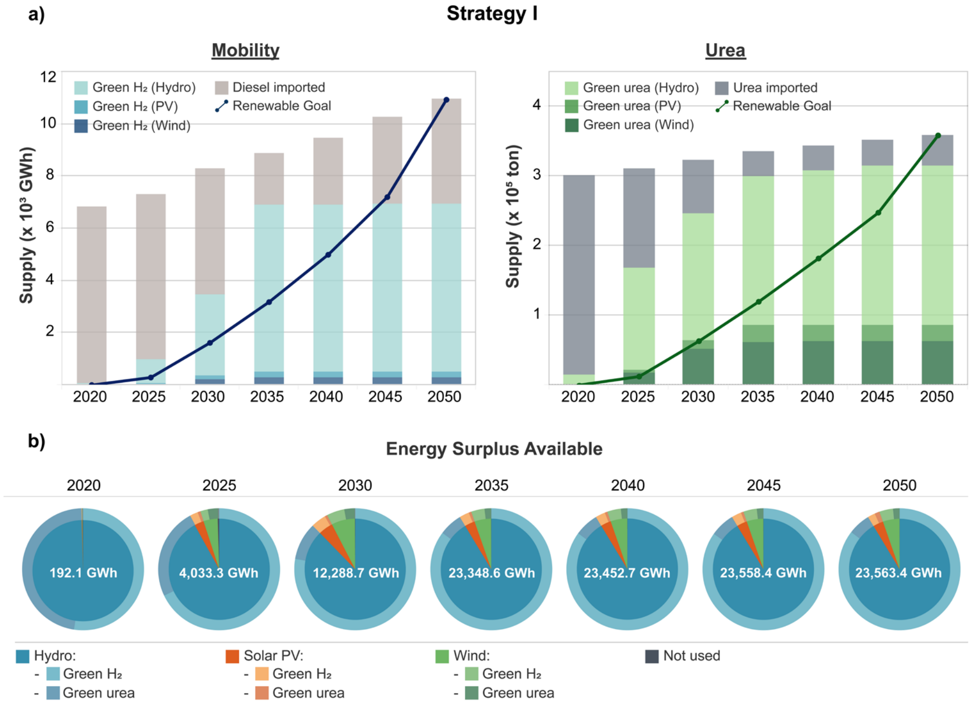

Fig. 2. Results of the optimal deployment of Strategy I: **a)** Decision variables, **b)** Use of energy surplus available for domestic production.

A comprehensive comparison of the results obtained for each deployment strategy is shown in Fig. 1. The initial period in 2020 reflects the current situation, with no strategy implemented during this phase due to its brevity. In each subsequent period (2025 – 2050), Strategy II consistently shows lower subsidy expenditure and CO_2 emissions than Strategy I. These results effectively minimize the subsidy expenditure and CO_2 emissions in each period. For instance, if the demand of these sectors in 2050 were to be met solely through imports, subsidies and emissions would total approximately $1,880 million and 15.51

million tons of CO_2, respectively. Strategy I reduces subsidy expenditure by up to 20.8% and emissions by 52.7%. In contrast, Strategy II outperforms Strategy I by achieving reductions of 24.1% and 81.5%, respectively.

As displayed in Fig.2, the energy surplus in Strategy I is fully utilized for the domestic production of commodities. Since the renewable energy mix mostly comes from hydropower, green hydrogen and green urea are mainly produced from this energy source. Moreover, the energy allocated solely for green hydrogen production for mobility exceeds that given for green urea by over 50% in all three RES. In this specific strategy, the actual Ecuadorian government plan is being evaluated. The integration of upcoming power facilities [11] spurs an exponential transition towards these green alternatives until 2035. Nevertheless, from 2040 onwards, this domestic production exhibits a more decelerated increase. This is attributed to the absence of new projects in the Electricity Master Program for these periods, as evident in the marginal increase in total available energy for 2040, 2045, and 2050 compared with 2035. In response to the unceasing growth in demand within these sectors, there is a noticeable rise in diesel and urea importation. This shift significantly impacts the trends illustrated in Fig. 1 for the objective functions. Initially, subsidy expenses and CO_2 emissions consistently decrease until 2035. However, this trend later reversed due to the increase in imports, suggesting that the influence of imports on both subsidy expenses and CO_2 emissions is more significant than that from domestic green hydrogen and urea.

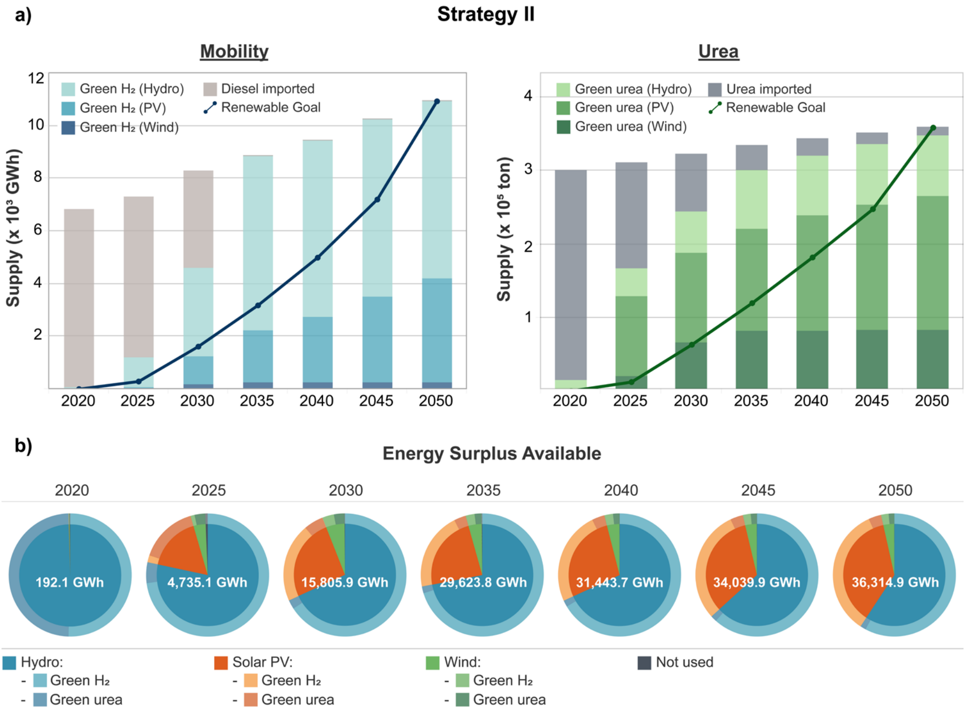

Fig. 3. Results of the optimal deployment of Strategy II: **a)** Decision variables, **b)** Use of energy surplus available for domestic production.

Fig. 3 (b) shows the availability of energy surplus allocated for the domestic production of green hydrogen for mobility and green urea. Notably, this allocation is greater than that of Strategy I throughout all periods. As new PV plants are being implemented periodically in this scenario, the share of energy generated by PV increases significantly, rising from 0.07% in 2020 to 37.25% in 2050. This growth in green hydrogen and urea production further reduces the dependence on imports, subsequently lowering CO_2 emissions, as illustrated in Fig. 1. Moreover, Fig.3 (a) indicates that the fertilizer sector primarily relies on green urea from available solar and wind energy. In fact, notwithstanding the continued import of urea until 2050, the quantity imported is lower than Strategy I. However, a complete transition to green urea has yet to be realized during any period. In contrast, the transport sector (freight and urban transport) will achieve a complete transition to green hydrogen by 2035 and maintain this status until 2050, primarily sourced from hydropower and solar power.

In 2021, the National Electromobility Strategy for Ecuador (ENEME) [18] was developed to decarbonize the transport sector. ENEME established targets for adopting electric vehicles in various automotive segments (i.e., public buses, taxis, light cargo trucks, and light vehicles) until 2040. In this context, the adoption targets for the market will be considered as if they were intended for hydrogen-powered fuel cell vehicles to achieve complete adoption by 2050. Since there are no specific green urea adoption strategies, the same mobility targets were applied.

These *Renewable Goals* are depicted in Fig. 2 (a) and Fig. 3 (a) for both sectors. Strategy I successfully meets the adoption targets in the transport sector until 2040, while Strategy II achieves a complete transition, and thus the subsequent adoption goals, in 2035. In the fertilizer sector, both strategies reach the target by 2045. However, it is crucial to note that further actions are necessary due to the 100% adoption target not being met by 2050 in the transport sector for Strategy I and in the fertilizer sector for any of the scenarios. Exploring options beyond PV plant construction, such as deploying other RES like wind, biomass, or geothermal [19], may be required. These findings provide insights into the effectiveness of the analyzed deployment strategies and their role in decarbonizing two crucial high-energy demand and subsidized sectors in Ecuador over time.

4 Conclusions

The proposed approach determined the optimal allocation of surplus RES energy to produce green hydrogen and green urea, thereby contributing to the long-term decarbonization efforts within the transport and fertilizer sectors in Ecuador. Through the evaluation of two hydrogen deployment strategies from 2020 to 2050, the algorithm effectively minimized annual subsidy expenditure and CO_2 emissions, presenting solutions that exhibited substantial reductions compared to an imports-only scenario. While both strategies contributed positively to adopting greener alternatives, Strategy II (PV expansion) demonstrated superior performance. However, achieving complete decarbonization of these sectors by 2050 may require additional measures. Thus, the proposed framework offers invaluable insights for policy decision-makers by providing a systematic methodology for forecasting and assessing green hydrogen deployment strategies. This structured approach enables decision-makers to navigate the complexities of the energy transition with clarity regarding the potential outcomes of various strategies and their implications for long-term sustainability goals. By empowering decision-makers to make informed policy decisions, this framework facilitates the identification of optimal pathways towards decarbonization. Moreover, decision-makers can adapt and refine strategies based on the evolving decarbonization objectives of their respective countries, ensuring alignment with broader sustainability agendas. In future work, optimization objectives could include considerations of social impact, energy efficiency, and resource consumption (e.g., water and land). Additionally, further exploration of coupling strategies with additional sectors (e.g., steel, chemicals, aviation, etc.) could be incorporated for a more comprehensive and integrated evaluation of these deployment strategies.

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