

# Process and Network Design for Sustainable Hydrogen Economy

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## ABSTRACT

This study presents a comprehensive approach to optimizing hydrogen supply chain network (HSCN), focusing initially on Texas, with potential scalability to national and global regions. Utilizing mixed-integer nonlinear programming (MINLP), the research decomposes into two distinct modeling stages: broad supply chain modeling and detailed hub-specific analysis. The first stage identifies optimal hydrogen hub locations, considering county-level hydrogen demand, renewable energy availability, and grid capacity. It determines the number and placement of hubs, county participation within these hubs, and the optimal sites for hydrogen production plants. The second stage delves into each selected hub, analyzing energy mixes under variable solar, wind, and grid profiles, sizing specific production and storage facilities, and scheduling to match energy availability. Iterative refinement incorporates detailed insights back into the broader model, updating costs and configurations to converge upon an optimal supply chain design. This design encapsulates macro-level network configurations, including centralization versus decentralization strategies, transportation cost analysis, and carbon footprint assessment, as well as micro-level operational specifics like renewable energy contributions, facility scale, and energy portfolio management. The methodology's robustness allows for strategic insights into hydrogen production facility siting, aligning with local energy resources and supply chain economics. This adaptable, multi-scale approach contributes to informed decision-making in the evolution of sustainable hydrogen-based energy systems, offering a roadmap for policy reforms and strategic supply chain development in diverse energy landscapes.

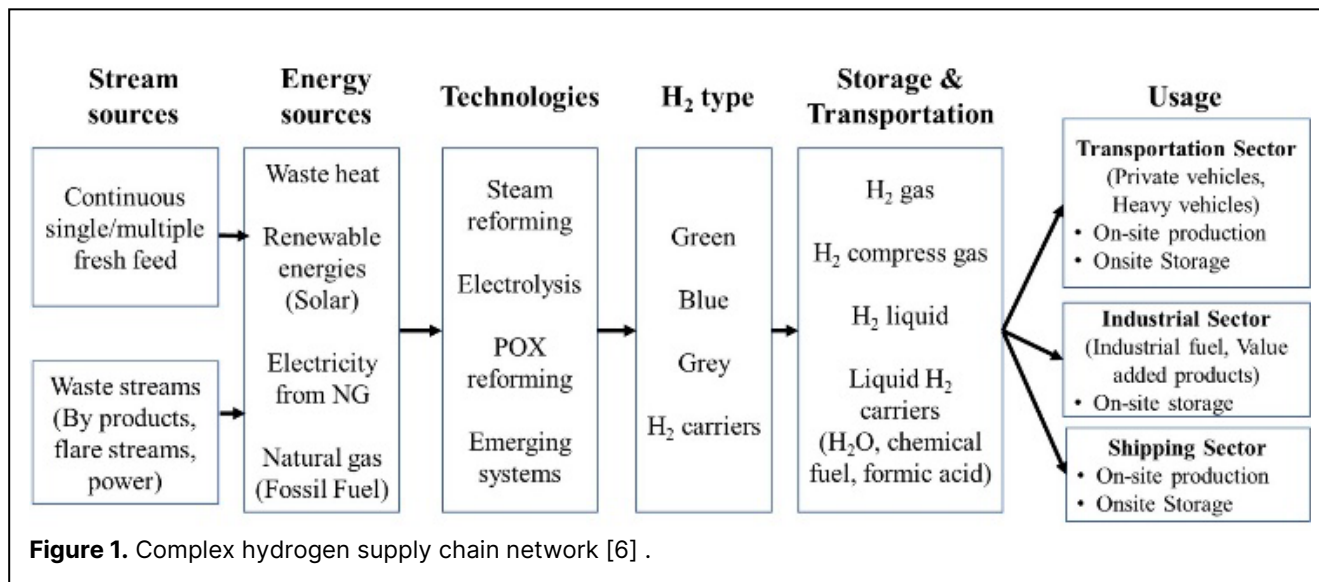
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**Keywords:** Energy Management, Hydrogen, Optimization, Renewable and Sustainable Energy, Supply Chain, Network Design.

## INTRODUCTION

The global energy landscape is undergoing a paradigm shift towards sustainable and clean energy sources, with hydrogen emerging as a pivotal player in this transition. Hydrogen, particularly green hydrogen produced from renewable energy sources, offers a promising solution to decarbonize various sectors, including transportation, industrial processes, and energy storage [1, 2]. The U.S. Department of Energy's (DOE) investment in hydrogen hubs underscores their pivotal role in advancing the nation's clean energy agenda. With a commitment of \$7 billion towards establishing H2Hubs, alongside \$1 billion to boost clean hydrogen demand and \$1.5 billion to enhance electrolysis technologies, the DOE aims to

significantly reduce the cost of clean hydrogen to \$1 per kilogram within a decade [3]. This initiative is not just an investment in sustainable energy but also a substantial job creator, promising to generate tens of thousands of well-paying jobs across the country. Moreover, the H2Hubs are expected to play a crucial role in environmental conservation by eliminating approximately 25 million metric tons of carbon dioxide emissions annually, equating to the emissions of about 5.5 million gasoline-powered cars [4]. This strategic move marks a significant step towards realizing a more sustainable, low-carbon future, positioning hydrogen hubs as a cornerstone in the transition to cleaner energy sources.



However, establishing an efficient hydrogen supply chain network (HSCN) poses significant challenges due to its complexity and the need for a multi-scale optimization approach encompassing production, storage, transportation, and distribution [5, 6]. The complexity stems from several key aspects: the geographical dispersion of supply and demand centers, the integration of diverse and intermittent renewable energy sources, and the need to align production with fluctuating energy availability. Additionally, the network comprises various interconnected components, including production sites, storage facilities, and distribution hubs, each with its own set of operational constraints and dependencies (see Fig. 1). The variability in renewable energy output, such as solar and wind, adds another layer of complexity, necessitating advanced planning and forecasting methods. This complexity is further amplified by the dynamic nature of market demands, technological advancements, and regulatory landscapes. Solving this multifaceted problem requires not only sophisticated computational models and optimization algorithms but also a deep understanding of the interplay between various elements of the hydrogen supply chain.

Pertinent literature reveals various approaches to modeling and optimizing Hydrogen Supply Chain Networks (HSCNs). Study such as by Vijayakumar et al. [7] have focused on geographic and economic aspects of hub placement. They highlight the importance of long-term planning in mitigating system costs and retail prices, but their deterministic approach overlooks uncertainties in demand and feedstock prices which are crucial for accurate forecasting. In contrast, Li et al. [8] provide an optimization-oriented review of hydrogen supply chain network design, noting gaps such as the treatment of uncertainty. Alkatheri et al. [9] address the intermittency challenges of renewable energies with a multiscale stochastic

programming approach for energy hub design, despite the computational complexity. Moran et al. [10] offer a flexible tool for analyzing regional hydrogen hubs, as exemplified by their Irish case study, but do not fully consider the implications of using grid electricity from non-renewable sources and the variability of the renewable integration. Additionally, Marouani et al. [11] delved into the integration of renewable energy sources into the supply chain. However, the dynamic and variable nature of renewable energy availability, particularly solar and wind, and its impact on hydrogen production and storage scheduling and sizing remains under-addressed.

To address these challenges, this study proposes a novel two-stage mixed-integer nonlinear programming (MINLP) approach. The first stage involves broad supply chain modeling to identify optimal hydrogen hub locations and configurations, considering county-level demand, renewable energy availability, and grid capabilities. The second stage focuses on detailed hub-specific modeling, specifying energy mixes, production and storage capacities, and schedules in alignment with variable energy inputs.

The results of this approach include the identification of optimal hub locations and configurations, tailored energy mixes for each hub, and detailed operational schedules that maximize efficiency and minimize costs. Moreover, the iterative refinement process employed in this study allows for the continuous updating of model parameters, leading to increasingly accurate and optimal solutions. This study not only contributes to the existing body of knowledge on HSCN optimization but also provides a practical and scalable framework for policymakers and industry stakeholders.

## PROBLEM STATEMENT

The central hypothesis of our study posits that by

addressing key research questions within Texas' hydrogen supply chain, the findings could be extrapolated to national or even international scales. McKinsey & Company's sustainability report projects that Texas' demand for clean hydrogen may increase to 21 million tonnes (MT) by 2050, up from the current 3.6 MT produced conventionally [12]. Our assumption is that all 254 counties in Texas will contribute to this demand based on factors such as local energy requirements, population, available land, and the variability of energy sources including the grid, wind, and solar. The target is to answer the following key research questions:

- What are the strategic locations for the hydrogen production plants?
- What constitutes the optimal energy mix for electrolytic hydrogen production, given variable electricity pricing, wind availability, and solar irradiance?
- What are the optimal size of H<sub>2</sub> production facilities, renewable farms, energy storage, considering the temporal variations in renewable energy availability?
- What is the comprehensive cost of the hydrogen supply chain, including production, storage, and transportation?
- What will be the optimal scheduling of the hydrogen production process to match energy availability?

## METHODOLOGICAL APPROACH

We adopt a multi-scale optimization framework that integrates both supply chain optimization (level 1) and process design and energy scheduling (level 2), ensuring convergence towards an optimal supply chain design that encapsulates macro-level network configuration and micro-level operational details.

### Level 1: Supply Chain Optimization

At the macro-level, the network configuration is informed by the optimization of strategic decisions such as site selection, facility sizing, hydrogen distribution, transportation costs to/from other counties, energy portfolio mix and management cost, guided by county-specific roles and requirements. In our supply chain optimization, we employ piecewise linearization to address the economies of scale inherent in hydrogen production. This mathematical technique allows us to model the cost benefits of scaling production facilities accurately. By breaking down the nonlinear cost structure into linear segments, we can analyze scenarios where a single large production facility or multiple smaller ones are more economically viable. This is crucial in evaluating the

feasibility of a hub approach to hydrogen production. Furthermore, this linearization facilitates the use of linear programming techniques, which significantly expedite the optimization process, ensuring a swift and efficient path to finding the optimal supply chain configuration.

$$\min \sum_i \sum_j c_{ij}^{trans,H_2} x_{ij}^{H_2} r_{ij} + \left(\frac{\varphi}{\beta}\right) \sum_i \sum_j c_{ij}^{trans,E} x_{ij}^E r_{ij} + \sum_p c_{i,p}^{prodH_2} \Delta x_{i,p}^{H_2} + \sum_i \sum_{sor} c_{i,sor}^{prodE} x_{i,sor}^E$$

Subject to

$$\begin{aligned} D_i &\leq \sum_j x_{ji}^{H_2} \\ e_i^{intensity} \sum_j x_{ij}^{H_2} &= \sum_{sor} \sum_j x_{j,i,sor}^E \\ \sum_j x_{j,i,sor}^E &\leq e_{i,sor}^{max} \\ \sum_p \lambda_{ip} &= 1 \\ x_{p-1}^L \lambda_{ip} &\leq \Delta x_{ip} \leq x_p^U \lambda_{ip} \\ \sum_j x_{ij}^{H_2} &= \sum_p \Delta x_{ip} \end{aligned}$$

### Level 2: Process Design and Energy Scheduling

The micro-level details focus on operational intricacies within individual counties. This includes determining the roles counties play within the network, scaling production and storage facilities, configuring the energy portfolio, aligning production timing with renewable energy availability, devising energy storage solutions, sizing renewable energy farms for grid independence, and formulating strategies to meet emissions reduction goals.

$$\min TC = C^{iv,tot} + C^{of,tot} + C^{ov,tot} + C^{ov,um}$$

Subject to,

$$\begin{aligned} LCOH &= \frac{C^{iv,tot} + C^{of,tot} + C^{ov,tot}}{\sum_t m_t^{out}} \\ P_t^g + \sum_{ren} P_{ren,t}^{sor} + \sum_i P_{i,t}^S &= P_t^{el} + P_t^{comp} \\ m_t^{dem} &= m_t^{out} + m_t^{um} - m_t^{excess} \\ C^{ov,grid} &= \sum_t \pi_t P_t^g \Delta t \\ C^{ov,um} &= \sum_t \lambda m_t^{um} \Delta t \\ C^{ov,co2} &= \sum_t P_t^g \gamma \varphi \Delta t \\ C^{iv,tot} &= C_{ren}^{iv,sor} + C^{iv,el} + C^{iv,comp} + C^{iv,tank} \\ &\quad + \sum_i C_i^{iv,stor} \\ C^{of,tot} &= C^{of,el} + C^{of,comp} + C^{of,tank} + \sum_i C_i^{of,stor} \\ C^{ov,tot} &= C^{ov,grid} + C^{ov,um} + C^{ov,co2} + \sum_i C_i^{ov,stortot} \end{aligned}$$

Renewable farm constraints,

$$\begin{aligned}
P_{ren,t}^{sor} &\leq eff_{ren} A_{ren} \\
Avail_{solar,t} &= ghi_t A_{total} \left( 1 - \max \left( \frac{PD_{th} - PD_{min}}{PD_{max} - PD_{min}}, \frac{PD - PD_{min}}{PD_{max} - PD_{min}} \right) \right) \\
Avail_{wind,t} &= 0.5 \pi \rho_{air} v_t^3 A_{total} \left( 1 - \max \left( \frac{PD_{th} - PD_{min}}{PD_{max} - PD_{min}}, \frac{PD - PD_{min}}{PD_{max} - PD_{min}} \right) \right) \\
C_{ren}^{iv,sor} &= CO_{ren} A_{ren} CRF \frac{T}{8760}
\end{aligned}$$

Electrolyzer constraints,

$$\begin{aligned}
N^{cell} &= \frac{1000 \Lambda^{el}}{nc_{h2}^{po,cell}} \\
m_t^{norm} &= \frac{m_t^{el}}{N^{cell} m_{cell,max}^{el}} \\
P_t^{el} &= (-8.5231 m_t^{norm2} + 23.995 m_t^{norm} + 47.752) m_t^{el} 10^{-3} \\
C^{iv,el} &= CO^{iv,el} \Lambda^{el} CRF \frac{T}{8760} \\
C^{of,el} &= CO^{of,el} C^{iv,el}
\end{aligned}$$

Hydrogen compressor constraints,

$$\begin{aligned}
P_t^{comp} &= m_t^{el} c_{h2}^{po,comp} \\
P_t^{comp} &\leq \Lambda^{comp} \\
C^{iv,comp} &= CO^{iv,comp} \Lambda^{comp} CRF \frac{T}{8760} \\
C^{of,comp} &= CO^{of,comp} C^{iv,comp}
\end{aligned}$$

Hydrogen storage constraints,

$$\begin{aligned}
m_{t+1}^{tank} &= m_t^{tank} + (m_t^{el} - m_t^{out}) \Delta t \\
0 &\leq m_t^{stor} \leq m^{tank,max} \\
C^{iv,tank} &= CO^{iv,tank} m^{tank,max} CRF \frac{T}{8760} \\
C^{of,tank} &= CO^{of,tank} C^{iv,tank}
\end{aligned}$$

Energy storage model,

$$\begin{aligned}
\sum_b z_{i,t,b}^{op} &= 1 \\
\epsilon y_i &\leq x_i \leq E_i^{ub} y_i \\
0 &\leq E_{i,t} \leq x_i \\
E_{i,t+1} &= E_{i,t} - (\eta_{i,t}^S z_{i,t,b=c}^{op} + z_{i,t,b=d}^{op}) P_{i,t}^S \Delta t \\
\eta_{i,t}^S &= n0_i s_{i,t}^{n1_i} \\
-z_{i,t,b=c}^{op} P_{i,t}^S &\leq P_{i,t}^{c,max} \leq P_{i,t}^{c,ub} y_i \\
z_{i,t,b=d}^{op} P_{i,t}^S &\leq P_{i,t}^{d,max} \leq P_{i,t}^{d,ub} y_i \\
\left| \frac{E_{i,t=NT+1} - E_{i,t=1}}{E_{i,t=1}} \right| &\leq cyclot \\
\left| (-z_{i,t+1,b=c}^{op} + z_{i,t+1,b=d}^{op}) P_{i,t+1}^S - (-z_{i,t,b=c}^{op} + z_{i,t,b=d}^{op}) P_{i,t}^S \right| &\leq rr_i^{stor} \\
P_{i,t}^S &= f1_{i,t} \\
E_{i,t} &= f2_{i,t} \\
s_i^{lb} &\leq s_{i,t} \leq s_i^{ub} \\
l_i^{lb} &\leq l_{i,t} \leq l_i^{ub} \\
tr^{lb} &\leq tr_i \leq tr^{ub}
\end{aligned}$$

$$\begin{aligned}
C_i^{iv,stor} &= (c11_i x_i^{\alpha11_i} + c12_i P_{d_i}^{max \alpha12_i} + c13_i P_{c_i}^{max \alpha13_i}) CRF_i \frac{T}{8760} \\
C_i^{of,stor} &= (c21_i x_i^{\alpha21_i} + c22_i P_{d_i}^{max \alpha22_i} + c23_i P_{c_i}^{max \alpha23_i}) \frac{T}{8760} \\
C_{i,t}^{ov,stor} &= (c31_i z_{i,t,b=d}^{op} - c32_i z_{i,t,b=c}^{op}) P_{i,t}^S \Delta t \\
C_i^{ov,stor,tot} &= \sum_t C_{i,t}^{ov,stor}
\end{aligned}$$

At its core, the model seeks to balance energy production and hydrogen generation across temporal and spatial dimensions, taking into account the variable nature of renewable energy sources and grid electricity prices. The model incorporates decision variables for energy management, renewable energy farms, energy storage, and hydrogen production and storage. These variables are optimized within a system of constraints that ensure energy balance, hydrogen balance, and operational feasibility (see Fig. 2). For example, the power purchased from the electricity grid at any given time is matched against the power consumed by electrolyzers and compressors, ensuring an overall energy balance. The constraints also enforce the physical and operational limitations of the system, such as the maximum hydrogen storage capacity and the power output limits of storage technologies. This detailed formulation allows for the examination of the economic and environmental implications of the supply chain, with the ultimate goal of minimizing costs and emissions while meeting the hydrogen demand.

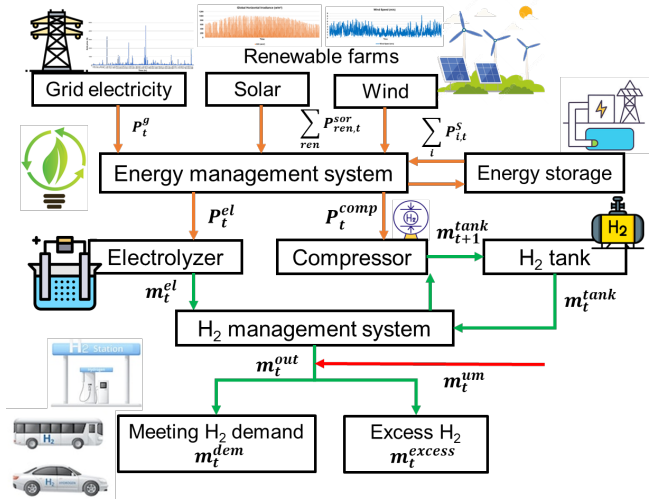
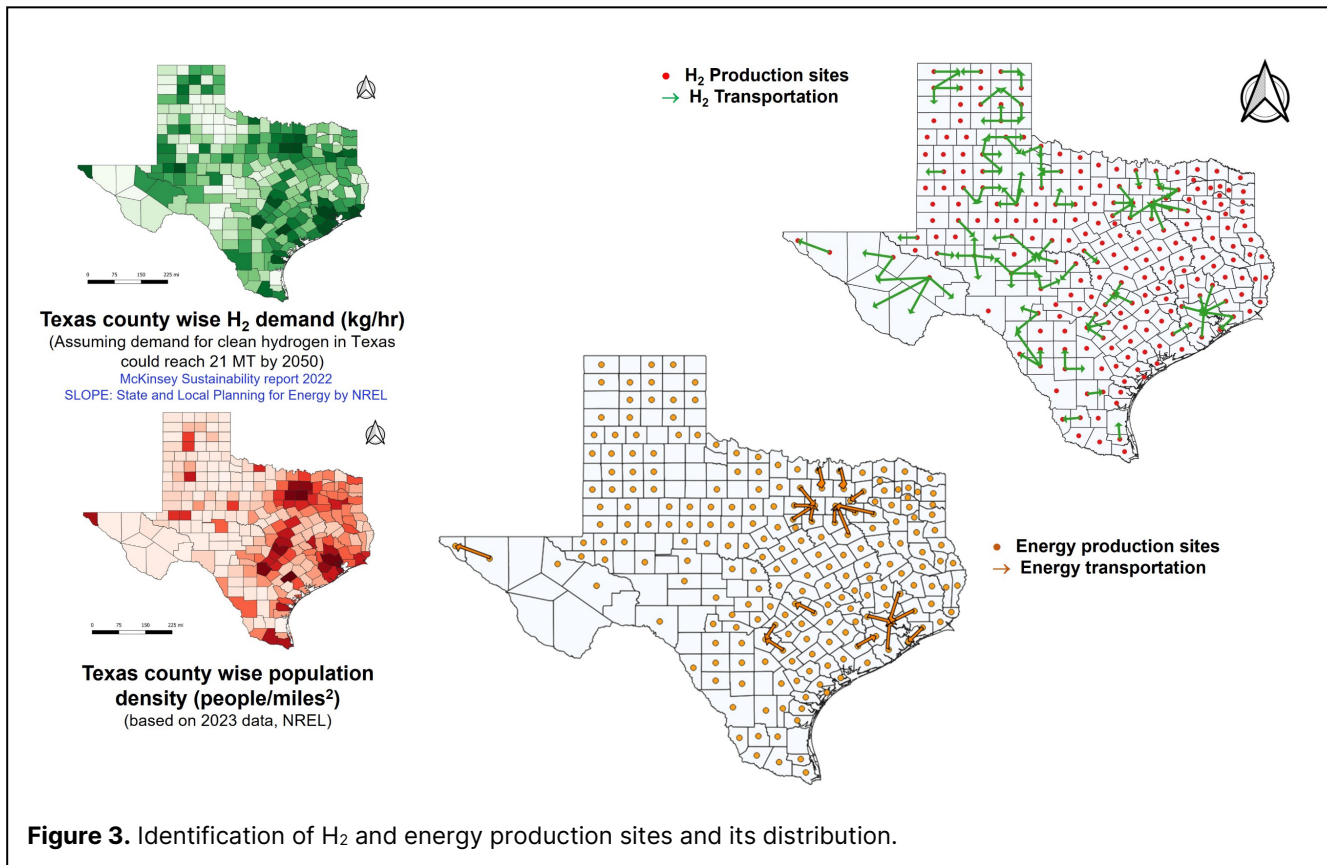


Figure 2. Green hydrogen production system.

This decomposition into two optimization levels allows for a structured breakdown of the complex supply chain problem. The output of level 1, which encapsulates



county-wise energy and hydrogen demand forecasts, informs level 2 decisions. This includes detailed cost assessments for hydrogen production at the county level, which are then fed back into level 1. The iterative feedback loop between the two levels propels the optimization process toward convergence, refining the network configuration with each iteration.

Recognizing the variable nature of energy availability across counties, our model incorporates a robust mechanism for inter-county energy flow. This mechanism dynamically channels surplus energy from counties with excess to those with deficits, thereby maintaining the balance necessary to meet each county's hydrogen production demands. This energy management strategy is integral to our comprehensive approach, affirming that all counties can achieve their hydrogen demand targets through cooperative energy sharing and sophisticated scheduling.

## RESULTS AND DISCUSSION

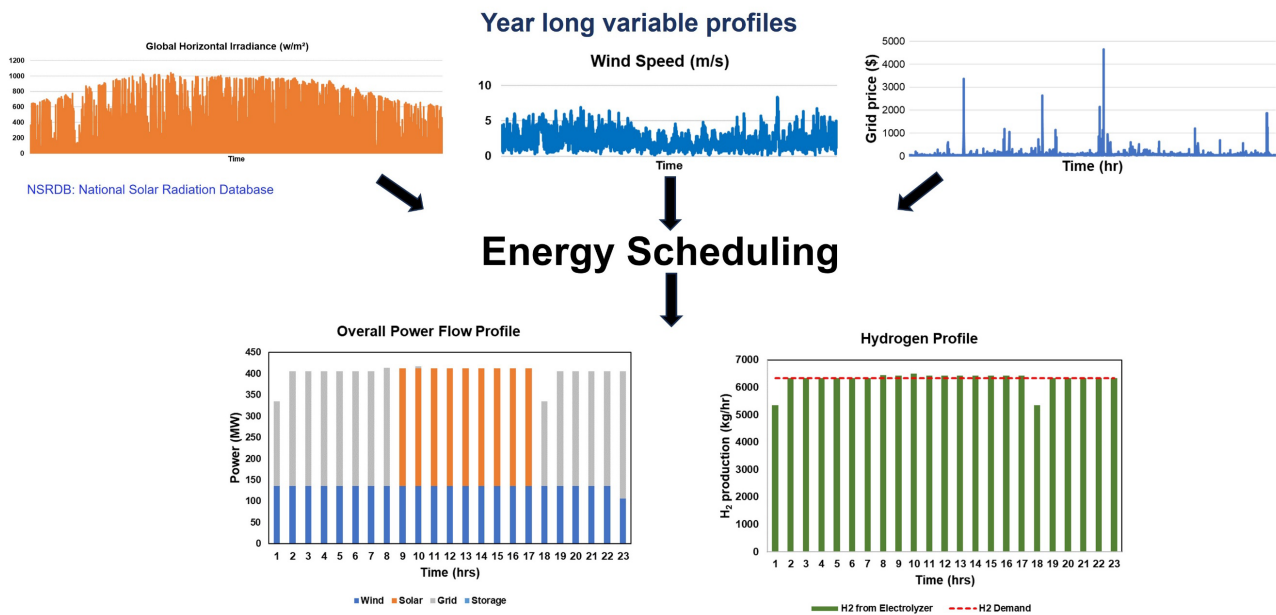
The broader supply chain optimization achieves strategic positioning of hydrogen production facilities across Texas, with significant concentrations in energy-rich counties. For instance, the production capacities ranged from 0.21 to 21 MT per year, aligning with the variable solar and wind profiles. In Fig. 3, we can see the location of the hydrogen production sites and the

distribution of produced hydrogen to other counties based on the given projected energy demand and population density of each county. We can observe that not every county is producing their H<sub>2</sub> rather few counties are taking the leverage of economics of scale by collaborating with the neighbouring counties. This also gives us the indication that if management or policy makers decided to build up the specific number of hubs for the hydrogen for Texas. Our supply chain optimization can find those locations with some additional constraints. The optimal energy mix was achieved with 35.46% wind, 34.3% solar, and 30.23% grid energy, illustrating a significant reliance on renewable sources.

The simulation results, derived from a year-long variability profile for solar irradiance and wind speed, indicate a consistent alignment between the overall power flow and the hydrogen production profile, which is crucial for maintaining a sustainable energy supply for hydrogen production (see Fig. 4). The hydrogen profile, compared with the demand, reveals that the production from electrolyzers is well-aligned with the demand pattern, suggesting an efficient design of the electrolyzer capacity and operational scheduling. Notably, peak production periods do not always coincide with peak demand times, indicating the necessity for robust storage solutions within the supply chain to balance the temporal discrepancies. In terms of energy supply, the integration of solar and wind energy contributes significantly to the overall

**Table 1:** Selected information on hydrogen production process design.

| County   | Max installed wind capacity (MW) | Max installed solar capacity (MW) | Installed electrolyzer capacity (MW) | LCOH (\$/kg) | Penalty on unmet H <sub>2</sub> demand (\$) | Total system cost (MM \$) | Emission penalty on grid bought electricity (MM \$) |
|----------|----------------------------------|-----------------------------------|--------------------------------------|--------------|---|---------------------------|---|
| Austin   | 528.831                          | 2563.51                           | 1602.3                               | 4.58         | -   | 992                       | 218   |
| Angelina | 1.93                             | 286.06                            | 159.73                               | 4.40         | -   | 92                        | 21.2  |
| Archer   | 194.43                           | 0                                 | 68.86                                | 3.39         | -   | 31.5                      | 0.5   |
| Austin   | 168.38                           | 4.01                              | 61.28                                | 3.51         | -   | 28.8                      | 0.69  |
| Bailey   | 0                                | 26.38                             | 14.54                                | 4.10         | -   | 6.32                      | 1.18  |
| Bastrop  | 0                                | 182.41                            | 105.68                               | 4.40         | -   | 61                        | 14.7  |
| Bee      | 788.58                           | 24.35                             | 290.05                               | 3.73         | -   | 145                       | 8.17  |
| Bell     | 915.15                           | 55.73                             | 351.74                               | 3.84         | -   | 181                       | 12.4  |
| Blanco   | 57.03                            | 0                                 | 20                                   | 3.27         | -   | 8.91                      | 0.02  |
| Borden   | 0                                | 0                                 | 1.80                                 | 5.46         | -   | 0.86                      | 0.36  |



**Figure 4:** Simultaneous design and scheduling model.

power flow, with grid energy supplementing the shortfall. However, the reliance on grid energy varies throughout the day, suggesting potential areas for further optimization of renewable energy sources or storage solutions to minimize grid dependence and enhance sustainability. Furthermore, our optimization model has successfully identified strategic locations for hydrogen production,

factoring in county-specific variables such as land area and energy profiles. This strategic placement, alongside an optimized energy mix, effectively minimizes transport costs and maximizes the use of local renewable energy, supporting the overarching goal of a resilient and sustainable hydrogen economy. Numerical insights obtained from the optimization highlight the potential for a

reduction in carbon footprint through optimized renewable energy use and strategic site placement. The proposed supply chain configuration promises to meet the projected 21 MT hydrogen demand by 2050, with a comprehensive cost analysis indicating a favorable comparison to current conventional hydrogen production costs.

The selective overview of Texas counties reveals a diversified approach to hydrogen production process design (see Table 1). For instance, Austin County showcases a substantial investment in renewable energy sources with impressive wind and solar capacities, facilitating a large-scale electrolyzer capacity that could cater to future hydrogen demands. However, the associated LCOH of \$4.58/kg suggests a higher production cost, potentially due to the scale of installed capacities and emission penalties. Conversely, counties like Archer, with a focus on wind energy, and Blanco, with a conservative renewable approach, indicate a more cost-effective production with their lower LCOH. Borden County's minimal figures might reflect an opportunity for growth or a strategic decision to maintain a small-scale operation. These data points indicate that while some counties are positioning themselves as potential leaders in hydrogen production, others may opt for a scaled approach or are in the early stages of infrastructure development. The diverse strategies underscore the need for a multifaceted, tailored approach in optimizing hydrogen production that balances cost, demand, and environmental impact.

## CONCLUSION

In our study, the placement of strategic hydrogen production sites was pivotal, with locations selected to align local demand with the availability of energy resources. The design of the network integrated insights from county-level contributions and renewable sources, setting a robust foundation for the configuration and scale of these production sites. Our analysis into the energy mix probed the feasibility of utilizing solar, wind, and grid sources to create a flexible energy portfolio for hydrogen production. By adopting an iterative, two-level optimization approach, we enhanced the supply chain model, ensuring economic feasibility and environmental sustainability. Our findings point to a future-adapted hydrogen supply network, resilient and scalable to meet the burgeoning demand and shifts in the energy sector. This synthesis of theoretical insights and numerical analysis underscores the viability of the proposed supply chain configuration, offering a viable pathway to achieving the DOE's goal of \$1 per kilogram of clean hydrogen within a decade.

## ACKNOWLEDGEMENTS

The authors acknowledge partial support for this

work from the Texas A&M Energy Institute.

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