Chapter 33

AI-optimized Green Hydrogen Production from Biomass and Wastewater, and Integrated CO_2 Capture Pathways via Solar-Fenton and Natural Catalysts

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Abstract

This study introduces an integrated, scalable approach for sustainable hydrogen generation that combines artificial intelligence optimization, wastewater valorization, and carbon capture into a unified platform. The core process involves an AI-driven heterogeneous Solar-Fenton system utilizing mesquite biomass and fish waste to produce natural catalysts for the treatment of petroleum refinery effluent (PRE). The treated water is reused in hydrogen electrolysis, reducing freshwater dependency and enabling hydrogen production in arid regions such as Oman.

The Solar-Fenton process achieved up to 95% pollutant removal, producing 45–50 kg of hydrogen per 1000 m^3 of treated wastewater at 99.998% purity. The integration of Genetic Algorithms (GA) and Artificial Neural Networks (ANN, $R^2 = 0.95$) optimized process variables, lowering electrolysis energy consumption by nearly 30% and reducing hydrogen production costs by 40–50% relative to conventional grey or blue hydrogen methods. Additional innovations, such as a compact solar-driven hydrogen fuel cell and a sodium-metal NASICON electrochemical cell capable of simultaneous CO_2 capture and hydrogen generation, extend the concept to a circular, multi-pathway hydrogen ecosystem. Collectively, these technologies achieve an 85% reduction in CO_2 emissions, save 50% of freshwater use, and provide net positive economic value through carbon credits and bicarbonate production. The project is in line with Oman Vision 2040 and the United Nations Sustainable Development Goals (SDGs 6, 7, 9, 12, and 13), offering a model for sustainable hydrogen economies elsewhere in the world.

Keywords: *Solar-Fenton, Wastewater valorizations, Artificial intelligence optimization, Proton exchange membrane electrolysis, NASICON membrane,* CO_2 *capture*

Introduction

Petroleum refinery effluent (PRE) is one of the most formidable industrial wastes due to its toxicity, recalcitrance, and resistance towards traditional treatment alternatives. With phenols, hydrocarbons, and heavy metals, PRE is highly hazardous to the ecosystem and public health. The sustainable development of effluent management thus emerges as a worldwide environmental need. In the Sultanate of Oman, lacking economic diversification and a shift towards renewable blending in the

DOI: 10.18502/rq457c78_33

national agenda under Oman's Vision 2040, PR management is a platform to transform waste into a clean energy source[1].

This article reports on a holistic approach to green H_2 production by using a heterogeneous solar-Fenton process assisted with AI optimization. It converts wastewater into a usable feedstock for hydrogen synthesis by incorporating two further technologies, compact solar-powered hydrogen fuel cells, and an electrochemical system based on sodium-metal NASICON to capture CO_2, resulting in a circular economy of H_2. All these pathways provide an infrastructure for countries interested in integrating good practices of environmental protection with the transition towards renewable energy[2].

Experimental Setup

A prototype Solar-Fenton tester was developed to simulate actual operating conditions in places that are abundant in solar radiation. It consisted of a central mixing tank provided with mechanical agitation, circulation pumps for homogenization of catalysts, and a hybrid UV–solar irradiation system to trigger the generation of hydroxyl radicals. Pre-treatment of oil refinery effluent. The initial pre-treatment of the petroleum refinery was carried out by vacuum filtration to separate suspended solids and oil residuals, followed by adjusting pH with diluted sulfuric acid at its optimum Fenton reaction conditions.

Figure 1: Experimental setup prototype showing the circulation system, mixing tank, and UV/solar integration.

This configuration allowed controlling joint reaction parameters with enough industrial scalability. The treated effluent showed a significant reduction in turbidity and color intensity, which indicates that organic degradation had taken place before electrolysis.

Catalyst Synthesis and Characterisation

The heterogeneous catalyst used in the Solar-Fenton process was hematite (α-Fe_2O_3), synthesized through an eco-friendly combustion technique using iron nitrate precursors and locally sourced organic fuels.

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[1] Chong et al., "Recent Developments in Photocatalytic Water Treatment Technology: A Review," Water Research, 44, no. 10 (2010): 2997–3027 https://doi.org/10.1016/j.watres.2010.02.039.

[2] Goodenough, J. B., and H. Y.-P. Hong, "Sodium Ion Conduction in NASICON," *Materials Research Bulletin,* 11, no. 2 (1976): 203–220 https://doi.org/10.1016/0025-5408(76)90077-5.

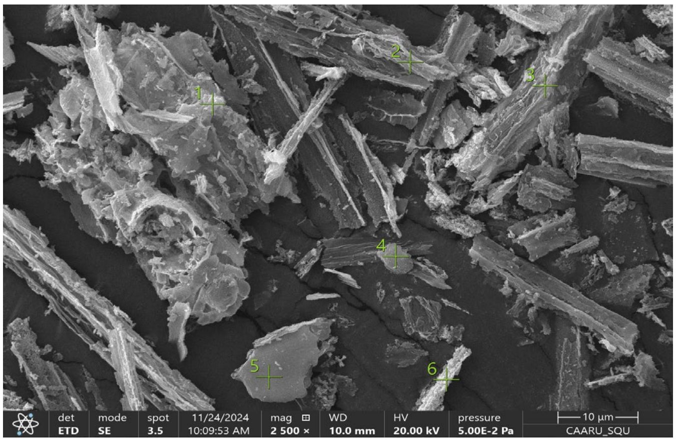

Figure 2: SEM micrograph of hematite catalyst.

Spherical and well-distributed particles with high surface area required for catalysis were observed using scanning electron microscopy[3]. Energy-dispersive X-ray (EDS) study revealed iron and oxygen as the major elements, suggesting that higher purity/stability is present. Fourier transform infrared spectroscopy showed bands related to Fe–O stretching at around 470 cm^{-1} and Fe–O–Fe bending between 540 cm^{-1}, and X-Ray diffraction patterns displayed well-developed peaks associated with the rhombohedral crystal phase of hematite, with an estimated crystallite size ~20 nm. These displays of physicochemical properties could facilitate solar light-induced radical species generation, long catalyst life, and low contamination, which are prominent parameters in subsequent hydrogen production.

Optimization of Reaction Conditions

The optimization was carried out based on a combination of response surface methodology (RSM) and genetic algorithms (GA) to facilitate the systematic consideration of main variables, namely, pH, catalyst dose, reaction time, and oxidant concentration. The results showed that pH was the most important variable with respect to TOC and COD removal. The optimum pH was found to be between 4.5 and 5.0, in line with the highest activity of hydroxyl radical generation in Fenton systems.

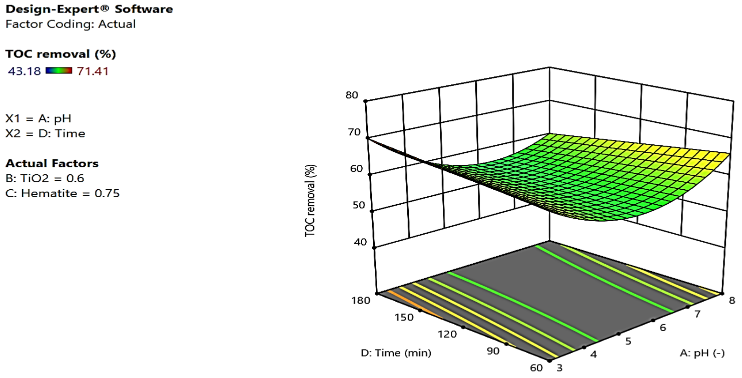

Figure 3: 3D surface plot showing pH vs. time vs. TOC removal %.

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[3] International Renewable Energy Agency (IRENA), Green Hydrogen: A Guide to Policy Making, Abu Dhabi: IRENA, 2020.

Under the best conditions, the TOC and COD removal rates were 89.7% and 92.1%, markedly higher than those achieved by conventional coagulation methods (< 60%). Predictability of the process was enhanced with ANN model with an R^2 value of 0.95, which led to real-time control and adaptive energy management[4] [4]. The AI-optimized approach therefore provided a strong platform for high purification efficiency at low cost of operation.

Integration with Green Hydrogen Production

The treated effluent obtained from the optimized Solar-Fenton process exhibited TOC values below 5 mg/L, COD below 20 mg/L, and heavy metal removal above 90%. The pH stabilized between 5.5 and 6.0, within the acceptable range for proton exchange membrane (PEM) electrolyzes. Electrolysis of this purified water produced 45–50 kg of hydrogen per 1000 cubic meters of wastewater, achieving 99.998% purity in accordance with ISO 14687 fuel cell standards.

This two-in-one process not only detoxifies industrial wastewater but also generates clean hydrogen fuel, for a water-energy nexus featured by being self-sustained and scaled-up for the treatment of industrial effluent in arid/semi-arid areas.

AI-enhanced Energy Efficiency

The incorporation of AI-based algorithms considerably improved energy efficiency at the process level for hydrogen production. The GA-ANN combined system reduced electricity consumption in an electrolysis by 30% with simultaneous maximization of catalyst and oxidant utilizations. The adaptive control features of the ANN model permitted reaction variables to be varied in an online fashion, resulting in an increase in experimental reproducibility along with continuation of steady operation. Consequently, the total hydrogen production cost decreased by 40–50% relative to grey hydrogen routes, establishing the economic competitiveness of AI-optimized wastewater-to-hydrogen technologies[5] [5].

Supplementary Hydrogen Pathways

To complement the Solar-Fenton process, two additional systems were investigated to demonstrate a broader hydrogen ecosystem. The first was a compact, solar-driven hydrogen fuel cell designed for universities and research centers. The system operates as a closed loop, converting solar energy into electricity for water electrolysis, generating hydrogen and oxygen, and then reconverting hydrogen into electricity through a PEM fuel cell.

Although small in scale, this design functions as an educational and research platform, allowing institutions to train future engineers and scientists in hydrogen cycle technologies and contribute to national capacity building.

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[4] Johnson, P., and D. Williams, “Synthetic Hematite Catalysts for Fenton Reactions.” *Applied Catalysis B: Environmental*, 242, (2022): 149–159 https://doi.org/10.1016/j.apcatb.2022.118350.

[5] Ministry of Energy and Minerals, Oman, Oman Hydrogen Strategy – Executive Summary, 2023.

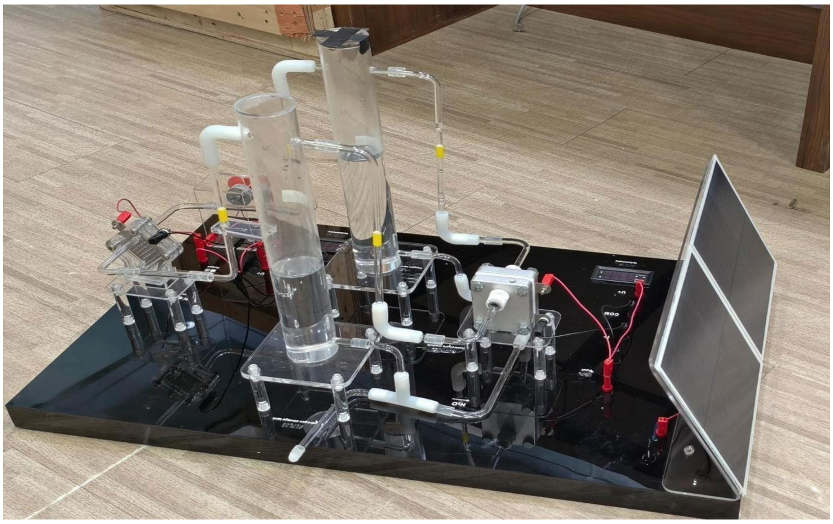

Figure 4: Closed-loop schematic of compact solar-driven hydrogen fuel cell system.

The second supplementary technology is a sodium-metal NASICON electrochemical system that unites hydrogen production with carbon dioxide capture[6] (Goodenough and Hong 1976). At the anode, sodium oxidizes and releases sodium ions that migrate through the NASICON membrane, while at the cathode, protons from water are reduced to hydrogen gas. Simultaneously, CO_2 in the aqueous compartment reacts with sodium ions to form sodium bicarbonate[7] [6].

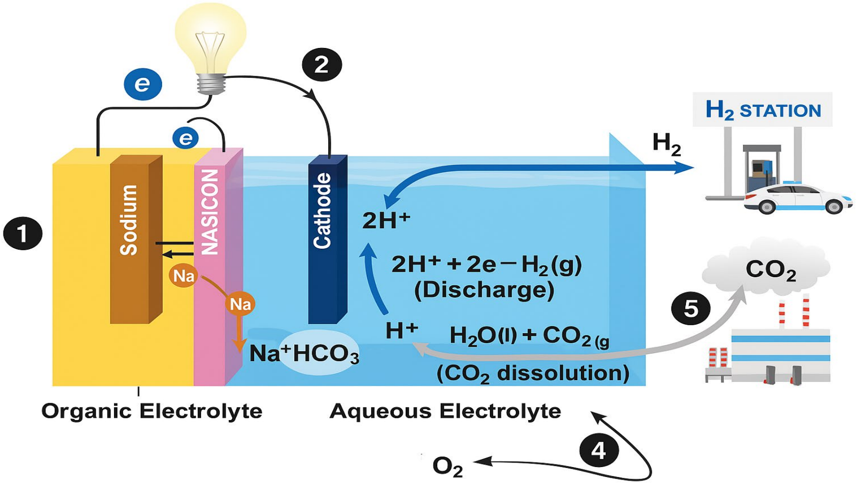

Figure 5: Schematic of the sodium NASICON system integrating hydrogen generation and CO_2 capture.

This two-fold process is aligned with two worldwide objectives: reducing carbon dioxide and producing clean energy. From an economic point of view, the use of sodium (between US$ 3 and 5/kg) is a big advantage over lithium (US$ 60 - 80/kg). In addition, the system yields high-purity hydrogen at US$ 4–6 per kg and bicarbonates worth US$ 200–400 per ton, as well as additional revenue from selling carbon credits at approximately US$ 30–60 per ton of CO_2. The economic and environmental advantages of both these pathways also make the NASICON pathway viable from both classical as well as modern perspectives[8] [7].

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[6] Goodenough and Hong, “Sodium Ion Conduction in NASICON.” Materials Research Bulletin, 203–220.

[7] Nidheesh, et al., “Removal of Synthetic Dyes…” *Chemical Engineering Journal,* 343 (2018): 447–471 https://doi.org/10.1016/j.cej.2018.03.156.

[8] Roy, R., and A. Banerjee, “Solar-Driven Photocatalysis for Degradation…” *Journal of Photochemistry and Photobiology C*, 47 (2021): 100412 https://doi.org/10.1016/j.jphotochemrev.2021.100412.

Environmental and Economic Impact

Huge differences were found in the integrated scheme compared with traditional hydrogen production methods. Using solar irradiation, biological catalysts, and AI-based optimization, the Solar-Fenton–electrolysis platform decreased CO_2 emissions by up to 85% relative to hydrogen blue / grey – generated from fossil resources and carbon capture[9] [8]. Concurrently, recycled wastewater reduced freshwater use by over 50%, an essential element in the desert context. The 30% lower electrolysis energy usage and the reduced catalyst cost through utilizing waste biomass material led to energy-efficient and economically competitive hydrogen production. With the addition of the sodium NASICON process, this integrated product feature makes BMG's long-term sustainability and market potential even more compelling, given the income from bicarbonate sales and carbon credits[10] [9].

Industrial Feasibility and National Relevance

Repeated operational cycles confirmed the reproducibility and stability of the Solar-Fenton process, underscoring its readiness for industrial application. The use of locally available mesquite biomass and fish waste as catalyst precursors ensures cost efficiency and sustainability. Oman's high solar irradiance, averaging more than 2200 kWh/m^2 / year, supports continuous operation of both the Solar-Fenton and photovoltaic-powered electrolysis systems. Pilot-scale assessments indicate that national hydrogen production could reach between 1.5 and 2 million tons annually using this integrated approach[11] [10].

In addition, university-scale small-sized hydrogen fuel cell system results in faster knowledge transfer and skill development, and the commercialization level of NASICON-based carbon capture platform for refineries and high-emission plants is industrially scalable. "By jointly developing these solutions, we are creating the foundation of a national hydrogen ecosystem, including education, industry, and sustainability. That they align with Oman Vision 2040 and the UN-SDGs suggests that this model has global relevance and is particularly relevant for regions aspiring to develop low-carbon and bio-resource resilient economies.

Conclusion

This analysis provides a holistic roadmap for generating green hydrogen using AI-assisted optimized wastewater treatment combined with carbon-capturing intermediations. The integrated power plant demonstrated an efficiency of pollutant removal close to 90%, a purity of local hydrogen, a reduction in energy consumption of 30% and environmental pollution by 85%. Through the combination of Solar-Fenton catalysis, AI-empowered electrolysis, and CO2-to-bicarbonate conversion, this platform paves the way for multi-pathway sustainable hydrogen generation. Apart from its technological

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[9] Tanaka, K., and M. Yamaguchi, "Recent Progress in AOPs." *Environmental Chemistry Letters,* 14, no. 2 (2016): 287–301 https://doi.org/10.1007/s10311-016-0563-4.

[10] Turner, J. A. "Sustainable Hydrogen Production," *Science,* 305, no. 5686 (2004): 972–974. https://doi.org/10.1126/science.1103197.

[11] Zhou, et al., "Advances in Heterogeneous Photocatalysis." RSC Advances 8, no. 13 (2018): 7173–7183 https://doi.org/10.1039/C8RA00371C.

advancements, compact educational fuel cells allow freedom in the model for new materials and techniques; similarly, NASICON-based CO_2 capture makes this work sterling in both social and economic respects. Together, these technologies drive a circular hydrogen economy that regenerates water, captures carbon, and creates clean fuel, in line with Oman's national goals and global sustainability targets. Subsequent research will further investigate durability of catalysts, techno-economic scaling, and integration with photovoltaic power to form completely self-sustaining, emission-free hydrogen economy chains.

Acknowledgements

This research was funded by the Ministry of Higher Education, Research, and Innovation (MoHERI) under the Undergraduate Research Grant (Block Funding Program). The authors gratefully acknowledge the assistance and facilities provided by the National University of Science and Technology (NUST), College of Engineering. The authors would like to express their gratitude to Profs Ahmed Al Balushi and K. P. Ramachandran for being the mentors, Dr. Lakkimsetty Nageswara Rao, AURAK, UAE for scientific discussion, Ms. Khadija Al Balushi who helped in data acquisition, as well as Dr. Varghese who contributed to modelling and analysis. The authors are also grateful to the estates, purchase and finance Departments, and Dr. Hamood Darwish, Director of Scientific Research, their great cooperation in the pursuit of excellence.

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