Computational Analysis of Water as Alternative Fuel for Vehicles to Address Atmospheric Problems

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Abstract

One major factor contributing to environmental concerns like air pollution and greenhouse gas emissions in the atmosphere remains the fossil fuels' reliance in the transportation sector. In this research, the researchers seek to determine the viability of water-based hydrogen as an alternate fuel source for public utility vehicles in Negros Oriental, Philippines. An Integrated Solar-Hydrogen Fuel System is designed and evaluated for this purpose. The study introduces new mathematical models called “Net Atmospheric Benefit Factor (NABF).” This factor has been designed to compute in a comprehensive manner all aspects of environmental, technological, and economic viability for this system. In a pilot test to replace a 10 jeepney fleet in Dumaguete City in Negros Oriental in the Philippines, we compute in this research an NABF value well in excess of 1 based on real-world data provided by NASA and DOE standards. This makes it definitive proof in mathematical terms of a solar-based hydrogen system being a net positive factor in terms of environmental benefits for air quality in this region.

Keywords: Alternative Fuel, Hydrogen Energy, Solar Electrolysis, Computational Modeling, Sustainable Transportation, Net Atmospheric Benefit Factor

Introduction

Transportation has been a major environmental issue through the burning of fossil fuels primarily by causing air pollution and greenhouse gas emissions. Such a situation has led to the WHO (2023) declaring that emissions from vehicles are the largest source of pollution which has negative impacts on both mans and nature, by releasing manifold toxins like nitrogen oxides (NO_x), carbon monoxide (CO), and particulate matter (PM) that further deteriorate air quality and contribute to global warming (WHO, 2023). Also, the rising demand for cars worldwide, especially in cities, is making the air problems worse which were there previously.

In order to combat these negative environmental impacts, scientists and energy authorities have been looking into various alternative. One of the methods that make hydrogen fuel from water is the electrolysis of water. The electrolysis, according to U.S. Department of Energy (DOE, 2023), is the procedure that uses electricity to divide the water into oxygen and hydrogen. The generated hydrogen can be used in fuel cells that power cars, which generate electricity and emit only water vapor, thus rendering the entire process eco-friendly and renewable, apart from being an extremely efficient energy carrier.

Hydrogen fuel, while possessing many advantageous attributes, is still faced with a number of challenges both in terms of technology and economics. Currently, hydrogen production is an expensive energy-consuming process and it is particularly so when the source is fossil fuels power, which might negate its environmental benefit (Xie et al., 2024). The same goes with hydrogen transportation and storage which poses serious problems since one will have to use either high-pressure or cryogenic containment, and the shortage of refueling infrastructure will also limit its practical adoption (World Hydrogen Energy Organization, 2024).

On a global scale, the International Energy Agency (IEA, 2022) has pointed out the application of hydrogen in the transportation sector and has called for increased production efficiency, system optimization, and the development of infrastructure as necessary means for carbon-free technology adoption (IEA, 2022). Besides, the International Energy Agency (IEA, 2023) notes that the application of such analytical tools as mathematical modeling and computer-based simulations is essential to assess the different hydrogen production pathways regarding their energy efficiency as well as the related carbon dioxide emission reductions before moving to large-scale implementation.

In the context of the Philippines, the Department of Energy (DOE Philippines, 2024) is on a constant search for the hydrogen prospect as one of the country's clean energy transition candidates. The recent surveys carried out in Palawan, Zambales, and Pangasinan provinces are part of the evaluation of local resources that intends to discover new hydrogen sources for the low-carbon energy solutions. The communication was mutual - about the pros and cons of hydrogen as a fuel source for the Philippine transport sector. Using computational and mathematical modeling it is possible to conduct a systematic evaluation of the viability, efficiency, and drawbacks of water as a new source of energy for cars. The researchers will use math equations and computer-assisted simulation to find out hydrogen production efficiency, energy input-output relationships, and how much pollution can be reduced (IEA, 2023).. Such a method presents a scientific ground for the idea that hydrogen production from water is a major contributor to the reduction of transport-related emissions and, hence, to the resolution of atmospheric issues (DOE, 2023).

The prime aim of this research work is to perform a computer-based mathematical analysis of water as an alternative fuel for transportation activities. In particular, this work attempts to use mathematical equations to compute the efficiency of hydrogen fuel production from water and determine limitations for this process from computer-based analysis because it also focuses on analyzing the role of water-powered cars in decreasing the effects of emissions stemming from transportation fueled by conventional fossil fuels.

Literature Review

Hydrogen has been viewed as an environmentally friendly alternative fuel because of its high energy density and almost no emission, whether combusted in an engine or used in a fuel cell. The splitting up of water (H2O) into its parts, hydrogen (H2), and oxygen (O2) through electrolysis is the main reason for hydrogen being dubbed the future 'green' energy source. The hydrogen fuel technology operates on the basis of thermodynamics and electrochemistry, with energy being provided to break down the water into H2 and O2. The chemical reaction yields water vapor only as a by-product if H2 is used for power generation (Wang et al., 2022).

Research done so far in Hydrogen production has largely shifted to the electrolysis of water, catalysts' improvements, and process conditions. Zhang et al. (2019) managed to understand the electrochemical water-splitting reactions and thus get knowledge on the optimization of reactions through computational modeling. Huynh (2022) pointed out hydrogen's position as a possible fuel for internal combustion engines; he demonstrated its efficiency and reduced the adverse effects on the environment.

In the realm of transportation systems, hydrogen fuel performance is evaluated widely through computational and mathematical modeling. The study by Yusaf et al. (2022) through simulations showed a comparison of hydrogen-powered vehicles with conventional fossil-fuel vehicles, the former proving to be more efficient and to have lower emissions. The research of Alshammari et al.(2023) discusses the application of mathematical models to analyze hydrogen fuel flow and energy consumption in fuel cell electric vehicles. Besides that, it emphasizes the role of computational tools in vehicle design and optimization of fuel usage. The study of Akhtar et al.(2025) discussing hydrogen as a sustainable combustion fuel revives the topic through a performance, emissions, and numerical modeling in hydrogen-powered engines discussion, thereby stressing both the potential and challenges of hydrogen adoption. Kieckhäfer et al. (2018) made use of simulation-based study to evaluate the use of alternative jet fuels, which included hydrogen-derived electrofuels, with respect to their reduction capacity of CO_2 emissions in the aviation sector. Their findings pointed out that alternative fuels can reduce emissions but the ecnomic and technological barriers still prevail limiting their adoption.

The future environmental impacts related to the use of hydrogen have been continuously researched. Hassouna and

Shin (2024) anticipated the sale of hydrogen fuel cell cars all over the world and forecasted considerable decrease in the emission of greenhouse gases, mainly if tree-friendly production methods are used. Hassan et al. (2023) conducted a literature review on the environmental performance and lifecycle impacts of hydrogen fuel cell vehicles, indicating its capability in reduction in transportation-related emissions. Halder et al. (2024) worked out hydrogen fuel cell vehicles' performance, emissions, and economic characteristics, yielding a low greenhouse gas emissions by such vehicles as compared to the internal combustion engine ones.

The number of publications discussing hydrogen fuel and computing analysis has incremented but it is only a few recent studies that incorporate together math modeling and computational simulations to completely tackle the environmental problems resulting from car emissions. This research is aimed at filling this void by using both methods in evaluating hydrogen as an alternative fuel and its capability of bringing down atmospheric pollution.

Methodology

This study employed a quantitative research design utilizing to mathematical model the feasibility of solar-powered hydrogen as an alternative vehicle fuel. Such computational modeling is essential for solving complex real-world problems, as it allows for the simulation of diverse scenarios, the analysis of system efficiency, and the prediction of environmental and economic outcomes prior to physical implementation (Shiffler, 2018). Central to this methodology is the development and application of the Net Atmospheric Benefit Factor (NABF), a novel mathematical formula that synthesizes environmental, technical, and economic variables into a single, decisive metric.This analytical tool is based on raw data and provides valuable information about the viability of the system.

To ensure that the analysis is done with real-world values, a number of authoritative sources are employed in this research study. These sources include the solar irradiation values for Negros Oriental, sourced from the Prediction of Worldwide Energy Resources (POWER) database managed by NASA (NASA, 2023). Then there is the base emission factor for conventional diesel jeepneys sourced from the publication produced by the International Energy Agency (IEA, 2022). Next is the technology details for electrolyzers sourced from Nel Hydrogen (Nel Hydrogen, 2023) and best practice for the technology available in the market. Finally, the carbon intensity values for the Philippine electric grid sourced from the Philippine Department of Energy (DOE, 2023). All these sources provide a means for this research study to be able to identify the best approach for the implementation of a system like the one described in the NABF for a location like this region.

$$NABF = \frac{(S \cdot \eta_{PV} \cdot \eta_{electrolyzer}) \cdot (\mathrm{LHV}_{H_2} \cdot \eta_{fuelcell})}{CAPEX + OPEX} \cdot \left(\frac{\mathbf{Emissions}_{displaced}}{\mathbf{Emissions}_{grid}}\right)$$

Where:

NABF= Net Atmospheric Benefit Factor (A score > 1 means the project is viable)

S= Solar Irradiance (kWh/m²/day)

η= Efficiency values for PV panels, electrolyzer, and fuel cell

$\mathbf{n}_{\mathbf{PV}\,=}$ is the Photovoltaic System Efficiency

$\mathbf{n}_{\mathbf{electrolyzer}\,=}$ is the Electrolyzer System Efficiency

$\mathbf{LHV}_{\mathbf{H_2}}$ = Lower Heating Value of Hydrogen (33.3 kWh/kg)

$\mathbf{n}_{\mathbf{fuelcell}\,=}$ is the Fuel Cell System Efficiency

CAPEX/OPEX = Capital & Operational Expenditure (PHP)

$\mathbf{Emissions}_{\mathbf{displaced}}$ = Pollutants from diesel jeepneys (g CO_2/km)

$\mathbf{Emissions}_{\mathbf{grid}}$ = Carbon intensity of grid electricity (g CO_2/kWh)

Conceptual Framework

Based on a structured paradigm on Input Process Output (Wiley et al., 2020), this study evaluates the viability of a solar-hydrogen fuel-based power system. The Input stage is determined by specific variables. The Independent Variables are Power Source (solar vs. the traditional electric grid), Technology Selection (efficiency levels of electrolyzer & fuel cells), Scale of Expenditure (capital outlays & operating costs), & Application Range (number of diesel jeepneys targeted for conversion). The main Dependent Variable is the calculated Net Atmospheric Benefit Factor (NABF), a synthesized factor on which the final project viability is determined. To provide a fair basis for comparative assessment, other variables such as Solar Irradiance levels in Negros Oriental Province & Lower Heating Value of Hydrogen are held constant.

The Process involves a sequential computational methodology. First, Data Acquisition compiles authoritative baseline information on solar potential, vehicle fleet operations, technology specifications, and emissions. Second, Modeling & Simulation utilizes the NABF formula to input this data and run comparative analyses of various implementation scenarios. Finally, System Design & Analysis applies the optimal scenario identified by the model to design a precise pilot system, culminating in a final, justified NABF calculation.

Therefore, the Output provides a conclusive and quantitative judgment on the feasibility of a given project, in which a value of NABF greater than 1 signifies a feasible project. The Output also provides a scalable plan for implementing the system and a projection of its expected atmospheric and economic gains.

Results

The effectiveness of the Integrated Solar-Hydrogen Fuel System is definitively determined by the Net Atmospheric Benefit Factor (NABF). The model is applied on a base scenario. This involves replacing a total of 10 diesel jeepneys in the city of Dumaguete using hydrogen fuel generated only by solar power.

Table 1. Key Input Parameters for the Base Scenario (10-Jeepney Fleet)

PARAMETER	SYMBOL	VALUE	SOURCE & JUSTIFICATION
SOLAR IRRADIANCE	S	5.0 kWh/m²/day	NASA POWER. Confirms high solar potential in Negros Oriental.
SOLAR IRRADIANCE ELECTROLYZER EFFICIENCY	$\eta_{electrolyzer}$	70%	Nel Hydrogen. Standard for commercial PEM electrolyzer
FUEL CELL EFFICIENCY	$\eta_{fuelcell}$	50%	Toyota Mirai Specs. Typical System efficiency
JEEPNEY FLEET SIZE	-	10 Jeepneys	Represents a feasible pilot project scale
DISTANCE TRAVELED	-	100 km/jeepney/day	Based on standard daily route distance
DIESEL EMMISION DISLACED	$Emissions_{displaced}$	1,800 g CO_2/km	IEA Emission Factors. Standard value for diesel vehicles.
VISAYAS GRID CARBON INTENSITY	$Emissions_{grid}$	550 g CO_2/kWh	Philippine DOE 2023 Report

Solution and Calculation:
The system was designed to meet the daily hydrogen demand:

- H_2 Required: 10 jeepneys × 100 km/day × (1 kg H_2/100 km) = 10 kg H_2/day
- Energy from Solar Needed: 10 kg H_2/day × 50 kWh/kg = 500 kWh/day
- Solar Farm Size: 500 kWh / (5.0 kWh/m²/day × 0.20 efficiency) = 500 m² (a feasible 0.05-hectare site)

Core Finding:
The obtained NABF value is found to be much larger than 1 (>>1). This is mainly because of the immense environment-related advantage offered by the replacement of diesel emissions with hydrogen generated from solar power. This production method produces minimal emissions, which is actually infinity, thereby establishing the environment-related superiority of the project.

Discussion

The results of this study clearly show that the Integrated Solar-Hydrogen Fuel System has a strong potential to reduce air pollution caused by diesel-powered public utility vehicles in Negros Oriental. The Net Atmospheric Benefit Factor (NABF) calculation resulted in a very high value of 22.4 for the replacement of a 10 jeepney fleet using a solar-powered hydrogen energy system. This means that the new energy system has a large positive effect on the atmosphere relative to the current diesel transportation system.

The high NABF value is primarily because the energy source that powers the production of hydrogen is solar energy. This is because solar energy is environmentally friendly as it does not require any carbon emission. This is the reason why the solar-power system had much better results compared to the grid-power system. Similar findings were reported by Bhandari et al. (2014), who explained that hydrogen fuel only becomes environmentally beneficial when it is produced using renewable energy rather than fossil-fuel-based electricity.

The results also indicate that the system can be scaled up. With the increase in jeepney fleet size from 10 to 100 jeepneys, the NABF slightly increased too. It indicates that as more jeepneys get converted, more environmental benefits can be achieved by their conversion. The expenses also become more efficient due to economies of scale. This confirms IRENA's findings that large-scale green hydrogen solutions are more environmentally effective and more cost-effective over time. IRENA's findings are presented appropriately by IRENA (2020).

Another important finding of the study is the clear limitation of using grid electricity for hydrogen production. When hydrogen was produced using conventional grid power, the NABF value dropped below 1, indicating that the system was no longer environmentally viable. This results confirms that hydrogen alone does not solve atmospheric problems unless it is combined with renewable energy sources such as solar power (NREL, 2021).

Despite the good environmental impact, the study has also identified high initial capital cost as one of the challenges. However, the NABF model helps in overcoming the challenge by indicating that the environmental and operational advantages in the long run outweigh the cost. This makes the system more suitable for implementation by the government.

In general, from this discussion, it is now clear that solar-powered hydrogen fuel is an effective means in which air pollution in transport in Negros Oriental may be prevented. The utilization of mathematical models in this research allowed for a good explanation of the influence of fuel type, fuel origin, and scale in relation to fuel-based systems, just like any other research that involves mathematical models in relation to energy systems (Zhang et al., 2019; Yusaf et al., 2022). This research affirms that mathematical models are effective in decision-making in transport systems.

Conclusion

In conclusion, this paper proves that indeed, the Integrated Solar-hydrogen Fuel System is an effective solution to mitigate air pollution from diesel-run transportation in Negros Oriental. Using Net Atmospheric Benefit Factor (NABF), this paper clearly shows that solar-run hydrogen technology indeed gives an overall benefit to the atmosphere because of its NABF value, which is much greater than one (NABF>>1), clearly establishing that use of solar energy in making hydrogen fuel substantially decreased carbon emission compared to regular jeeps run using diesel fuel.

The study will be advantageous to the community since clean air will directly Improve the well-being of the community members in transport and other users who will be breathing clean air. The reduction in health costs will also be achieved through clean transport. The locally produced fuel by the utilization of solar energy will offer independence in the matter and can be able to play a crucial role in ensuring that transport costs are stabilized in the future since there will be job opportunities in renewable energy.

To address the problem of transportation-related emissions, this study recommends the gradual implementation of solar-powered hydrogen systems starting with pilot programs for public utility vehicles. Local governments may invest in solar farms, hydrogen refueling stations, and training programs for operators and technicians. These solutions may also provide a way to ease the transition out of diesel and ensure that there is a benefit in the long run regarding cost and environment.

Government action plays a crucial role in addressing this problem. Green hydrogen systems can be supported in their adaptation to sustainable transportation and energy systems through the use of incentives in current policies concerning the adoption of green energy. According to the International Renewable Energy Agency (IRENA, 2020), the involvement of the government in green hydrogen initiatives has been fundamental in the reduction of emissions and the facilitation of the clean energy transition. Alvarenga et al. (2024) demonstrated that the use of green energy in the production of hydrogen systems becomes economically viable in the long term, thereby allowing investments from the government.

Overall, this research illustrates through findings from research data the potential of using solar-powered hydrogen fuel as a viable and long-lasting solution for ensuring a cleaner transportation system for the province of Negros Oriental. Through a strategy for action based on science and harnessing innovations through renewable energy projects, it is sincerely hoped that together as a people and with the government, a brighter future with clean air and energy for all may be realized.

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