Hydrogen as a Sustainable Energy Vector in Transport: Supply Chain Optimization via Mixed-Integer Linear Programming

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***Abstract*— The global transformation toward a low-carbon economy has intensified interest in hydrogen as a sustainable energy vector in the transport sector. However, designing an efficient and environmentally sound hydrogen supply chain (HSC) remains a complex challenge due to the variety of production methods, storage requirements, transportation options, and environmental constraints. This study presents a mathematical model for optimal strategic design of HSC based on hydrogen production via water electrolysis. Particular focus is placed on the location of hydrogen fueling stations. The model is formulated as a mixed-integer linear programming (MILP) problem and can be solved using GAMS. It integrates economic, environmental, and social criteria to minimize carbon footprint and overall costs while supporting investment and logistical decisions in the transport sector. The proposed optimization framework offers a flexible tool for planning sustainable hydrogen infrastructure and addresses key challenges in the transition toward a hydrogen-based economy.**

***Keywords*— Electrolysis, Hydrogen Supply Chain, Mixed-Integer Linear Programming, Optimization, Sustainable Transport**

I. Introduction

The decarbonization of the transport sector is crucial for achieving the global climate goals set out in the European Climate Law [1]. In this context, hydrogen is outlined as a strategic energy carrier due to its high energy density, zero carbon emissions in usage, and flexibility for integration into various types of transport systems. Today, the transport sector is the only one whose greenhouse gas emissions are higher than in 1990 and continue to grow. The carbon intensity of this sector in Bulgaria is 3.5 times higher than the average for the European Union (EU) [2]. The main reasons for this are the high average age of the light-duty vehicle fleet (19 years) and the use of gasoline and diesel as the main sources of energy in transport.

A significant part of the barriers to the large-scale implementation of hydrogen technologies is gradually being overcome, due to technological advancements. This is making hydrogen an increasingly accessible and applicable solution [3]. Despite the growing attention to hydrogen as an energy carrier, not all of its 'colors' meet sustainability standards. This is because the production of some color of hydrogen emits significant amounts of greenhouse gases and incurs relatively high production costs. Given these considerations, green hydrogen is appearing as a key solution to overcoming the environmental challenges associated with the energy transition. Green hydrogen is a low-carbon energy source produced through water electrolysis using renewable energy [4]. It can serve as a perfect energy carrier for decarbonizing power grids and transportation networks [5,6].

To realize the potential of hydrogen in carbon-intensive sectors such as road transport, it is necessary to build a sustainable workable hydrogen supply chain (HSC).

This study proposes a sustainable optimization model for the design of HSC based on water electrolysis. It's included feedstocks, production, storage, end usage, also transport. The model integrates environmental, economic and social indicators into Mixed – integer linear programming (MILP) framework. It aims are to determine optimal configurations for hydrogen production, storage, and distribution while meeting sustainability and cost objectives.

II. Hydrogen in the Transport

Hydrogen is considered as a strategic energy carrier with potential to contribute significantly to the decarbonization of the transport sector, which is one of the primary sources of global carbon emissions. Its application in the transport is based on two main technological directions: fuel cell electric vehicles (FCEVs) and internal combustion engines adapted for hydrogen fuel (H_2-ICEs).

Hydrogen fuel cells FCEVs convert the chemical potential of reactants into electricity [7]. Typically, a hydrogen fuel cell consists of electrodes (anode and cathode) separated by a proton exchange membrane (PEM), also known as an electrolyte. The operating temperature is in the range of 333–353 K. Hydrogen and oxygen enter the fuel cell in the anode and cathode compartments, respectively. Hydrogen is an electron donor. Oxygen is an electron acceptor. At the anode, protons are formed which migrate through the membrane and react with oxygen at the cathode, producing water vapor and releasing heat. The electron transfer occurs via an external circuit as electric current, driven by the electromotive force generated between the electrodes.

One of the primary advantages of FCEVs is their high energy efficiency, which can reach up to 60%, significantly exceeding that of traditional engines. FCEVs operate with minimal noise and emit only water as a byproduct, making them environmentally friendly. Another benefit is the rapid refueling time—approximately 3 minutes for a passenger car and around 10 minutes for a bus—rendering them suitable for long-distance transportation.

However, FCEVs also present certain limitations. The cost of fuel cells is still high, mainly due to the use of platinum and complex membranes. Hydrogen refueling infrastructure is also limited or completely absent, making their mass deployment difficult.

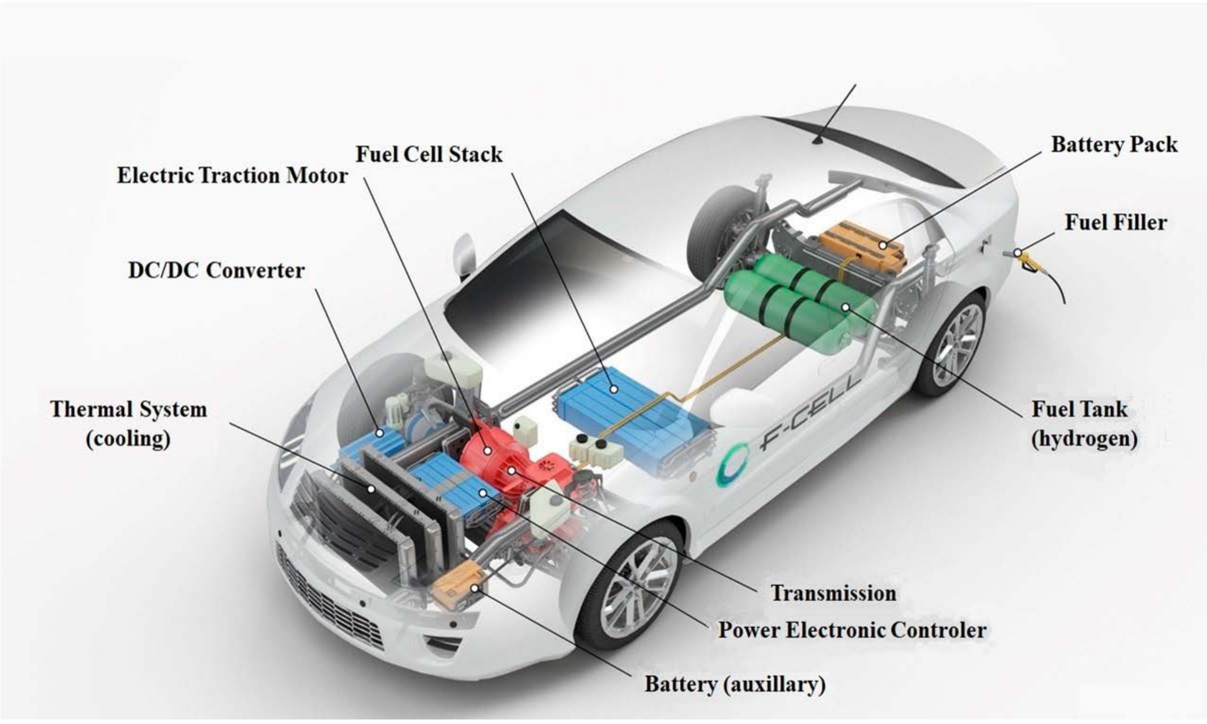

Fig. 1 The design of a fuel cell-powered vehicle [8]

The design of a fuel cell-powered vehicle is presented in Fig. 1. The hydrogen is charged and stored in a high-pressure tank. It is fed to a battery of fuel cells (usually called “a stack”), where the chemical energy is converted into direct current (DC) electricity. The generated constant electrical voltage is fed to a DC/DC converter, which powers the speed regulator (a powerful electronic controller). The driver uses the speed controller to set the required instantaneous rotational speed of the traction electric motor.

Hydrogen internal combustion engines (H_2-ICEs) are modified versions of conventional gasoline or diesel engines, adapted to operate using hydrogen as fuel [9]. They function on the principle of igniting a hydrogen–air mixture, with the released energy being converted into mechanical work.

The main advantage of H_2-ICE is their compatibility with existing technologies, which makes the transition to hydrogen easier and more cost-effective. These engines can operate with lean mixtures, which reduces the formation of nitrogen oxides (NO_x). Moreover, they are particularly suitable for heavy-duty vehicles and industrial applications, where high power and durability are critical.

The drawbacks of H_2-ICEs include lower efficiency (typically ranging from 25% to 45%) compared to fuel cells, as well as challenges related to NO_x emissions at high combustion temperatures. Additionally, hydrogen can cause hydrogen embrittlement of metals, necessitating the use of specialized materials in engine construction.

Both approaches have their respective roles in the future of hydrogen-based energy systems. Fuel cells offer high efficiency and zero emissions, making them particularly suitable for passenger vehicles and urban transportation. A major challenge to the commercialization of fuel cell electric vehicles (FCEVs) is the construction of charging stations, implemented in a sustainable supply chain and taking into account the environmental, economic and social aspects.

III. Problem statement

Hydrogen Refueling Stations (HRS) produce hydrogen through the process of electrolysis. The following raw materials are used in their operation:

- electricity from renewable sources (solar, wind);
- electricity from a centralized nuclear power plant (if necessary);
- water supplied by a national supplier.

For the purposes of this study, the following data are assumed to be known: the cost of electricity and water used as raw materials; the possible types of HRSs that can be installed at acceptable locations; and the associated operation and maintenance costs. It is also assumed that the technologies for the utilization of waste products when producing hydrogen in HRSs are known. Additionally, the potential locations of end users are identified, along with the greenhouse gas emissions generated at each stage of the supply chain life cycle, as well as government incentives for hydrogen production and consumption, and the applicable carbon tax.

If additional hydrogen is needed to meet the needs of end customers, hydrogen produced by steam reforming methane from the relevant hydrogen storage facilities is delivered to HRSs.

Fig.2. shows a generalized superstructure of a hydrogen supply chain obtained through the electrolysis process.

Fig. 2. A generalized superstructure of a hydrogen supply chain obtained through the electrolysis process

The presented supply chain includes feedstocks, storage of hydrogen produced by steam reforming, hydrogen refueling stations, end users.

IV. General Formulation of the Optimization Problem

Given the above-described data, the task is to determine the optimal operating conditions for the system as a whole, which includes determining the sets and location of hydrogen refueling stations that should be built at designated locations; the sets and location of hydrogen storage facilities (from steam reforming of methane) that should be built at designated locations; a transport delivery scheme; the total number of jobs created as a result of the operation of all elements of the system during its operation.

The optimal operating conditions of the system should provide a minimum of the objective function, which includes all costs for the supply of raw materials, production and transportation costs, as well as costs for the construction of the necessary facilities. At the same time, it is necessary to observe technological, environmental, social and time constraints i.e., the optimization criterion is defined in terms of economic sustainability, and data for environmental and social assessment are implemented as part of it.

The optimization task can be solved using the GAMS application software and can be used to make comprehensive intelligent decisions. After modifying the necessary data, the proposed plan can be adapted to different territories.

V. Formulation of the Mathematical Model

MILP optimization model including data sets, decision variables, mathematical models of the environmental and economic performance of the considered supply chain, constraints and optimization criterion is defined. A supply chain for a long planning horizon H (10 years) is considered. The entire time horizon H is divided into a set of 5 discrete time intervals t. This time interval is divided into several equal time subintervals t={0,1,2,…T} , each of which has a duration ∇t. During the planning horizon, it is assumed that hydrogen consumption will change by a predicted value. The mathematical model describing the optimal configuration of the sustainable supply chain is given as follows:

A. The model of the environmental impact of hydrogen supply chain

The model assesses multiple environmental impact factors across the complete HSC, encompassing all stages from production and storage to transportation and final distribution. The primary objective involves optimizing the ecological footprint of the HSC while maintaining compliance with both sustainability targets and established regulatory requirements.

The total emissions represent the cumulative environmental impact across all lifecycle phases [10]. For each operational period, greenhouse gas emissions are typically quantified using the following methodology:

$$eTEI_t = eELD_t + eETT_t + eEAPP_t + eEPP_t, \forall t \quad (1)$$

where:

$eTEI_t$ - The total environmental impact of the HSC operation over its entire life cycle, $[\mathrm{kg_{CO_2eq}}/\mathrm{y}]$;

$eELD_t$ - Total greenhouse gas emissions from the production of diesel fuel, associated with diesel, $[\mathrm{kg_{CO_2eq}}/\mathrm{y}]$;

$eETT_t$ - Greenhouse gas emissions associated with the transportation of raw materials and product, $[\mathrm{kg_{CO_2eq}}/\mathrm{y}]$;

$eEAPP_t$ - Greenhouse gas emissions associated with the use of hydrogen as a fuel, $[\mathrm{kg_{CO_2eq}}/\mathrm{y}]$;

$eEPP_t$ - Greenhouse gas emissions released during hydrogen production through the electrolysis process, $[\mathrm{kg_{CO_2eq}}/\mathrm{y}]$.

B. *The model of the social impact of hydrogen supply chain*

The social impact model for the operation of the HSC defines the expected total number of jobs created (J_t) as a result of the actions of all the elements of the system during its operation:

$$eJob_t = eNJ1_t + eLT_tNJ12_t + eNJ2_t + eLT_tNJ21_t,\ \ \forall t \tag{2}$$

where: the terms of (2) are defined according to the relationships for each time interval $t \in T$, [\$/y]:

$eNJ1_t$ - The costs for creating jobs related to the installation of hydrogen production facilities, [\$/y];

eLT_tNJ12_t - The costs for creating jobs related to the operation of the hydrogen facilities, [\$/y];

$eNJ2_t$ - The costs for creating jobs related to the installation of hydrogen refueling stations, [\$/y];

eLT_tNJ21_t - The costs for creating jobs related to the operation of hydrogen refueling stations, [\$/y].

Equation (2) can be considered as a simplified model of the social assessment criterion [11].

C. *The model of the economic impact of hydrogen supply chain*

The model takes into account annual operating costs. The annual operational budget integrates all supply chain components from raw material acquisition to final product distribution.

$$\begin{aligned} eTHC_t = {} & eTIC_t + eTPC_t \\ & + eTHH_t + eTHE_t + eTHHH_t \\ & + eTMO_t + eTPW_t + eTTC_t \\ & + eTTAXB_t + eTHSC_t + eTOEC_t \\ & - eT1L_t - eT2L_t \\ & - eTH_t, \forall t \end{aligned} \tag{3}$$

where:

$eTHC_t$ - Total annual costs of the HSC, [\$/y];

$eTIC_T$ - Total investment costs for the production capacity of the HSC are related to the operational period of exploitation and the buyout of the installation per year, [\$/y]

$eTPC_t$ - Production costs in hydrogen production, [\$/y];

$eTHH_t$ - Costs for raw material purchase – water, [\$/y];

$eTHE_t$ - Costs for raw material purchase – electricity, [\$/y];

$eTHHH_t$ - Costs for hydrogen produced in a nuclear power plant, [\$/y];

$eTMO_t$ - Costs for maintenance and operation of the hydrogen fueling stations, [\$/y];

$eTPW_t$ - Production costs for waste disposal from hydrogen production, [\$/y];

$eTHSC_t$ - Total investment costs for the commercial capacity of the HSC relative to the operational period of operation and the acquisition of the hydrogen station per year,[\$/y];

$eTOEC_t$ - Operating costs for hydrogen retailers,[\$/y];

$eTTC_t$ - Total transportation costs of the HSC [\$/y];

$eTTAXB_t$ - Carbon tax levied according to the total amount of CO_2 generated during the operation of the HSC, [\$/y];

$eT1L_t$ - Government incentives for hydrogen consumption, [\$/y];

$eT2L_t$ - Government incentives for hydrogen production, [\$/y];

eTH_t - Revenue from the sale of produced hydrogen from all installed refueling stations, [\$/y];

D. *Constraints*

To ensure the workability of the derived optimal solutions, the following constraints must be satisfied:

- *Capacity limits* – Facility operations must remain within defined minimum and maximum limits.
- *Flow feasibility* – All material and product flows must adhere to acceptable conditions.
- *Regional hydrogen demand* – The system must meet the fuel requirements of all demand regions.
- *Resource availability* – Sufficient inputs (water, electricity) must be provided for hydrogen production.
- *Transport and logistics* – Distribution networks must comply with logistical limitations.
- *Material balance* – The entire hydrogen supply chain (HSC) must maintain balance in material flows.
- *Annual production capacity* – Facility outputs must be leveled with yearly operational limits.
- *Demand fulfillment* – End-user product requirements must be fully satisfied.
- *Social impact enhancement* – HSC operations should contribute positively to societal benefits.

E. *Objective function*

The optimal operating conditions for HSC should ensure the minimization of the objective function, which includes several key aspects. First, it involves reducing environmental impact by optimizing the use of renewable energy sources and minimizing emissions associated with hydrogen production, storage, and transportation. In addition, achieving the lowest possible costs across all stages of the supply chain is essential (from production and storage to the development of the necessary infrastructure) taking into account capital, operational, and maintenance expenses. Alongside environmental and economic aims, emphasis is also placed on the social and economic benefits, such as job creation, economic growth, and positive effects on local communities, while maintaining a balance between environmental sustainability and economic viability.

$$COST = \sum_{t\epsilon T}(LT_t eTHC_t) \quad (4)$$
$$Find: X_t[Decision\ variables]$$
$$MINIMIZE\{COST(X_t)\} \rightarrow (Eq.4) s.t.: \{\text{Constraints}\}$$

where: LT_t - duration of time intervals $t \in T$, [y].

The mathematical optimization problem can be effectively addressed through implementation in the GAMS (General Algebraic Modeling System) computational environment. This modeling platform enables comprehensive decision-support analysis through its robust optimization capabilities. Following appropriate data parameterization and model calibration, the developed optimization framework can be adapted to different areas.

VI. Conclusion

This study presents a generalized structure of the hydrogen supply chain (HSC) based on electrolysis. The demonstrated supply chain structure includes all key elements as a feedstocks, storage of hydrogen produced by steam reforming, hydrogen refueling stations, end users. The proposed model for HSC design is grounded in the three pillars of sustainability—economic, environmental, and social. The environmental dimension considers the impact of the entire supply chain on the environment. The economic aspect reflects the operational and investment costs. The social criterion evaluates the potential for job creation across the system.

Formulated as a Mixed-Integer Linear Programming (MILP) problem, the model serves as a strategic decision-support tool for hydrogen infrastructure planning. The presented model can be solved using specialized software such as GAMS.

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References

[1] https://climate.ec.europa.eu/eu-action/european-climate-law_bg

[2] Center for the Study of Democracy, „Switching the Gears of Decarbonisation: Policy Action for a Low-Carbon Transformation of the Bulgarian Economy, 2021, https://csd.bg/bg/publications/publication/switching-the-gears-of-decarbonisation/

[3] D. Greene, J. Ogden, Z. Lin, Challenges in the designing, planning and deployment of hydrogen refueling infrastructure for fuel cell electric vehicles, *ETransportation*, 2020, 6:100086, https://doi.org/10.1016/j.etran.2020.100086

[4] Q. Hassan, S. Algburi, A.Z. Sameen, H.M. Salman, M. Jaszczur, Green hydrogen: a pathway to a sustainable energy future, *Int. J. Hydrog. Energy*, 50, 2024, 310–333.

[5] Z. Yang, K. Li, J. Chen, Robust scheduling of virtual power plant with power-tohydrogen considering a flexible carbon emission mechanism, *Electr. Power Syst.Res.* 226, 2024, 109868.

[6] Y. Wang, J. Liu, Z. Qu, Multi-stage collaborative planning of electricity-hydrogentransportation coupling network considering carbon emission reduction, *Electr. Power Syst. Res.* 228, 2024 110071

[7] F. Günaydın, S. Topçu, A. Aksoy, Hydrogen fuel cell vehicles: Overview and current status of hydrogen mobility, *International Journal of Hydrogen Energy*, 2025, https://doi.org/10.1016/j.ijhydene.2025.01.412

[8] How Do Fuel Cell Electric Vehicles Work Using Hydrogen? U.S. Department of Energy—Energy Efficiency and Renewable Energy. Available online: https://afdc.energy.gov/vehicles/how-do-fuel-cell-electric-cars-work

[9] C.M. White, R.R. Steeper, A.E. Lutz, The hydrogen-fueled internal combustion engine: a technical review, *International Journal of Hydrogen Energy*, 2006, Volume 31, Issue 10, https://doi.org/10.1016/j.ijhydene.2005.12.001

[10] E. Ganev, D. Nikolova, E. Kirilova, R. Vladova, V. Beschkov, T. Valkanova, B. Burdin, E. Slavcheva, J. Iliev, Sustainable design approach of a hydrogen production supply chain through water electrolysis, *Bulg.Chem.Com*., Volume 57, Issue 2, 2025, “to be published”

[11] E. Ganev, B. Ivanov, N. Vaklieva-Bancheva, E. Kirilova, Y. Dzhelil, A Multi-Objective Approach toward Optimal Design of Sustainable Integrated Biodiesel/Diesel Supply Chain Based on First- and Second-Generation Feedstock with Solid Waste Use , *Energies*, **14(8)**, 2261, 2021, https://doi.org/10.3390/en14082261