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OPTIMAL DESIGN OF HYDROGEN INFRASTRUCTURE BASED ON ECOLOGICAL, ECONOMIC AND SOCIAL FRAMEWORKS

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Abstract: *The transition towards a sustainable hydrogen economy requires a comprehensive approach to infrastructure planning that balances ecological, economic, and social considerations. This study presents an integrated optimization framework for the design of the hydrogen supply chain. The paper explores the development of a Mixed-Integer Linear Programming (MILP) mathematical model for the location optimization of hydrogen infrastructure elements, including hydrogen production, storage, distribution, and end-use in fuel cell vehicles. A superstructure of the hydrogen supply chain is proposed. The research incorporates different production pathways, including electrolysis and steam methane reforming. The proposed methodology identifies the optimal hydrogen infrastructure configuration that ensures environmentally, economically, and socially sustainable outcomes.*

Keywords: *MILP, Supply chain, Sustainability, Hydrogen, Hydrogen fuel cell vehicle*

INTRODUCTION

The optimal design of a sustainable hydrogen infrastructure is directly linked to the Sustainable Development Goals (SDGs) set out in the 2030 Agenda for Sustainable Development (United Nations, SDGs, 2015). Hydrogen production via electrolysis can provide low-carbon and reliable energy, reducing dependence on fossil fuels. (Martins, F. P., 2024). Optimal design promotes technological progress and innovation (Martins, F. P., 2024), and hydrogen mobility supports the decarbonization of transport (Halder, P., 2024). The integration of hydrogen technologies is key to achieving carbon neutrality (Mac Kinnon, M. A., 2016) and requires collaboration between institutions, industry and the scientific community (United Nations, SDGs, 2015). Additionally, careful planning of hydrogen infrastructure can enhance energy resilience and support long-term system stability.

The use of hydrogen in the transport sector is a multidimensional process that combines environmental, economic and social priorities in support of the UN's global goals for sustainable development. The optimal design of such infrastructure can accelerate decarbonization, stimulate innovation and industrial production, which necessitates the need for integrated models for optimizing the hydrogen supply chain.

In recent years, there has been a growing interest among researchers in the field of hydrogen infrastructure. Fig. 1 shows the publication activity on this topic over the past ten years. (scopus.com, 2025). This trend reflects the increasing meaning of hydrogen as a basic element in the transition to low-carbon energy systems.

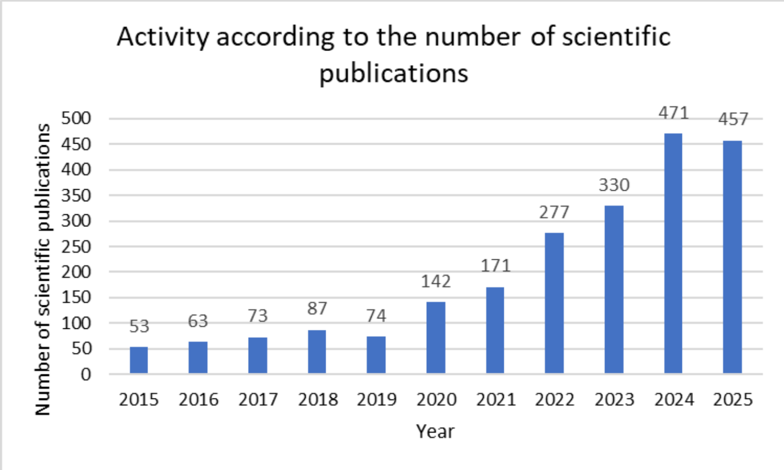

Fig. 1. Activity according to the number of scientific publications related to hydrogen supply chain for the period 2015 – 2025

In their work, authors often use approaches that include mixed-integer linear programming (MILP) (Timalsina, S. 2025), multi-objective optimization (Han, Jee-Hoon, 2013), and technical- economic analyses (Kim, S., 2024).

Despite progress in the field, integrated models that simultaneously address the three pillars of sustainability and include different hydrogen production technologies are still lacking. Existing research often focuses on economic efficiency, with environmental and social aspects remaining secondary. There is also a lack of spatio-temporal integration between the stages of production, storage, transport and refueling. A unified model is needed that integrates economic, environmental and social objectives into a common optimization framework for the sustainable development of hydrogen infrastructure in the transport sector.

This study aims to develop an integrated optimization framework for hydrogen infrastructure design, taking into account environmental, economic and social factors equally. It proposes an upgrade of the supply chain by integrating different hydrogen production technologies (electrolysis, steam methane reforming) into a common superstructure, as well as developing a MILP model for optimal determination of locations and capacities of infrastructure elements.

EXPOSITION

Integrated Superstructure of the Hydrogen Supply Chain

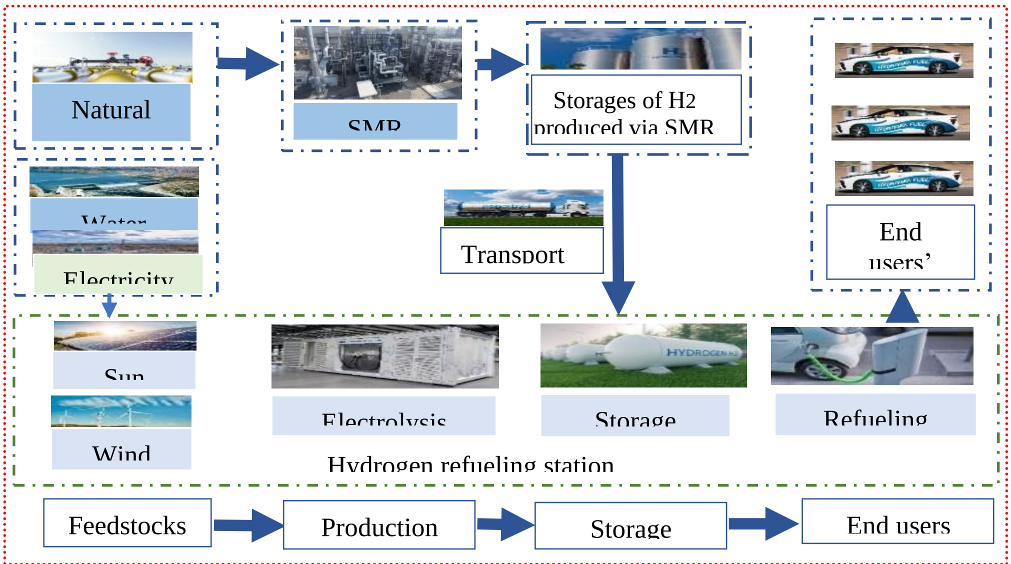

Fig. 2. An integrated superstructure of the hydrogen supply chain

Fig. 2 shows an integrated superstructure of the hydrogen supply chain. The presented hydrogen infrastructure integrates various technological options to ensure flexibility in resource utilization. The focus of this development is on a hydrogen prodused via electrolysis powered by renewable energy sources and steam methane reforming (SMR). The proposed integrated superstructure includes feedstocks, production, storage, end user's areas, and it considers the system as a whole.

Problem definition

The problem considered in this work can be formulated as follows and comes down to determining the optimal operating conditions for the system as a whole:

Given are:

- the location and production capacity of plants for hydrogen production by steam methane reforming (SMR)
- the potential locations and capacity of storage facilities for hydrogen produced via SMR;
- potential locations of charging stations and their production capacity;
- potential demand nodes (regions)
- price of raw materials (water, electricity and natural gas);
- selling price of hydrogen produced;
- hydrogen production technologies (electrolysis and SMR);
- demand for hydrogen as a fuel for vehicles;
- mode of transport for delivery;
- greenhouse gas emissions for each stage of the life cycle;
- transport costs for each transport link and mode of transport;
- government incentives for hydrogen consumption and production;
- carbon tax;
- maintenance and operation costs of charging stations;
- labor cost;
- population of region J (number of people);
- time intervals.

Under the conditions described above, the objective is to determine the optimal operating parameters of the system as a whole. This includes identifying the set, scale, and locations of refueling stations that must be built at designated locations; the set, scale, and locations of hydrogen storage facilities (from steam methane reforming) that must be built at designated locations; the transport delivery scheme; the total labor cost as a result of the operation of all system during its operation.

The optimal operating conditions of the system should ensure 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.

Mathematical Model Formulation

The model is formulated as a mixed-integer linear programming (MILP) problem, which can be solved using the GAMS application software. After modifying the necessary data, the proposed plan can be adapted to different territories. The mathematical model describing the optimal configuration of a sustainable hydrogen infrastructure is given as follows:

- *Life-Cycle Environmental Impact Model*

The environmental impact model aims to quantify the total emissions generated throughout the hydrogen supply chain, encompassing all key stages of its life cycle — production, storage, distribution, and end use. The calculated emissions are converted into carbon credits by multiplying them by the market price of carbon emissions. The aim is to minimise the total amount of equivalent greenhouse gas emissions.

Greenhouse gas emissions are determined as follows for each time interval: $t \in T$.

$$E_t = EProd_t + EStor_t + EOwn_t + ETrans_t + EFossil_t \ , \ \forall t \qquad (1)$$

where:

E_t - The total environmental impact of the Hydrogen Supply Chain operation over its entire life cycle, $[\mathrm{kg}_{CO_2eq} / y]$;

$EProd_t$ - Greenhouse gas emissions released during hydrogen production via SMR, $[\mathrm{kg}_{CO_2eq} / y]$;

$EStor_t$ - Greenhouse gas emissions released during hydrogen storage, $[\mathrm{kg}_{CO_2eq} / y]$;

$EOwn_t$ - Greenhouse gas emissions released during hydrogen production via the electrolysis process, $[\mathrm{kg}_{CO_2eq} / y]$.

$ETrans_t$ - Greenhouse gas emissions released during the transportion of hydrogen (Tank-to-Whell), $[\mathrm{kg}_{CO_2eq} / y]$;

$EFossil_t$ - Greenhouse gas emissions released during from the production of diesel fuel, associated with diesel (Well-to-Tank), $[\mathrm{kg}_{CO_2eq} / y]$;

Fig. 3 presents a structural scheme of emissions for the entire life cycle of hydrogen infrastructure.

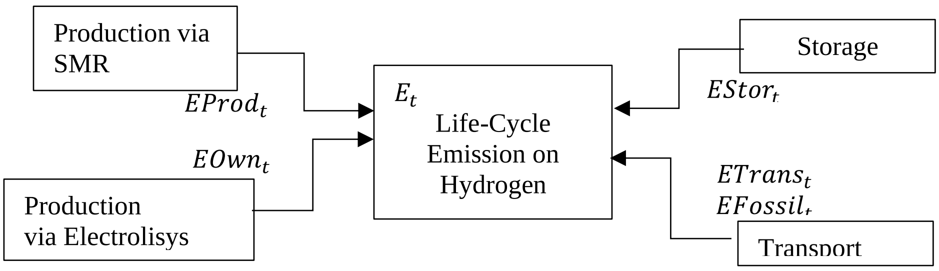

Fig. 3. Structural scheme of greenhouse gas emissions

➢ *Life-Cycle Social Impact Model*

The social impact model assesses the contribution of hydrogen infrastructure development to employment creation along the entire supply chain. Labor costs, or social benefits, are calculated for each stage - production, storage, transport, and local production — as a function of the amount of hydrogen processed and the labor intensity of the respective technology. Labor costs are determined as follows for each time interval $t \in T$.

$$L_t = LProd_t + LStor_t + LOwn_t + LTrans_t \ , \ \forall t \qquad (2)$$

where:

L_t - The total social impact of the Hydrogen Supply Chain operation over its entire life cycle, [\$/y];
$LProd_t$ - Labor costs in hydrogen production via SMR, [\$/y];
$LStor_t$ - Labor costs for hydrogen storage, [\$/y];
$EOwn_t$ - Labor costs in hydrogen production via the electrolysis process, [\$/y];
$ETrans_t$- Labor costs for hydrogen transportation, [\$/y];

Fig. 4 presents a structural scheme of labor costs throughout the life cycle of hydrogen infrastructure.

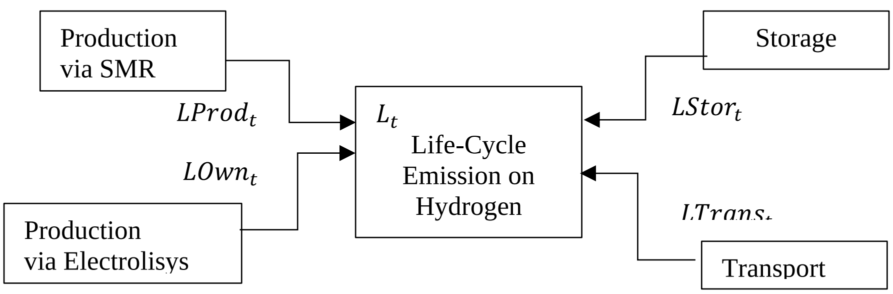

Fig. 4. Structural scheme of labor costs

- *Life-Cycle Economic Impact Model*

The Life-Cycle Economic Impact Model includes the full economic costs of the hydrogen supply chain - from production to final consumption. The model takes into account both operational costs (energy, raw materials, transport, labor) and investment costs for building the infrastructure. The model also includes government subsidies and a carbon tax, which affect the net costs of the system. This model is expressed via next dependency for each time interval $t \in T$.

$$TC_t = TCProd_t + TCStor_t + TCOwn_t + TCTrans_t + \\ + TCOwn_t^{inv} + TCStor_t^{inv} + CarbTax_t - Sub_t, \ \forall t \qquad (3)$$

where:

TC_t - The total economic impact of the Hydrogen Supply Chain operation over its entire life cycle, [$/y];

$TCProd_t$- Operating expenditure (OPEX) for hydrogen production via SMR, [$/y];

$TCStor_t$- Operating expenditure (OPEX) for hydrogen storage, [$/y];

$TCOwn_t$- Operating expenditure (OPEX) for hydrogen production via the electrolysis process, [$/y];

$TCTrans_t$- Transportation expenditure, [$/y];

$TCOwn_t^{inv}$- Capital expenditure (CAPEX) for HRS, [$/y];

$TCStor_t^{inv}$- Capital expenditure (CAPEX) for Storages, [$/y];

$CarbTax_t$- Carbon tax, [$/y];

Sub_t, -Government incentives, [$/y];

Fig. 5 presents a a structural scheme of the total costs over the entire life cycle of hydrogen infrastructure

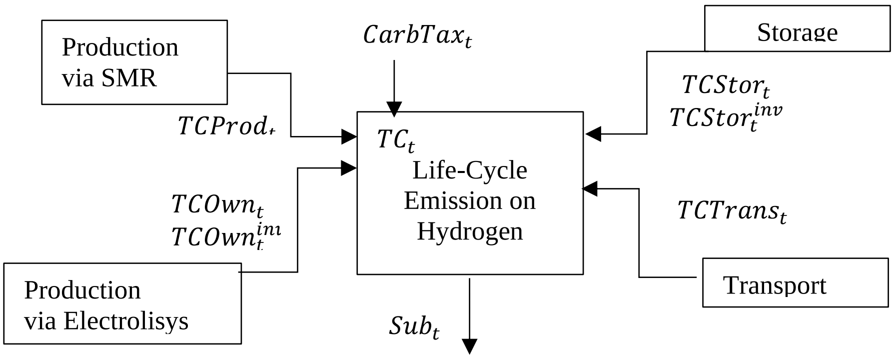

Fig. 5. Structural scheme of total costs

- *Model constraints*

The constraints ensuring the execution of the task are linear functions with respect to all independent variables. The planning period considered is 5 years.

- *Objective function*

The objective function Z minimizes the total value of economic, environmental and social factors by weighted combination of the three criteria:

$$Z = \alpha . TC_t + \beta . E_t + \gamma . L_t \qquad (4)$$

α, β, γ – weighting factors that determine the priority of each criterion.

$$Find: X_t[Decision\ variables]MINIMIZE\{Z(X_t)\} \rightarrow (Eq.4)s.t.:\{\text{Constraints}\}$$

The objective is to identify decision variables that, subject to the system of constraints, minimize the objective function Z.

The model aims to achieve an optimal balance among economic efficiency, environmental sustainability, and social impact in the design of hydrogen infrastructure. By integrating these three dimensions through weighted coefficients, the approach enables a comprehensive assessment of overall sustainability.

The optimization problem can be solved using the GAMS application software, and it is possible to use it for making comprehensive intelligent decisions. After modifying the necessary data, the proposed plan can be adapted to different areas.

CONCLUSION

An approach for optimal design of hydrogen infrastructure based on ecological, economic and social frameworks has been developed. It includes a mathematical model and its software implementation on the GAMS platform. A superstructure of an integrated supply chain for hydrogen produced by different technologies has been proposed.

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