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Sustainable design approach of a hydrogen production supply chain through water electrolysis

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Among the many alternative energy sources, hydrogen emerges as a key vector in the future energy mix due to its flexibility, high energy content, and significant potential for decarbonization. Among the various hydrogen production methods, electrolysis stands out as a promising and sustainable solution. However, realizing the full potential of hydrogen as a transportation fuel requires the development of an efficient and sustainable supply chain infrastructure capable of addressing the unique challenges associated with production, storage, transportation, and distribution.

This study focuses on developing a mathematical model for the sustainable design of a hydrogen supply chain produced through electrolysis. The proposed model is formulated within the framework of mixed-integer linear programming. A generalized superstructure of a resource-secured hydrogen supply chain, obtained through the electrolysis process, is presented.

Keywords: supply chain, GHG, hydrogen, electrolysis, hydrogen fuel cell vehicle

INTRODUCTION

Globally, hydrogen is well known as a sustainable energy source that can help bring the world closer to achieving net zero emissions (NZE) by 2050. It is also considered a promising energy carrier for decarbonizing a wide range of industrial sectors, transportation, and heating [1]. For this reason, in recent years, the concept of using hydrogen as an energy carrier has been gaining increasing popularity. Significant progress has been made in overcoming the technological and economic barriers to its large-scale implementation, making hydrogen an increasingly accessible solution [2]. Moreover, hydrogen is known as one of the few energy carriers capable of meeting the energy demands of many energy-intensive and hard-to-abate sectors, while its consumption is associated with zero emissions. The use of hydrogen as a fuel is crucial for reducing emissions in the transportation sector.

Depending on the level of hydrogen production "sustainability" and the primary energy source, a "color" classification has been introduced. The technologies for producing so-called "green" hydrogen are identified as the cleanest, resulting in zero emissions. This implies the generation of hydrogen using renewable energy sources (RES), as it does not involve greenhouse gases and is environmentally clean [3].

This type of hydrogen is considered a potential solution to overcoming the barriers in the transition to a sustainable future. The high cost, uneven distribution, and insufficient amount of energy from RES hinder its commercial use in hydrogen production for the needs of modern industry and transportation. On the other hand, hydrogen production using nuclear energy could also be considered a potential low-carbon technology. Hydrogen production using nuclear energy can generally be achieved through five methods: hybrid thermochemical water splitting, high-temperature steam electrolysis, radiolysis, and electrolysis.

To split water into hydrogen and oxygen, radiolysis uses nuclear radiation; electrolysis uses electricity generated from nuclear energy; high-temperature steam electrolysis and hybrid thermochemical water splitting are referred to as hybrid methods, as they split water using both electricity and high-temperature heat; and thermochemical water splitting directly uses high-temperature heat [4].

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The low-emission hydrogen market is expected to grow by 70% by 2030 [5]. It is believed that a mixture of 15% by volume of hydrogen and compressed natural gas (CNG) will reduce carbon dioxide (CO_2) emissions from the use of gas by 6% globally. The net zero emissions (NZE) scenario significantly alters hydrogen production. By generating 200 million tons of hydrogen by 2030, it is expected that around 70% of this will be the result of electrolysis, which could lead to a reduction in carbon dioxide emissions. By 2050, approximately 500 million tons of hydrogen will be produced using advanced low-carbon technologies. To achieve these goals, the installed capacity of electrolysis must be maximized from its current level of 0.3 GW to approximately 850 GW and 3600 GW by 2030 and 2050, respectively. Between 2022 and 2030, the generated CO_2 per kg of hydrogen will decrease from 12-13.5 kg to 6-7.5 kg.

Although with great potential, the hydrogen industry is still in its early stages of development and faces various challenges. They include low production efficiency, high storage and transportation costs, and, not least, an unbalanced supply and demand structure. Therefore, it is crucial to develop a model for designing the hydrogen supply chain infrastructure (HSC) to support the sustainable development of the hydrogen industry and its application in the transportation sector. In this context, there has been an increase in research interest in the field of HSC by about 8-9 times [6], Figure 1.

In their developments, the author teams researching this topic have reported literature reviews, studies, analyses, comparisons, research, technological solutions, and mathematical models for optimal design of HSC.

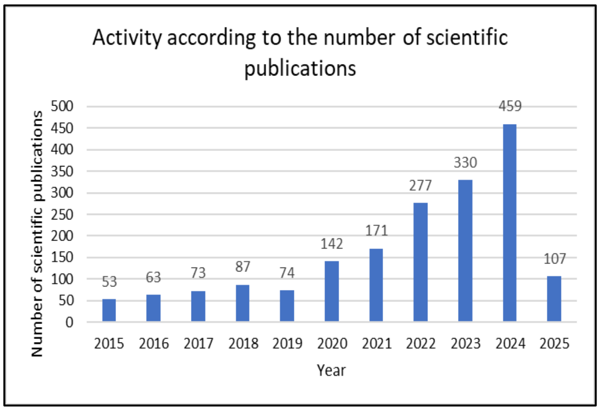

Figure 1. Activity according to the number of scientific publications related to hydrogen supply chain for the period 2015 – 2025.

Studies related to mathematical models describing HSC infrastructure can be divided into two categories [7]. The first category of research is related to the development of mathematical models for optimal design of the HSC. These models mainly focus on the production, transportation, and storage of hydrogen, offering solutions regarding the location and capacity of the infrastructure. The second category of research mainly focuses on developing mathematical models describing the location of hydrogen refueling stations, aiming to meet the requirements of fuel cell vehicles while considering the capacity of the stations. In cases where refueling stations are considered, the required electrical energy mostly comes from the main power grid, which facilitates decision-making [8]. There are no known developments in the literature offering solutions for the sustainable design of an HSC produced through electrolysis, taking into account the location and capacity of refueling stations.

This study presents a generalized model for the optimal design of an HSC, produced through the electrolysis process, simultaneously considering the three aspects of sustainability—economic, environmental, and social. The developed model is formulated in terms of mixed-integer linear programming (MILP) and could be solved using specialized optimization software, such as GAMS.

COLOR CLASSIFICATION OF HYDROGEN

At standard temperature and pressure, hydrogen is a colorless, non-toxic, tasteless, and highly flammable diatomic gas with the molecular formula H_2. Depending on the method of production, 12 different colors of hydrogen are recognized today [5].

Standard colors of hydrogen

"Green" hydrogen is produced through water electrolysis, which requires electrical energy. When this energy is sourced from renewable energy sources, the hydrogen production process results in zero carbon dioxide emissions. For this reason, green hydrogen is also referred to as clean, low-carbon, or renewable hydrogen. It is well known that green hydrogen plays a vital role in the ongoing energy transition toward more sustainable energy sources. Currently, this type of hydrogen has a high production cost, but the fact that it results in zero carbon emissions still makes it the fuel of the future [9].

"Gray" hydrogen currently represents the majority of hydrogen production. It is most commonly produced through steam methane reforming (SMR), a process that also generates carbon dioxide, which is ultimately released into the atmosphere. Almost 40% of gray hydrogen is a byproduct of various chemical reactions. According to the International Energy Agency (IEA), approximately 60% of the hydrogen produced is gray [1].

Globally, approximately 2% of coal and 6% of natural gas are used for the production of gray hydrogen, generating 830 million tons of carbon dioxide per year. However, carbon dioxide emissions from gray hydrogen are still lower than those from "black" and "brown" hydrogen production [10].

Black or brown hydrogen is produced from coal. Black hydrogen is derived from bituminous (black) coal, while brown hydrogen comes from lignite (brown) coal. Coal gasification is the method used for hydrogen production. This approach results in significant carbon dioxide emissions, approximately 20 kg of carbon dioxide per kg of hydrogen [5].

During the biomass gasification process, hydrogen is also produced, and some researchers argue that this hydrogen should also be considered "green." This is because biomass is a renewable resource, and its use can contribute to a more sustainable energy system.

"Blue" hydrogen is produced from fossil fuels, but unlike gray hydrogen, its production is associated with the capture and storage of greenhouse gases in underground storage sites. It is sometimes referred to as "carbon-neutral," but in practice, the amount of carbon dioxide captured is less than 100%.

Innovative hydrogen colors

"Turquoise" hydrogen can be produced through the thermal splitting of methane *via* pyrolysis. Compared to methane reforming (SMR - steam methane reforming), methane pyrolysis produces both hydrogen (H_2) and carbon (C) as a byproduct. The carbon produced can be easily stored and utilized. In this way, turquoise hydrogen demonstrates a reduced carbon footprint. Techniques such as plasma, thermal, and catalytic decomposition have been known for years but are still not well studied for industrial-scale hydrogen production.

A common issue with turquoise and blue hydrogen is the use of natural gas. Compared to blue hydrogen, the production of turquoise hydrogen is smaller. Additionally, during the production process of turquoise hydrogen, 3 kg of soot are produced for every 1 kg of hydrogen, which creates a need for a suitable market for the soot [11]. For this reason, compared to blue and green hydrogen, turquoise hydrogen has a smaller commercialization potential in the medium term.

"Pink," "red," and "purple" hydrogen can be compared in terms of production volume with green hydrogen, with one exception - nuclear energy which can be considered a carbon-neutral source instead of renewable electricity [12]. Nuclear energy can be considered a consistent and continuous source of electricity, which supports the production of pink hydrogen. This could lead to stable and flexible energy grids. However, there are challenges associated with the radioactive waste generated during this process.

"Golden" hydrogen is produced through biological processes that transform natural hydrocarbons obtained from deep oil wells. In this case, the richness of nature is combined with technological innovations. Golden hydrogen is a low-carbon hydrogen, but it is less cost-effective compared to green hydrogen in terms of production expenses. It also provides the opportunity for underground storage and utilization of the produced carbon dioxide , making it carbon-neutral.

"Yellow" hydrogen is produced through water electrolysis powered by a mix of electricity from various sources. For example, in 2021, Spain used 23.3% of wind and 21% of nuclear sources to generate yellow hydrogen through electrolysis powered by grid electricity. This was followed by 21% of energy generation from hydropower, 8% from photovoltaic systems, and 1% from water-to-electricity conversion [13]. In another example, Iceland uses 30% of its grid energy from geothermal sources, while 70% comes from hydro sources, leading to nearly zero carbon dioxide emissions.

"White" hydrogen is naturally occurring hydrogen. It is found naturally in geysers, hydrothermal systems, volcanic gases, layers of continental or oceanic crust, or as free gas. Degassing from the Earth's core, the reaction of water with rocks, radiolysis, and the breakdown of organic matter are the responsible processes for naturally occurring hydrogen. White hydrogen is an abundant, carbon-free resource that requires minimal infrastructure to be utilized, thus offering hydrogen energy without carbon emissions. However, there is a lack of sufficient research on white hydrogen.

To achieve the goal of NZE by 2050, green and pink hydrogen are considered key to long-term sustainability. All other forms of hydrogen also play a significant role in transitioning to a low-carbon future to achieve the ultimate goal.

Figure 2 summarizes the color codes of hydrogen in the so-called hydrogen rainbow.

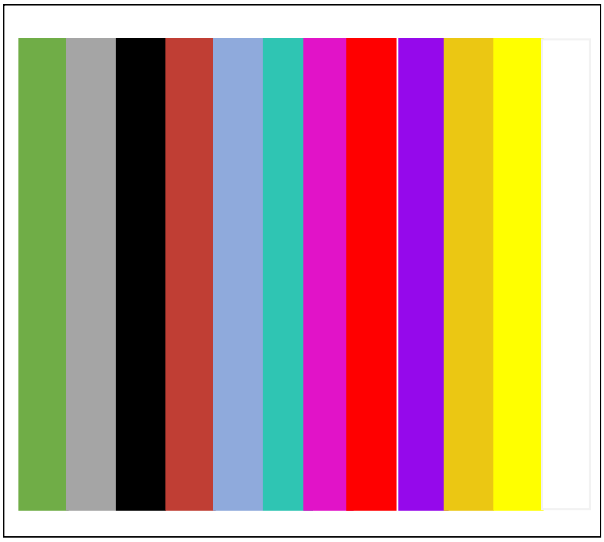

Figure 2. The hydrogen rainbow.

HYDROGEN PRODUCTION THROUGH ELECTROLYSIS

The production of hydrogen through electrolysis involves the following key stages:

1. Water treatment: The water is purified and deionized to obtain a clean electrolyte. This ensures that impurities do not interfere with the electrolysis process and helps to improve the efficiency and lifespan of the electrolyzer.

2. Electrolysis process: An electric current is passed through the aqueous solution in the electrolyzer. Typically, two electrodes – an anode and a cathode – are immersed in the electrolyte. When the electric current is applied, water molecules break down into hydrogen and oxygen. The reactions occur as follows:

- *At the anode (positive electrode):* Water molecules (H_2O) lose electrons and are oxidized to produce oxygen gas (O_2) and hydrogen ions (H^+):
  $2H_2O \rightarrow O_2 + 4H^+ + 4e^-$
- *At the cathode (negative electrode):* Hydrogen ions (H^+) gain electrons and are reduced to form hydrogen gas (H_2):
  $2H^+ + 2e^- \rightarrow H_2$

Thus, oxygen is released at the anode, and hydrogen gas is generated at the cathode. These reactions occur simultaneously, resulting in the production of hydrogen and oxygen gases.

3. Collection of gases: The produced hydrogen and oxygen gases are collected separately. They can either be used directly for various applications or stored for later use.

- *Hydrogen:* Typically, hydrogen gas is stored under pressure or in liquid form for transportation and storage. It can be used in industries, energy production, or as fuel in hydrogen-powered vehicles.
- *Oxygen:* Oxygen can be vented into the atmosphere or captured for industrial applications, such as in medical or metallurgical processes.

Electrolysis can be classified into several categories.

According to the type of electrolyte:

1. Alkaline electrolysis: Uses an aqueous solution of alkali (usually potassium hydroxide or sodium hydroxide) as the electrolyte. This technology is one of the oldest and most widely used for industrial hydrogen production. Alkaline electrolysis has high efficiency and long component life.

2. Proton exchange membrane (PEM) electrolysis: Uses a polymer membrane that conducts protons (hydrogen ions) but not electrons. PEM electrolysis operates at lower temperatures and pressures compared to alkaline electrolysis, making it suitable for small and medium-sized installations. It also offers fast start-up and shut-down, which is beneficial for integration with renewable energy sources.

3. Solid oxide electrolysis (SOE): Uses solid oxide ceramic materials as electrolytes. SOE electrolysis operates at very high temperatures (around 800-1000°C), which allows for high efficiency and the potential for cogeneration of heat and electricity. However, this technology is still in the development stage and is not as widely deployed.

According to the type of cell:

1. Monopolar cell: Consists of multiple parallel cells connected in series. Each unit has its own anode and cathode, which results in greater flexibility and reliability.

2. Bipolar cell: Uses a common bipolar plate between each pair of anode and cathode. This reduces the number of required connections and simplifies the arrangement of the cells, resulting in a more compact design.

According to the type of application:

1. Industrial electrolysis: Used for large-scale hydrogen production for industrial purposes, such as in the chemical industry, refineries, and other sectors.

2. Stationary electrolysis: Designed for fixed installations, often connected to renewable energy sources such as solar or wind power.

3. Portable electrolysis: Small and mobile devices that can produce hydrogen on-site.

According to some authors, hydrogen production through electrolysis amounts to about 2% per year [14].

The production of energy from hydrogen fuel cells is a highly efficient and environmentally friendly method for the direct conversion of the chemical potential of reactants into electrical energy. A hydrogen fuel cell typically consists of separated electrodes (anode and cathode) through a proton exchange membrane (PEM), also referred to as the electrolyte [15] (Figure 3).

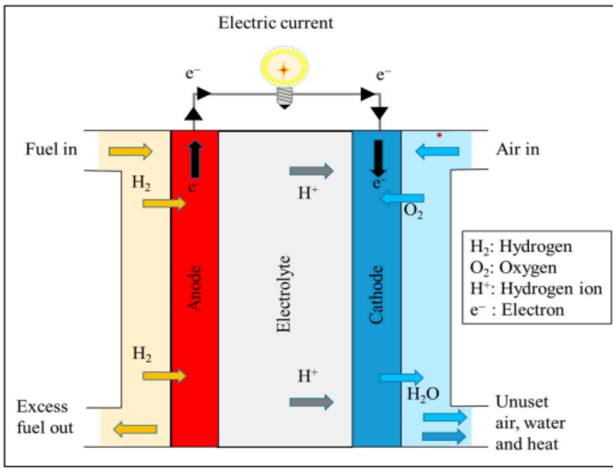

Figure 3. Hydrogen fuel cell [16].

The operating temperature is within the range of 333–353 K. Hydrogen and oxygen enter the fuel cell in the anode and cathode chambers, respectively. Hydrogen acts as an electron donor, while oxygen acts as an electron acceptor. At the anode, protons are formed, which pass through the membrane and react with oxygen at the cathode, resulting in the formation of water vapor and the release of heat.

Despite the numerous advantages of hydrogen energy, challenges still exist for the scientific community that must be addressed in order to achieve the sustainable application of hydrogen in the transportation sector. One possible solution is the development of hydrogen supply chains (HSC) that take into account the economic, environmental, and social aspects of sustainability.

SUPERSTRUCTURE OF A HYDROGEN SUPPLY CHAIN OBTAINED THROUGH ELECTROLYSIS PROCESS

Figure 4 presents a generalized superstructure of the hydrogen supply chain obtained through the electrolysis process. It includes feedstocks, production, storage, end usage, also transport. This structure allows for the identification of key decision points and optimization opportunities across the entire supply chain.

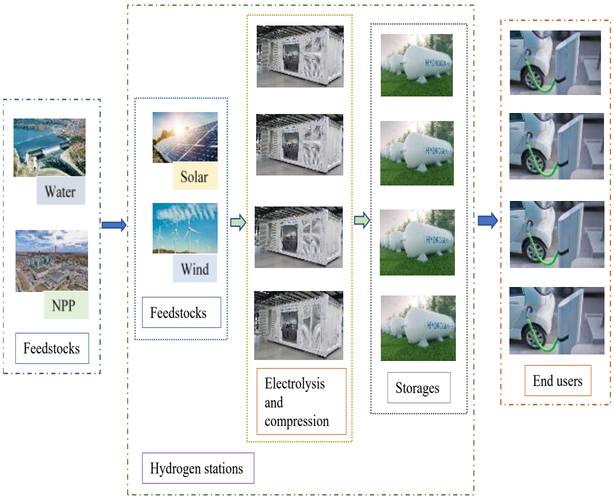

Figure 4. Generalized superstructure of a HSC for the supply of hydrogen produced through the electrolysis process.

AN OPTIMIZATION MODEL FOR DESIGNING A SUSTAINABLE HYDROGEN SUPPLY CHAIN THROUGH ELECTROLYSIS PROCESS

To formulate the mathematical model for the optimal design of a sustainable hydrogen supply chain (HSC), the following data are required:

Necessary data

1. *Hydrogen Demand Data:*
- Hydrogen demand: the required hydrogen demand (kg H_2) over a specific period, considering the energy needs of industries, transportation, and other sectors.
- Time horizon: The time period over which the hydrogen supply chain is evaluated (e.g., annually, monthly).
2. Hydrogen Production Data:
- Efficiency of electrolysis technologies: Energy efficiency for different electrolyzer types (alkaline, PEM, SOE).
- Electrolyzer capacity: The capacity of each type of electrolyzer (kg H_2/day or year).
- Energy consumption: Energy required for hydrogen production (kWh per kg H_2).
- Renewable energy source availability: The availability of renewable energy sources (solar, wind, hydro) for powering the electrolysis process (kWh/year).
3. *Costs Data:*
- Capital costs: Initial investment required for hydrogen production, storage, and transportation infrastructure.
- Operating costs: Ongoing costs for maintenance, electricity, labor, and other operational expenses.

- Transportation costs: Costs associated with hydrogen transportation (trucks, etc.).
- Storage costs: Costs related to hydrogen storage systems (e.g., compression, liquefaction, etc.).
- Carbon taxes/credits: Cost of CO_2 emissions or potential credits earned through the use of low-carbon technologies.
- Energy costs: Cost of renewable energy required for electrolysis and cost of hydrogen produced in a nuclear power plant.

4. *Environmental Data:*

- Carbon emission factors: Emission levels per unit of hydrogen produced, considering the use of renewable and non-renewable energy sources.
- Energy efficiency and emissions per transportation mode: Emission factors for hydrogen transport via different methods (trucks, etc.).
- Emissions from storage: Any emissions resulting from storage processes (e.g., leakage, energy consumption).

5. *Infrastructure Data:*

- Storage capacity: Maximum storage capacity for hydrogen in different storage technologies (kg H_2).
- Transportation capacity: Maximum hydrogen transportation capacity for the trucks, and other methods of transportation (kg H_2/day).

6. *Social and Economic Data:*

- Labor costs: Employment and wage data for workforce required in hydrogen production, storage, and transportation sectors.
- Job creation impact: Estimations on the number of jobs created within the hydrogen supply chain.
- Economic benefits: Potential for local economic growth, considering the hydrogen value chain's impact on local communities.

7. *Regulatory Data:*

- Government policies: Regulations, subsidies, or incentives for hydrogen production, transportation, and use, especially for renewable hydrogen.
- Carbon emission reduction targets: National or regional carbon reduction targets and guidelines for hydrogen production.

8. *Technical Constraints:*

- Capacity limits for different production, storage, and transportation facilities.
- Technological advancements: Expected improvements in technology efficiency, storage, or transportation costs.

Goal of optimization

The goal of solving the optimization problem is to be determined the optimal operating conditions, as follows:

1. Structure of the Hydrogen Supply Chain (HSC);
2. Production capacity for hydrogen from electrolysis systems, considering the available renewable energy sources and technological efficiency, to meet the hydrogen demand;
3. Number, location, and capacity of the charging stations that need to be built;
4. Performance of the charging stations;
5. Number, location, and capacity of the hydrogen storage facilities that need to be built;
6. Design of the hydrogen transportation network (trucks, etc.), including the capacity, route selection, and distribution methods;
7. Number of jobs created as a result of the operation of all HSC elements during its operating.
8. Energy source allocation. It is related to the distribution of renewable energy sources (e.g., wind, solar, hydropower) to the electrolysis systems for hydrogen production, maximizing energy utilization and minimizing operational costs.
9. Operational schedules for hydrogen production, storage, and transportation, ensuring system flexibility to handle varying demand patterns, renewable energy availability, and operational downtime.

The solution to this optimization problem provides a comprehensive design that ensures the most efficient, cost-effective, and environmentally friendly hydrogen supply chain while meeting all demand, regulatory, and social considerations.

MATHEMATICAL MODEL

The HSC is considered with a long planning horizon H (10 years). The entire time horizon H is divided into a set of discrete time intervals t. This time interval is divided into several equal subintervals, each with a duration of ∇t.

Over the planning horizon, it is assumed that the hydrogen consumption will change with a forecasted value. The mathematical model describing the optimal configuration of the sustainable hydrogen supply chain (HSC) is given as follows:

Model of the environmental impact of HSC e TEI_t, $\left[\mathrm{kg}_{\mathrm{CO_2eq}}/\mathrm{d}\right]$

This model takes into account various factors influencing the environment throughout the entire hydrogen supply chain (HSC), including hydrogen production, storage, transportation, and distribution. The goal is to minimize the environmental footprint of the HSC while ensuring that energy production aligns with sustainability goals and regulatory standards.

These emissions are equal to the sum of the impact of each stage of the life cycle on the environment. Greenhouse gas emissions are typically determined as follows for each time interval $t \in T$ [16]:

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

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, $[\mathrm{kg_{CO_2eq}}/\mathrm{y}]$.

Model of the economic impact of HSC $eTHC_t$, $[\$/\mathrm{y}]$

Annual operating costs include the costs of raw material acquisition, local costs for the final product, production costs of the final products, and transportation costs for raw materials and final products. Production costs take into account both the fixed annual operating costs, which are given as a percentage of the corresponding total capital investment, as well as the net variable cost, which is proportional to the processing amount. Transportation costs account for both fixed distances and distances with variable costs. The economic optimization criterion will be the operating costs of the enterprise, which include the total investment costs for production facilities and the operation of the HSC. This cost is expressed through a dependency for each time interval $t \in T$:

$$\begin{aligned} eTHC_t = eTIC_t + eTPC_t &+ eTHH_t + eTHE_t + eTHHH_t \\ &+ eTMO_t + eTPW_t + eTTC_t \\ &+ eTTAXB_t + eTHSC_t \\ &+ eTOEC_t - eT1L_t - eT2L_t \\ &- eTH_t, \forall t \end{aligned} \quad (2)$$

where:

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

$eTIC_T$ - 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, $[\$/\mathrm{y}]$

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

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

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

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

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

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

$eTHSC_t$ - 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, $[\$/\mathrm{y}]$;

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

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

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

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

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

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

Model of the social impact of HSC $\mathrm{eJob_t}$, $[\text{Number of Jobs}/\mathrm{y}]$

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:

$$\begin{aligned} &eJob_t \\ &= eNJ1_t + eLT_tNJ12_t + eNJ2_t \\ &+ eLT_tNJ21_t, \ \forall t \end{aligned} \quad (3)$$

where: the terms of (3) 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, $[\$/\mathrm{y}]$;

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 (3) can be considered as a simplified model of the social assessment criterion [17].

Model constraints

The constraints ensuring the feasibility of the obtained optimal solutions are as follows:

- Constraints regarding the capacity of the facilities, limited by the lower and upper boundaries;
- Constraints ensuring the flows admissibility;
- Constraints ensuring the hydrogen fuel needs of all regions;
- Constraints ensuring the necessary quantities of raw materials (water, electricity) for hydrogen production;
- Logistical and transportation constraints;
- Constraints ensuring the material balance for the entire HSC;
- Constraints ensuring the fulfillment of the annual capacities of the facilities;
- Constraints ensuring the satisfaction of product demand;
- Constraints ensuring the increase of social impact during the operation of the HSC as a whole.

Objective function

The optimal operating conditions for the HSC should ensure a minimum of the objective function, which includes:

1. *Environmental Impact Reduction:* The reduction of the overall carbon footprint of the hydrogen supply chain by optimizing the use of renewable energy sources, minimizing emissions from production, storage, and transportation processes.
2. *Cost Minimization:* The minimization of total costs across all stages of the hydrogen supply chain, including production, storage, transportation, and infrastructure development, while considering capital, operating, and maintenance costs.
3. *Social and Economic Objectives:* Maximizing the social and economic benefits of the hydrogen supply chain, such as job creation, economic growth, and local community impacts, while maintaining a balance between environmental sustainability and economic viability.

$$COST = \sum_{t \epsilon T}(LT_t eTHC_t) \tag{4}$$

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

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

The 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.

CONCLUSIONS

1. The color scale for classifying H_2 were generalized, which determines the method of its production. The color codes for H_2 are presented in the so-called hydrogen spectrum. The standard colors for hydrogen are: green, gray, brown, black, and blue, while the new/innovative ones are: turquoise, pink, red, purple, gold, yellow, and white. To achieve the goal of net zero emissions (NZE) by 2050, green and pink H_2 are considered essential for long-term sustainability.
2. The hydrogen production process through electrolysis has been considered. Energy generation from hydrogen fuel cells is a highly efficient and environmentally friendly method for directly converting the chemical potential of the reactants into electrical energy.
3. A generalized structure of the supply chain for hydrogen produced through electrolysis has been proposed. The HSC includes feedstocks, production, storage, end usage, also transport.
4. A model for designing the HSC was proposed, taking into account the three pillars of the sustainability concept: economic, environmental, and social.
5. The environmental criterion includes the impact on the environment during the operation of the considered hydrogen supply chain.
6. The economic criterion includes the operating costs of the enterprise, which consist of the total investment costs for production capacities and the operation of the HSC.
7. The social criterion includes the expected total number of jobs created as a result of the operation of all system elements during its functioning.
8. The developed model is formulated in terms of Mixed-Integer Linear Programming (MILP) and can be solved using specialized optimization software, such as GAMS.

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