Mathematical modeling of the hydrogen supply chain — an integrated approach for sustainable transport

Desislava Nikolova, Tanya Valkanova
Burgas State University "Prof. dr Assen Zlatarov" – Bulgaria
desislava-nikolova@uniburgas.bg

Abstract: *This study proposes a mathematical model for design and optimization of a hydrogen supply chain, covering all stages of the life cycle - feedstocks, production, storage, distribution, end-use in the transport sector. The developed methodology integrates different hydrogen production technologies and takes into account environmental, economic and social impacts in order to identify the most efficient and sustainable configuration. The focus in this work falls on hydrogen production by steam reforming of methane and hydrogen production by electrolysis of water in hydrogen refueling stations. The mathematical model is formulated in terms of MILP programming and can be solved using the GAMS software product. The aim is to find an optimal balance between economic efficiency, environmental sustainability and social impact by using weighted coefficients (weights). The proposed concept provides a decision-making tool for planning hydrogen infrastructure in line with European decarbonization and sustainable transport goals.*
Keywords*: MILP, OPTIMIZATION, SUSTAINABLE, SUPPLY CHAIN, HYDROGEN*

1. Introduction

Energy conservation has emerged as one of the key challenges of the modern world. This is due to the gradual but inevitable depletion of natural feedstocks, as well as the complex economic, political and social situation in different regions, also affecting ecosystems. These circumstances have prompted the scientific community to seek solutions to global problems, such as the development of alternative energy sources and the promotion of sustainable use of energy carriers. Recently, the integration of hydrogen technologies has been seen as a key factor in achieving carbon neutrality [1] and requires cooperation between scientific institutions, industry and political structures [2]. Especially in the transport sector, the use of hydrogen as a fuel is essential for reducing GHG emissions and increasing sustainability, and strategic planning of hydrogen supply chain can ensure the long-term stability of energy systems. Hydrogen technologies are expected to play a crucial role in the transformation towards a sustainable energy future in terms of transport. Over the past few years, the fuel and energy systems in transportation have been evolving from conventional fossil fuels to renewable energy sources [3]. However, there are problems with regard to high cost, inconsistent supply, and reliability [4].

Although atomic hydrogen is the most abundant chemical element in the universe [5], it is very rarely found in its pure form. Hydrogen can be produced through various technological processes, such as water electrolysis or steam methane reforming. The choice of hydrogen production method largely determines its environmental impact, energy efficiency, and economic feasibility. Among the most widely applied technologies, water electrolysis and steam methane reforming (SMR) differ significantly in terms of carbon footprint and energy input. Electrolysis, when powered by renewable energy sources, enables the production of nearly carbon-free hydrogen, making it one of the most promising pathways for achieving climate neutrality. Conversely, SMR remains the dominant industrial method due to its high efficiency and lower production costs, although it is associated with considerable CO_2 emissions. Other emerging technologies, such as biomass gasification, photoelectrochemical water splitting, and thermochemical cycles, are being investigated as potential alternatives that could enhance sustainability and reduce reliance on fossil fuels. The integration of these production pathways within a unified hydrogen economy requires comprehensive assessment of technical performance, cost efficiency, and environmental compatibility to ensure a balanced transition toward sustainable energy systems.

Depending on the technological production methods, hydrogen is classified into several color categories [6]. These colors categories are in turn divided into standard and innovative. The standard colors of hydrogen include "green hydrogen" - produced via electrolysis using renewable energy sources; "gray hydrogen" - produced via steam methane reforming (SMR), a process that also generates carbon dioxide, which is ultimately released into the atmosphere; "blue hydrogen" - produced from fossil fuels, but unlike gray hydrogen, its production is associated with the capture and storage of greenhouse gases in underground storage sites; "black/brown hydrogen" - produced from coal. The innovative color categories of hydrogen include pink, gold, yellow, turquoise and white.

The use of hydrogen as an energy carrier has its advantages and disadvantages [7]. Some of the main positive properties of hydrogen are high gravimetric energy density, decarbonization potential, flexible energy storage, good integration in the existing energy infrastructure [8], diversification of energy sources and reduced dependence on fossil fuels [9]. From another perspective, hydrogen also has disadvantages, such as low volumetric energy density, high production costs [10], high energy losses as a result of compression and transportation, stringent safety requirements.

Currently, the implementation of hydrogen in the energy infrastructure around the world remains expensive and difficult. Although there is an increase in the number of hydrogens refueling stations [11] (mainly in Japan, South Korea, the USA and parts of the EU), the design of sustainable supply chains is still in its early stages. In order to enable the widespread adoption of hydrogen technology in the transport sector, it is necessary to develop a stable and sustainable supply chain. Such a hydrogen infrastructure must ensure the three pillars of sustainability – environmental, economic and social.

The scientific community has increasingly focused on developments on issues related to the hydrogen supply chain. Various methodologies and mathematical models have been proposed, with the studies most often emphasizing economic efficiency, while social and environmental aspects remain secondary. In addition, there is a lack of spatio-temporal integration between the stages of production, storage, transport and refueling. It is in this context that our study is positioned - developing a unified optimization framework that equally takes into account economic, environmental and social criteria.

The focus of the present work falls on green hydrogen – produced by electrolysis of water and using renewable energy sources and gray hydrogen, produced by steam reforming of methane. These two technologies represent the most established and contrasting hydrogen production pathways—SMR for its economic efficiency and maturity, and electrolysis for its environmental sustainability and renewable potential. Both production methods are integrated into a combined resource security chain. The present study proposes a MILP-based approach for sustainable design of an integrated superstructure of a supply chain. Optimization problem has been formulated and solved either at in terms of economic, social and environmental sustainability. The purpose of the defined mathematical model is to obtain optimal operating conditions of the considered an integrated supply chain. The proposed approach has been solved using GAMS software, and the results can serve as a decision-support tool.

2. Formulation of the optimization problem

This study presents an integrated superstructure of a supply chain of hydrogen production via various technologies. The focus here is on hydrogen produced via steam methane reforming (SMR), as well as via electrolysis using renewable energy. The proposed superstructure views the supply chain system as a whole. It comprises feedstocks, production, storage, end user's areas and is represented in Fig. 1.

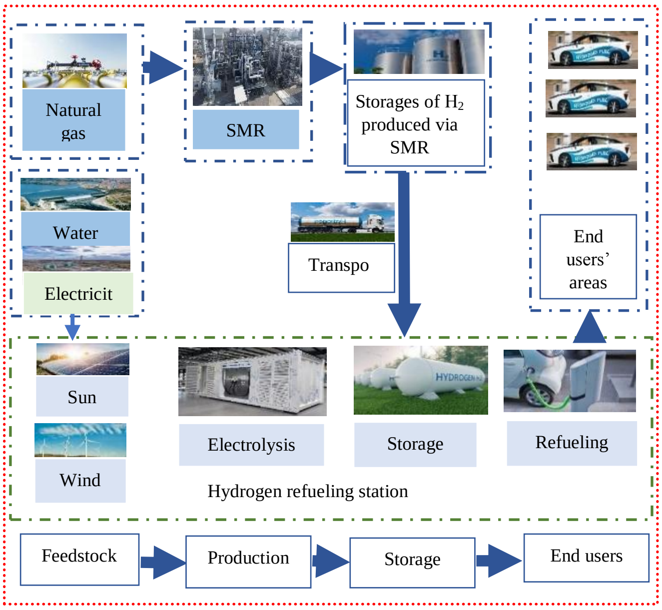

Fig. 1 *An integrated superstructure of a supply chain*

The problem considered in this paper can be formulated as follows Table 1:

Table 1: *Problem statement*

Given are:	Determine the optimal parameters of the supply chain as:
the location and production capacity of plants for hydrogen production via SMR	size, capacity and location of refueling stations
the potential location and capacity of storage facilities	size, capacity and location of hydrogen storage facilities
the potential locations of charging stations and their production capacity	the transport delivery scheme
the technologies for production of hydrogen via SMR and electrolysis	the total environmental impact as a result of the operation of all system during its operation
the price of raw materials (water, electricity and natural gas) and selling price of hydrogen	the total social impact as a result of the operation of all system during its operation
The type of transport for hydrogen delivery and transport costs	the total economic impact as a result of the operation of all system during its operation
greenhouse gas emissions for each stage of the life cycle and carbon tax	
government incentives for hydrogen consumption and production	
maintenance and operation costs of charging stations and labor cost	
demand at regions	

The problem is formulated as an optimization procedure in terms of mixed integer linear programming. The aim is to identify such decision variables that, subject to the system of constraints, minimize the objective function Z. The constraints guaranteeing the performance of the task are linear functions with respect to all independent variables. The model aims to achieve an optimal balance between environmental sustainability, economic efficiency, and social impact when designing the hydrogen supply chain for the transportation sector.

The presented optimization procedure, which generates the mathematical model of a sustainable supply chain for hydrogen production for transport sector, is accompanied by preliminary collection and processing of the necessary data. In this case, two different technologies for hydrogen production are considered. Specifically, hydrogen production by steam methane reforming (SMR) and hydrogen production by electrolysis in hydrogen refueling stations (HRS) powered by renewable energy sources.

2.1. *Input data for the test example*

This part of the paper presents some of the necessary data.

- *Territorial distribution*

According to Geodesy, Cartography and Cadaster Agency [12] under the Ministry of Regional Development and Public Works, the total area of the Republic of Bulgaria is 111,002 km^2. In the case under consideration, Bulgaria is territorially divided into 28 administrative-territorial units (Fig.2).

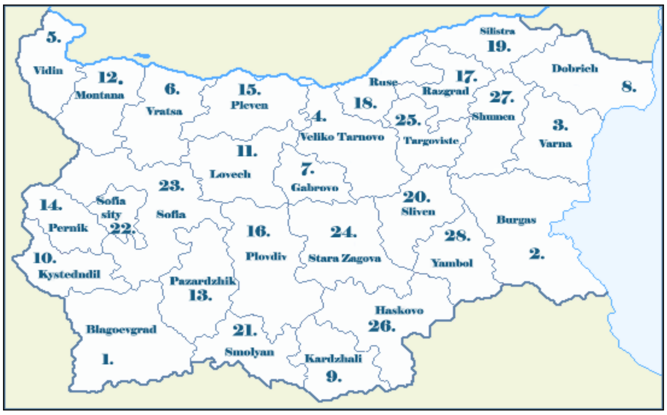

Fig. 2 *Administrative - territorial units of Bulgaria*

The hydrogen supply chain consists of 28 potential storage sites for hydrogen produced via steam reforming of methane, 28 potential sites for hydrogen production via electrolysis in Hydrogen Refueling Stations (HRS), 28 potential customer areas and 3 areas for hydrogen production by steam reforming. It is possible to build more than one Hydrogen Refueling Station in individual areas.

- *Data on the actual delivery distance between*

The distances in kilometers between regions in Bulgaria for the purposes of this study were taken from the Ministry of Regional Development and Public Works, Road Infrastructure Agency [13] for each mode of transport.

- *Data on the type of transport for hydrogen delivery*

According to the Agreement on the International Carriage of Dangerous Goods by Road (ADR), mandatory for the EU, including Bulgaria [14], gaseous hydrogen (flammable gas Class 2.1.) must be transported in special tanks or cylinders.

- *Data on transport cost*

It is assumed that all transportation will be carried out by land roads. Transportation costs include three main components: loading and unloading costs, time-dependent costs, and costs dependent on the distance between regions.

- *Data on environmental parameters*

Carbon emissions [kg CO2-eq per kg H2 per km] emitted during hydrogen transport are calculated taking into account the average fuel consumption for the respective type of transport, the emission factor of the fuel (diesel) and the capacity of the trucks. The emission factor for the combustion of petroleum diesel (direct emissions - tank-to-wheel), the emission factor for the production of diesel, the emission factor for the entire life cycle of petroleum diesel, including production (gray emissions - well-to-wheel) are taken into account.

- *Capital Expenditure Data*

The capital costs of individual structures themselves represent fixed and variable capital costs.

- *Data on the type of hydrogen refueling stations*

For the purposes of this study, hydrogen refueling stations intended only for vehicles that meet the requirements of Regulation (EC) No 79/2009 of the European Parliament and of the Council on type-approval of hydrogen-powered motor vehicles are considered.

- *Data on demand*

Hydrogen market demand data presents a forecast of the market demand for hydrogen as an automotive fuel based on the population size of a given area. Calculations have been made for a scenario where 0.5% of cars would be hydrogen-powered, given the available infrastructure and incentives.

- *Data on monetary parameters in hydrogen production by electrolysis*

It is assumed that the envisaged fixed premium for the production of green hydrogen is between €0.37 and €0.48 per kg of H_2 , with a ceiling of €4.5/kg. ($0.43 - $0.56 with a ceiling of $5.24 per kilogram of hydrogen) [15].

- *Data on time intervals*

According to the strategic legislative package "Fit for 55" [16] developed by the European Commission, the rules for integrated and transparent network planning across the EU according to the "energy efficiency first" principle and with a future-oriented approach, gas and hydrogen network operators will have to prepare a 10-year EU network development plan. For the purposes of this task, a 5-year time frame is considered. The entire time horizon H is divided into a set of discrete time intervals t. This time interval is divided into several equal time subintervals t={0,1,2,…,T}, each of which lasts ∇t.

2.2. Environmental assessment model

The environmental assessment model of the integrated hydrogen supply chain is represented as the total greenhouse gas emissions generated over the whole live. They are converted into carbon credits multiplied by the price of carbon emissions on the market.

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

Where:

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

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

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

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

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

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

2.3. Social assessment model

The social assessment model of the integrated hydrogen supply chain is represented as the total labor costs 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.

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

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];

2.4. Economic assessment model

For definition of the economic assessment model of the supply chain operation the annual operating costs are used. The economic criterion includes the total investment costs, 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 for the planned time period. They define for each time interval t∈T as:

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

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];

2.5. Constraints

The constraints that guarantee the completion of the task are linear functions of all independent variables. The constraints that guarantee the completion of the task are linear functions of all independent variables. These constraints are related to the capacity of the facilities, the material balance, flows admissibility, needs of hydrogen as fuel, logistical and transportation constraints and others. The planning horizon is set to 5 years.

2.6. Objective function

The optimization problem for determining the optimal location of the plants in the regions and their parameters is formulated as:

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

$$Find: X_t[Decision\ variables]MINIMIZE\{Z(X_t)\} \rightarrow (Eq.4)s.t.:\{Constraints\} \quad \ldots\ldots(5)$$

Where

$\alpha, \beta, \gamma -$ weighting factors that determine the priority of each criterion.

The objective function Z aims to minimize the overall value derived from a weighted combination of economic, environmental, and social factors.

The optimization problem can be solved using the GAMS software, which enables comprehensive and intelligent decision-making.

The results obtained from the developed methodology will be presented and discussed in a forthcoming paper. Further research will elaborate on the implementation and analysis of the proposed approach.

In addition, by adjusting the required data, the proposed model can be adapted to various regions.

4. Conclusion

The study proposes an integrated approach for design of hydrogen supply chain. The proposed mathematical model is formulated in terms of MILP. Sustainability is considered from the perspective of economic, environmental and social factors. It is proposed an integrated superstructure of a supply chain including various technologies for hydrogen production and considering the supply chain as a whole from feedstock to end users. The proposed task is solved using the GAMS software platform, which can serve as a decision-support tool.

Acknowledgments

The study has been carried out by the financial support of National Science Fund, Ministry of Education and Science of the Republic of Bulgaria, Contract № КП-06-Н89/6/09.12.2024

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