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Hydrogen Production System Design considering the Water-Energy-Carbon Nexus and Cost

Juan C. González Palencia*, Yuta Itoi, Mikiya Araki

Division of Mechanical Science and Technology, Graduate School of Science and Technology, Gunma University, 29-1 Honcho, Ota, Gunma 373-0057, Japan

* Corresponding Author. E-mail address: gonzalez@gunma-u.ac.jp

ABSTRACT

Replacing steam methane reforming with electrolysis using renewable electricity for hydrogen production can reduce CO_2 emissions with a trade-off of larger energy use, water use and cost. A linear programming optimization model that accounts for energy use, water use, CO_2 emissions and cost was developed to optimize the configuration of a hydrogen production system; considering Japan in 2030 as a case of study. Four scenarios were considered, prioritizing 1) cost, 2) energy use, 3) Water-Energy-Carbon nexus and 4) Water-Energy-Carbon nexus and cost; under maximum CO_2 intensities for hydrogen production between 0 and 18 kg-CO_2/kg-H_2. Hydrogen production routes include steam methane reforming; and electrolysis using grid electricity, wind electricity, solar photovoltaic electricity, geothermal electricity and hydroelectricity. For CO_2 intensities higher than 8 kg-CO_2/kg-H_2, steam methane reforming accounts for more than 50% of hydrogen production in all scenarios. For a CO_2 intensity of 0 kg-CO_2/kg-H_2, hydroelectricity represents more than 76% of hydrogen production when energy use or cost are prioritized. Including water use in the priorities drives the share of wind electricity in hydrogen production to 37.6%. The remaining hydrogen is produced using solar electricity if cost is not prioritized; or 23.7% geothermal electricity and 38.7% hydroelectricity if cost is prioritized simultaneously.

Keywords: Hydrogen Production, Water-Energy-Carbon Nexus, Hydrogen Economy, Low-Carbon Hydrogen Production, Linear Programming Optimization

NOMENCLATURE

Abbreviations	
PV	Photovoltaic
SEC	Specific Energy Consumption
SMR	Steam Methane Reforming
WEC	Water-Energy-Carbon
Symbols	
α	Share of hydrogen production technology in hydrogen production
Attribute	Specific energy consumption, specific water consumption, specific CO_2 emissions and specific production cost
c	Category for evaluation
Dmd	Hydrogen demand
j	Hydrogen production technology
H_2	Amount of hydrogen produced
Maximum	Maximum value for each attribute
Minimum	Minimum value for each attribute
S	Score
w	Weighting coefficient
Z	Hydrogen production system overall score

1. INTRODUCTION

Hydrogen can contribute to achieve climate change and energy security goals in transport, industry, buildings and other sectors of the energy system [1]. However, hydrogen supply chain development remains as one of the main challenges for the widespread adoption of hydrogen on a scale similar to the scale in which fossil fuels are used in the present.

The hydrogen supply chain has been studied extensively. For instance, El-Emam and Özcan [2] reported more than 180 economic studies about hydrogen production during the year 2017. Similarly, the Water-Energy-Carbon (WEC) nexus is an active area of research; with studies assessing problems such as the potential for water saving in electricity generation [3]; and the Water-Energy nexus for electricity generation in Europe [4]. To the authors' best knowledge, there are no previous studies about the design of hydrogen production systems considering the WEC nexus and cost.

In this research, a hydrogen production system is designed using a linear programming optimization model considering energy use, water use, CO_2 emissions and cost. Japan in 2030 is considered as a case of study. The rest of the paper is organized as follows: the linear programming optimization model is presented in section 2; results for the hydrogen production system design are presented and discussed in section 3; and conclusions are presented in section 4.

2. METHODS

A Bottom-up, linear programming optimization model was developed to determine the optimum design of a hydrogen production system. The model was developed using GAMS [5] and solved using CPLEX [6]. A brief description of the model is provided below.

Considering the production of 1 kg-H_2 as the calculation basis, the specific energy consumption, specific water consumption, specific CO_2 emissions and specific production cost are estimated, including energy resource production, feedstock production and hydrogen production process.

Similar to Acar and Dincer [7], hydrogen production technologies are normalized and ranked within each category against the top performer. The overall score of the hydrogen production system is estimated considering the importance of each category through a weighting coefficient, similar to the approach developed in [8]. The weighting coefficients are defined in each scenario according to the priorities of the stakeholders in the design of the hydrogen production system.

2.1 Objective function

The objective function corresponds to the overall score of the hydrogen production system evaluated in terms of energy use, water use, CO_2 emissions and cost, as indicated in Eqs. (1, 2):

$$Z = \sum_j \sum_c \alpha_j S_{j,c} w_c \tag{1}$$

$$\alpha_j = \frac{H_{2,j}}{Dmd} \tag{2}$$

Hydrogen production technologies were ranked in each one of the categories for evaluation using Eq. (3) [7]:

$$S_{j,c} = \frac{Maximum_c - Attribute_{j,c}}{Maximum_c - Minimum_c} \tag{3}$$

2.2 Constraints

Due to space limitations, the constraints for the optimization model are only described qualitatively. 1) Hydrogen demand satisfaction, hydrogen produced should be equal or larger than hydrogen demand; 2) feedstock availability, the amount of feedstock used for hydrogen production cannot exceed the amount of feedstock available; 3) energy resource availability, the amount of energy resource used for hydrogen production cannot exceed the amount of energy resource available; 4) non-negativity constraint, the share of each technology in hydrogen production cannot be negative; 5) non-viable combinations, the amount of hydrogen production using energy resource-hydrogen production technology-feedstock combinations that are not viable is zero; 6) maximum CO_2 intensity for hydrogen production, CO_2 intensity for hydrogen production cannot exceed the maximum CO_2 intensity set.

2.3 Scenarios

Scenarios represent the priorities of the stakeholders for designing the hydrogen production system, expressed in terms of the weighting coefficients.

Low Cost (LC). Prioritizes low cost; with a weighting coefficient of 1 for cost, and zero for other categories.

Low Energy Use (LEU). Prioritizes low energy use; with a weighting coefficient of 1 for energy use, and zero for other categories.

Water-Energy-Carbon (WEC). Prioritizes water use, energy use and CO_2 emissions; with weighting coefficients of 0.333 for water use, energy use and CO_2 emissions, and zero for cost.

Water-Energy-Carbon Cost (WECC). Prioritizes water use, energy use, CO_2 emissions and cost; with weighting coefficients of 0.250 for all categories.

Calculations were performed for each scenario varying the maximum CO_2 intensity for hydrogen production between 0 and 18 kg-CO_2/kg-H_2 in steps of 1 kg-CO_2/kg-H_2.

2.4 Input data

Hydrogen demand was set exogenously at 300,000 t-H_2/year, corresponding to the national hydrogen production target for Japan in 2030 [9]. It was assumed that hydrogen was produced using only national energy resources, due to energy security concerns. Therefore, maximum natural gas availability was limited to domestic natural gas, estimated in 2.29 Mt/year [10,11]. Water availability was limited to 10% of water consumed in the industrial sector, 1.11 billion m^3/year [12].

Hydrogen production routes include steam methane reforming (SMR); and electrolysis using grid electricity, wind electricity, solar PV electricity, geothermal electricity and hydroelectricity. The data for specific energy consumption and yield for hydrogen production are shown in Table 1. Data for energy resource production are presented in Table 2.

Table 1. Specific energy consumption (SEC) and yield for hydrogen production [11,13–15].

	SEC [MJ/kg-H_2]		Yield [kg-H_2/unit]	
	Natural gas	Electricity	Natural gas [kg]	Water [m^3]
SMR	46.3	2.05	0.500	110
Electrolysis	0	195	0	64.4

Table 2. Maximum available energy resource, energy consumption factor and feedstock consumption factor during energy resource production [10,16–21].

	Availability [PJ]	Energy use [MJ/MJ]	Feedstock use [unit/MJ]	
			Water [L]	Natural gas [kg]
Natural gas	110	0.066	0.004	0.0012
Wind electricity	22.1	1.857	0	0
PV electricity	132	6.042	0.006	0
Geothermal electricity	13.9	7.333	0.487	0
Hydroelectricity	420	0.294	4.267	0
Grid electricity	1444	1.530	0.632	0

All costs were estimated in 2017 USD. Feedstock costs were estimated in 0.203 USD/m^3 for water [22] and 0.437 USD/kg for natural gas [23]. Renewable electricity prices were 38.7, 52.0, 27.0 and 42.7 USD/GJ for wind electricity, solar PV electricity, geothermal electricity and hydroelectricity [24]. Regarding grid electricity, the price for industrial electricity of 35.7 USD/GJ was used [23].

Capital costs for SMR and electrolysis were assumed equal to 121 USD/kW and 800 USD/kW, respectively [25,26]. Service lives for SMR and electrolysis were assumed equal to 25 and 10 years, respectively. The capital costs were annualized throughout the service lives of the hydrogen production technologies using a discount rate of 10%. Capacity factors for SMR and electrolysis are 0.90 and 0.97 [11]. The capacity factors for electrolysis using different electricity sources was estimated as the product of the capacity factor for electrolysis and the capacity factor for the electricity source from [16,24]. Only centralized electrolysis was considered.

Natural gas production emits 2.29 kg-CO_2/kg-natural gas [11]; while water production emits 0.453 kg-CO_2/m^3 when the CO_2 emission factor for grid electricity of 142 g-CO_2/MJ [27] is considered. Electricity production using renewable energy sources produces zero CO_2 emissions. CO_2 emissions for hydrogen production using SMR result from heat production using methane, 57.0 g-CO_2/MJ; and from the chemistry process, 5.7 kg-CO_2/kg-H_2 [14]. CO_2 emissions during hydrogen production are zero for all routes using electrolysis.

3. RESULTS AND DISCUSSION

3.1 Configuration of the hydrogen production system

The configuration of the hydrogen production system is presented in Fig. 1. SMR is used in all scenarios to produce hydrogen as much as the CO_2 intensity constraint allows; accounting for more than 50% of hydrogen production for CO_2 intensities higher than 8 kg-CO_2/kg-H_2 in all scenarios. For lower CO_2 intensities, electrolysis using renewable electricity is preferred.

For a CO_2 intensity of 0 kg-CO_2/kg-H_2, hydroelectricity represents more than 76% of hydrogen production when energy use or cost are prioritized. Including water use in the priorities drives the share of wind electricity in hydrogen production to 37.6%. The remaining hydrogen is produced using solar electricity if cost is not prioritized; or 23.7% geothermal electricity and 38.7% hydroelectricity if cost is prioritized simultaneously.

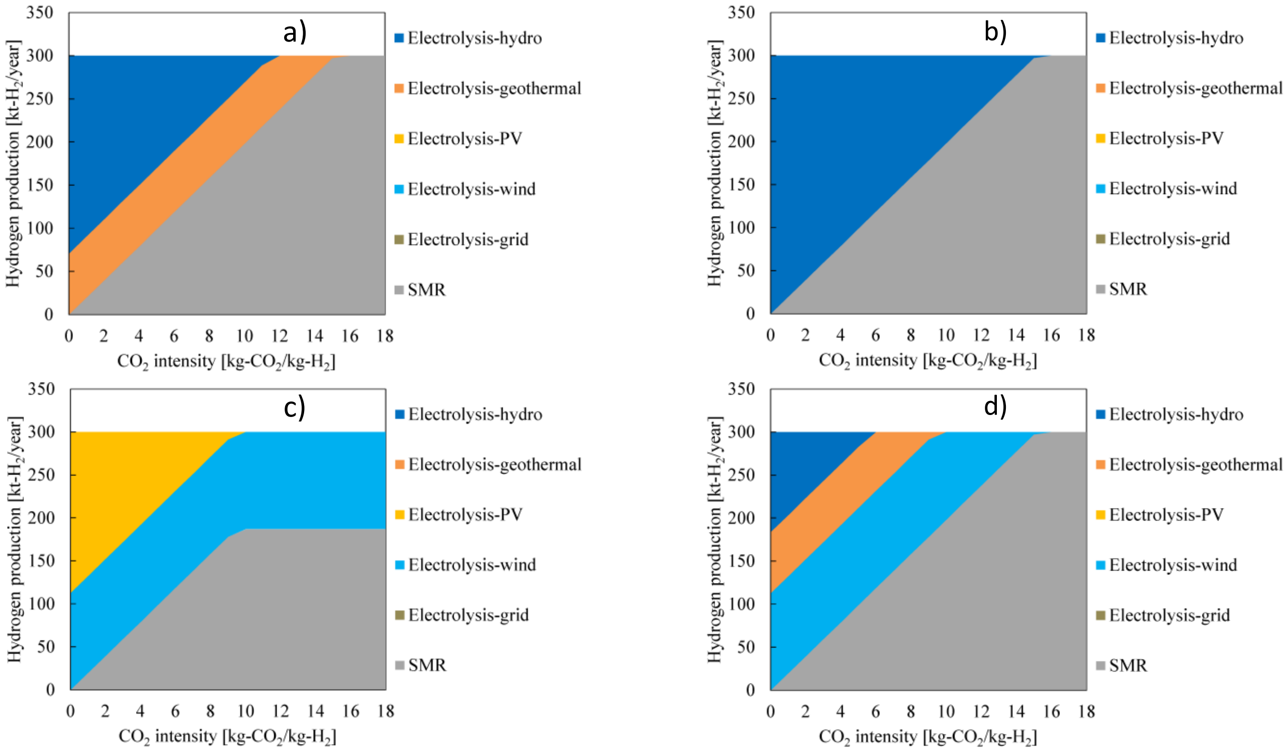

Fig 1 Hydrogen production system configuration. a) LC scenario; b) LEU scenario; c) WEC scenario; d) WECC scenario.

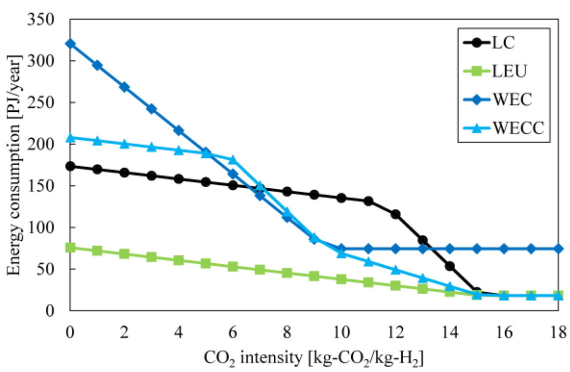

Fig 2 Energy consumption

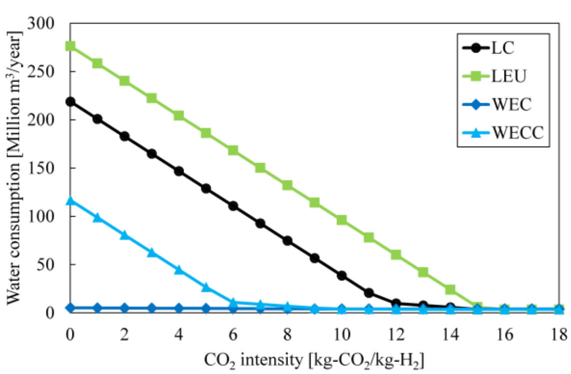

Fig 3 Water consumption

3.2 Energy consumption and water consumption

Energy consumption and water consumption are presented in Figs. 2 and 3, including energy resource production, feedstock production and hydrogen production process. In all scenarios, energy consumption increases as CO_2 intensity decreases, since SMR is replaced with electrolysis, which has a larger specific energy consumption for hydrogen production. Additionally, renewable electricity generation consumes more energy than natural gas production, contributing to the increase of energy consumption for hydrogen production on a Well to Wheel basis. Differences across scenarios using electrolysis are explained by energy consumption associated with electricity generation.

Water consumption increases as the CO_2 intensity constraint decreases; since SMR is replaced with electrolysis, which has larger water consumption for hydrogen production; and renewable electricity generation consumes more water than natural gas production, excepting wind electricity and solar PV electricity.

3.3 Hydrogen production cost

The specific cost of hydrogen production is presented in Fig. 4. The cost of hydrogen production in all scenarios increases as the CO_2 intensity decreases; as SMR is replaced by electrolysis using renewable electricity, which has higher energy costs, higher capital costs and lower capacity factors than natural gas.

The LC scenario has the lowest cost for hydrogen production, going from 1.59 to 8.81 USD/kg-H_2 when the CO_2 intensity decreases from 18 to 0 kg-CO_2/kg-H_2. Prioritizing the WEC nexus has the largest cost for hydrogen production, going from 5.03 to 13.6 USD/kg-H_2 when the CO_2 intensity decreases from 18 to 0 kg-CO_2/kg-H_2. In contrast, prioritizing the WEC nexus and cost simultaneously causes a smaller increase in the cost for hydrogen production, 1.59 to 9.23 USD/kg-H_2 when the CO_2 intensity decreases from 18 to 0 kg-CO_2/kg-H_2.

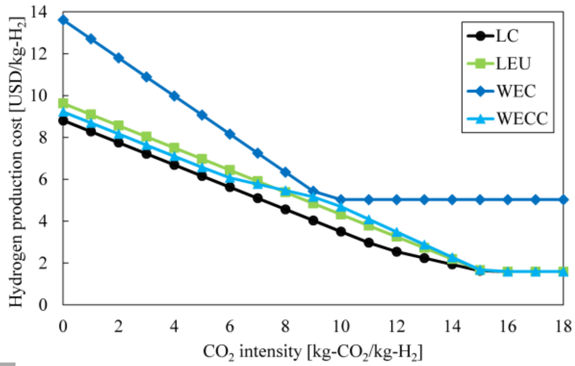

Fig 4 Specific cost for hydrogen production

4. CONCLUSIONS

- SMR is used in all scenarios to produce hydrogen as much as the CO_2 intensity constraint allows; accounting for more than 50% of hydrogen production for CO_2 intensities higher than 8 kg-CO_2/kg-H_2 in all scenarios. For lower CO_2 intensities, electrolysis using renewable electricity is preferred.
- Energy consumption, water consumption and cost increase in all scenarios as CO_2 intensity decreases, since electrolysis using renewable energy has higher energy consumption, higher water consumption and higher cost than SMR.
- Producing hydrogen with a maximum CO_2 intensity of 18 kg-CO_2/kg-H_2 can be achieved at a specific cost for hydrogen production as low as 1.59 USD/kg-H_2. Zero-emission hydrogen production is significantly more expensive, with the specific cost for hydrogen production ranging between 9.23 and 13.6 USD/kg-H_2.

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