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Optimum Design of a Hydrogen Production System Under Different Constraints for CO_2 Emissions

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ABSTRACT

An optimization model is used to design a hydrogen production system under different constraints for CO_2 emissions, focusing on Japan as case of study. Two scenarios were considered: Base scenario, focusing on minimizing cost; and WEC scenario focusing on balancing energy use, water use and CO_2 emissions. Domestic natural gas alone is not enough to produce 1 Mt-H_2/year and electrolysis is used for all CO_2 intensities. For low CO_2 intensities, Base scenario uses hydroelectricity and geothermal electricity; while WEC scenario uses solar electricity and wind electricity. Zero-emission hydrogen production needs installed capacities for electrolyzers of 8.45 and 30.3 GW in Base and WEC scenarios, respectively.

Keywords: Hydrogen Production System, Hydrogen, Water-Energy-Carbon Nexus, Hydrogen Economy

NONMENCLATURE

Abbreviations	
CTG	Craddle to gate
LP	Linear programming
SMR	Steam methane reforming
Symbols	
α	Share of a given hydrogen production route in total hydrogen production
c	Category for evaluation
Dmd	Hydrogen demand
j	Hydrogen production route
S	Normalized indicator
w	Weighting coefficient
Z	Overall score hydrogen production

1. INTRODUCTION

As energy carrier, hydrogen is expected to play an important role in the transition to a decarbonized energy system[1]; particularly in sectors such as transportation, industry and buildings[2]. Transition to an energy system where hydrogen is used at the same scale that fossil fuels are used in the present requires the development of infrastructure for producing, transporting and storing hydrogen. Nevertheless, lack of development of hydrogen infrastructure is a barrier to widespread use of hydrogen in the energy system[3].

Research about the hydrogen supply chain is extensive, with most of the studies focusing on designing or evaluating hydrogen supply chains and hydrogen production systems considering CO_2 emissions, energy use and cost [4–9]. However, these studies did not take water use into account.

More recently, several studies considered water use as feedstock [10,11]; and the nexus between water use, energy use and CO_2 emissions in hydrogen production [12]. These studies contribute to designing sustainable hydrogen supply chains that reduce CO_2 emissions in the energy system without increasing pressure on water supply. This research follows that direction and aims to contribute to the assessment of the water-energy-carbon nexus in the design of hydrogen supply chains by analyzing the effect of the CO_2 emissions constraint on the optimum design of a hydrogen production system.

The objective of this research is to determine the optimum design of a hydrogen production system under different constrains for CO_2 emissions; focusing on Japan in 2030 as case of study. The rest of the paper is organized as follows: methods used to design the hydrogen production system are presented in section 2; results for the hydrogen system design are presented

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and discussed in section 3; and conclusions are presented in section 4.

2. METHODS

2.1 Hydrogen production system

As shown in Fig. 1, hydrogen production was assessed on a cradle to gate (CTG) basis, considering hydrogen production process, production of feedstock and production of energy carriers.

Hydrogen can be produced using steam methane reforming (SMR) or electrolysis. In that sense, feedstock used in hydrogen production corresponds to natural gas and water. SMR uses natural gas and grid electricity as energy carriers; while energy resources used to generate electricity used in electrolysis are sunlight, wind, geothermal energy and water. In addition, grid electricity can also be used in electrolysis.

2.2 Model formulation

A static bottom-up linear programming (LP) optimization model developed in the General Algebraic Modeling Systems (GAMS) software was used. The optimization model was solved using the solver CPLEX. The complete model formulation is presented in [12]. A brief description of the model is presented below. The model estimates the optimum share of each hydrogen production route in total hydrogen production, considering simultaneously energy consumption, water consumption, CO_2 emissions and cost, as indicated in Eqs. (1, 2).

$$Z = \sum_j \sum_c \propto_j S_{j,c} w_c \quad (1)$$

$$\propto_j = \frac{H_{2,j}}{Dmd} \quad (2)$$

Similar to Acar and Dincer [13], simultaneous optimization of the hydrogen production system considering these four categories is performed using a normalized indicator that evaluates how each hydrogen production route performs against the best performer in each category. The normalized indicator is estimated using Eq. (3).

$$S_{j,c} = \frac{Maximum_c - Attribute_{j,c}}{Maximum_c - Minimum_c} \quad (3)$$

The objective function described in Eq. (1) is solved under the following constraints:

1. Non-negativity constraint for α_j.
2. Hydrogen production demand must be satisfied.
3. Feedstock used cannot exceed the maximum available amount of feedstock.
4. Energy carriers used cannot exceed the maximum amount of energy carriers available.

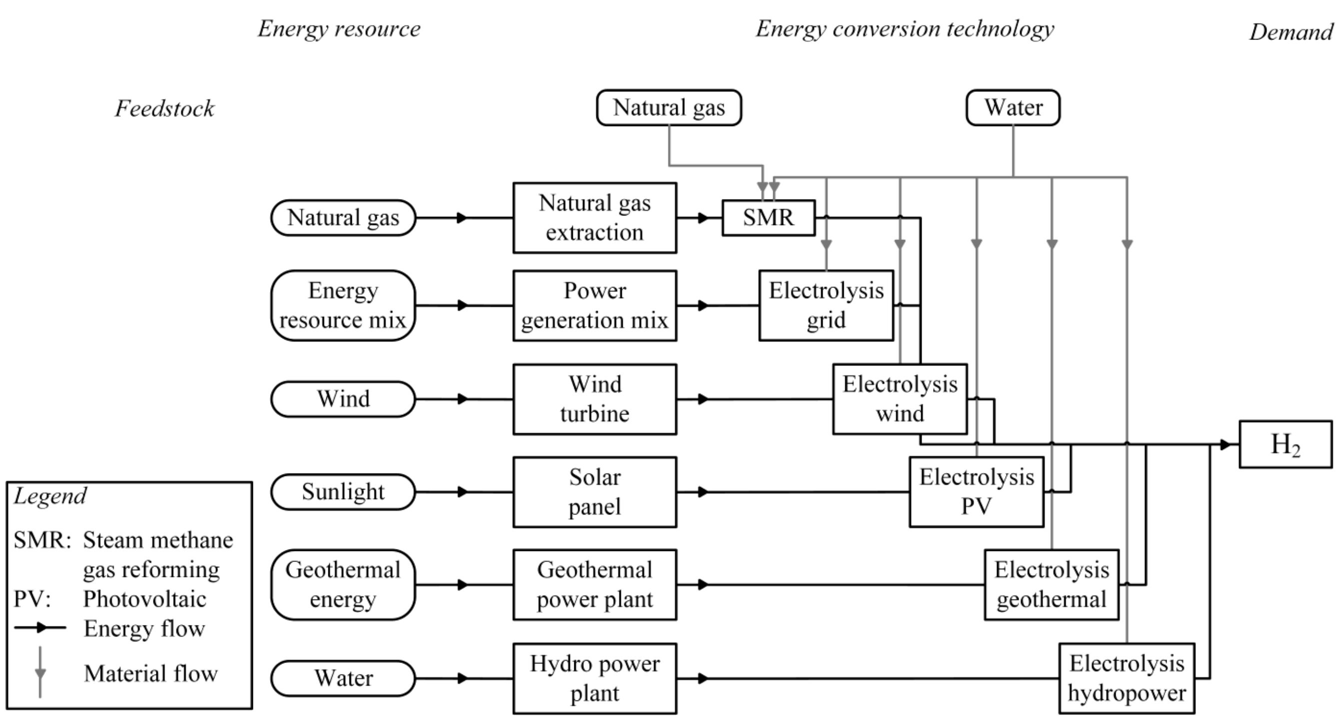


Fig. 1. System boundary in hydrogen production assessment on a cradle to gate basis

5. Combinations of feedstocks, energy carriers and hydrogen production technologies that are not feasible are excluded.
6. CO_2 intensity for hydrogen production cannot exceed the maximum CO_2 intensity constraint.

2.3 Scenarios for hydrogen production in Japan

As part of the efforts to mitigate climate change, Japan aims to promote the widespread use of hydrogen in the energy system. In 2017, the Japanese government formulated the first national strategy to promote the use of hydrogen on a large scale in the national energy system "Basic Hydrogen strategy"[14]; targeting the supply of 0.3 Mt-H_2/year by 2030. In 2021, the Sixth Strategic Energy Plan updated this target from 2 Mt-H_2/year used in 2020 (mostly in the industrial sector) to 3 Mt-H_2/year by 2030; [15]. The target of hydrogen supply as energy carrier is 1 Mt-H_2/year; corresponding to 0.8 Mt-H_2/year to achieve 1% share in electricity production by co-firing hydrogen and/or ammonia in existing thermal power plants; and 0.2 Mt-H_2/year for use in fuel cell vehicles [16]. The newest revision of the "Basic Hydrogen Strategy" was made in June 2023, keeping the target of 1% share of hydrogen and/or ammonia use in electricity generation[17]. However, the target for hydrogen use in mobility was not set explicitly. In this research, hydrogen demand was set in 1 Mt-H_2/year, keeping the target set in the Sixth Energy Strategic Plan.

Two scenarios that represent different priorities in the design of the hydrogen production system were considered: Base scenario and WEC scenario. The Base scenario uses a value of 1.0 for the weighting coefficient of cost and zero for all the other categories in the objective function in Eq. (1). The Base scenario focuses on achieving the lowest cost for the hydrogen production system, without considering energy consumption, water consumption or CO_2 emissions. It represents the business as usual scenario. The WEC scenario uses a value of 1/3 for the weighting coefficients of energy consumption, water consumption and CO_2 emissions and zero for cost in the objective function in Eq. (1). The WEC scenario focuses on achieving a balance between energy use, water use and CO_2 emissions in the design of the hydrogen system, without considering cost.

The optimum design of the hydrogen production system was estimated for CO_2 intensities between 0 and 18 kg-CO_2/kg-H_2 on a CTG basis, using steps of 1 kg-CO_2/kg-H_2. 18 kg-CO_2/kg-H_2 corresponds to the maximum value of the CO_2 intensity for the hydrogen production system for the hydrogen production routes considered. Since grid electricity is used for water processing, the minimum value for the CO_2 intensity was 0.007 kg-CO_2/kg-H_2. This value was considered 0 kg-CO_2/kg-H_2 in the calculations.

2.4 Input data

With the aim of improving energy security, it was assumed that only domestic energy resources are used for hydrogen production. Natural gas availability was estimated in 2.29 Mt-natural gas/year, based on [18,19]. Water availability was limited to 1.11 billion m^3-H_2O/year; corresponding to 10% of water consumption in the industrial sector, based on [20]. Main characteristics of hydrogen production routes are presented in Table 1.

All costs were estimated in 2017 USD. The average exchange rate for the Fiscal Year 2017 of 112.1 JPY/USD was used [21]. Feedstock costs were 0.203 USD/m^3-H_2O for water [22] and 0.437 USD/kg-natural gas for natural gas [23]. Service lives for SMR and electrolysis were assumed equal to 25 and 10 years, respectively. A

Table 1. Main characteristics of hydrogen production routes. Estimated using data from [18,23,24,27–32].

		Electrolysis				
	SMR	Grid	Wind	Solar PV	Geothermal	Hydro
Natural gas consumption [MJ/kg-H_2]	46.3	0	0	0	0	0
Grid electricity consumption [MJ/kg-H_2]	2.1	195	0	0	0	0
Wind electricity consumption [MJ/kg-H_2]	0	0	195	0	0	0
Solar electricity consumption [MJ/kg-H_2]	0	0	0	195	0	0
Geothermal electricity consumption [MJ/kg-H_2]	0	0	0	0	195	0
Hydroelectricity consumption [MJ/kg-H_2]	0	0	0	0	0	195
Natural gas yield [kg-H_2/kg-natural gas]	0.5	0	0	0	0	0
Water yield [kg-H_2/m^3]	110	64.4	64.4	64.4	64.4	64.4
Capacity factor [-]	0.90	0.97	0.19	0.12	0.78	0.52
Electricity price [USD/GJ]	-	35.7	38.7	52.0	27.0	42.7
Capital cost [USD/kW]	121	800	800	800	800	800

discount rate of 10% was used to annualize the capital costs of SMR and electrolysis throughout their services lives. Operating and maintenance costs of 0.212 and 0.150 USD/kg-H_2 were assumed for SMR and electrolysis, respectively [24,25].

Natural gas production emits 2.29 kg-CO_2/kg-natural gas [19]. Water production emits 0.453 kg-CO_2/m^3-H_2O, (only grid electricity is used in water production). Grid electricity has a CO_2 emission factor of 0.142 kg-CO_2/MJ [26]; while renewable electricity generation has zero CO_2 emissions. Hydrogen production process for SMR emits 8.34 kg-CO_2/kg-H_2 [27]; while electrolysis has zero CO_2 emissions.

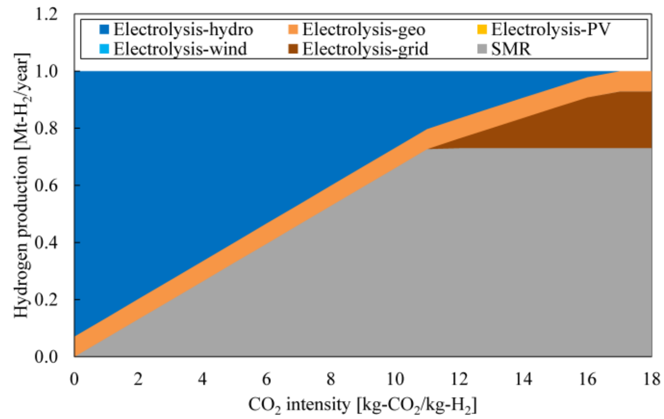
3. RESULTS

3.1 Optimum desing of the hydrogen production system

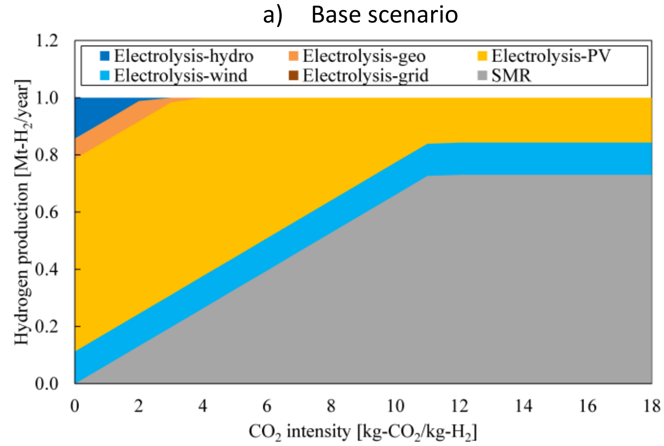
The optimum designs of the hydrogen production system for CO_2 intensities between 0 and 18 kg-CO_2/kg-H_2 for the Base and WEC scenarios are presented in Fig. 2. All natural gas available is used in SMR to produce hydrogen for CO_2 intensities higher than 11 kg-CO_2/kg-H_2 in both scenarios. For lower values, SMR is replaced by electrolysis using renewable electricity as the CO_2 intensity constraint becomes stricter. In the Base scenario, geothermal electricity and hydroelectricity are the preferred sources of electricity; while in the WEC scenario solar PV electricity and wind electricity are utilized. However, due to limitations in the availability of solar PV electricity, geothermal electricity and hydroelectricity are also used as electricity sources for CO_2 intensity constraints lower than 3 kg-CO_2/kg-H_2.

The resulting installed capacity for the hydrogen production system is shown in Fig. 3. As general trend, installed capacity for the hydrogen production system increases as the CO_2 intensity decreases due to the substitution of SMR with electrolysis using renewable electricity, which has lower capacity factors than SMR. In the Base scenario, installed capacity varies between 4.98 to 8.45 GW when CO_2 intensity decreases from 18 to 0 kg-CO_2/kg-H_2; with installed capacity for electrolyzers increasing from 1.33 to 8.45 GW. In the WEC scenario, installed capacity increases from 12.3 to 30.3 GW when CO_2 intensity decreases from 18 to 0 kg-CO_2/kg-H_2; while installed capacity for electrolyzers increases from 8.69 to 30.3 GW. Shifting the priorities in the design of the hydrogen production system from cost minimization to achieving balance between energy use, water use and CO_2 emissions causes an increase in the installed capacity as solar PV electrolysis and wind electrolysis have lower capacity factors than hydro electrolysis and geothermal electrolysis.

From the point of view of policy making, the Japanese government set the target of reaching an installed capacity for electrolyzers of 15 GW by 2030 [17]. In the Base scenario, zero-emission hydrogen production is possible with this installed capacity for electrolyzers. However, in the WEC scenario, the minimum CO_2 intensity possible is about 9 kg-CO_2/kg-H_2. This highlights the necessity to increase the installed



a) Base scenario



b) WEC scenario

Fig. 2. Optimum share of hydrogen production routes

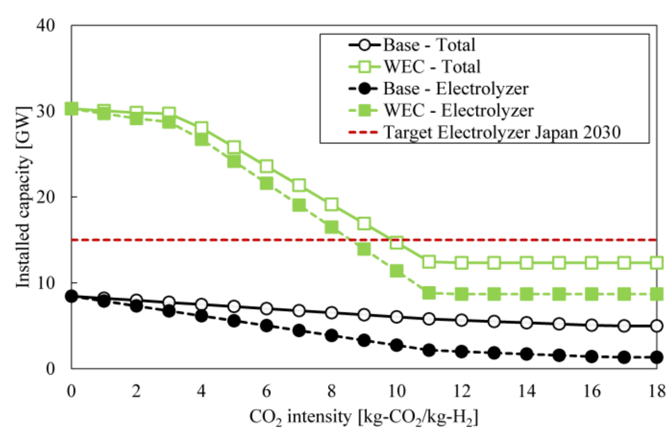


Fig. 3. Installed capacity

capacity of electrolyzers and improve the low capacity factors for electricity generation using solar PV and wind.

3.2 Energy consumption

Energy consumption associated with hydrogen production is presented in Fig. 4. In general terms, energy consumption increases as the CO_2 intensity decreases. This occurs due to the larger values for energy consumption in energy carrier production and hydrogen production process of electrolysis using renewable electricity compared with SMR.

However, in the Base scenario, as slight reduction in energy consumption from 259 to 211 PJ/year was observed when the CO_2 intensity decreased from 18 to 11 kg-CO_2/kg-H_2. This is caused by the substitution of electrolysis using grid electricity with electrolysis using hydroelectricity, which has lower energy consumption for energy carrier production. As the CO_2 intensity decreases from 11 to 0 kg-CO_2/kg-H_2, energy consumption increases from 211 to 351 PJ/year. Shifting the priority from minimizing cost to achieving balance energy use, water use and CO_2 emissions in the hydrogen production system design causes the increase of energy consumption. In the WEC scenario energy consumption remains constant at 328 PJ/year as the CO_2 intensity decreases from 18 to 11 kg-CO_2/kg-H_2, since the optimum configuration of the hydrogen production system in this range of CO_2 intensities is not changed. As the CO_2 intensity decreases from 11 to 0 kg-CO_2/kg-H_2, energy consumption increases from 328 to 1141 PJ/year. The latter value is 3.3 times the energy consumption in the Base scenario for zero-emission hydrogen production.

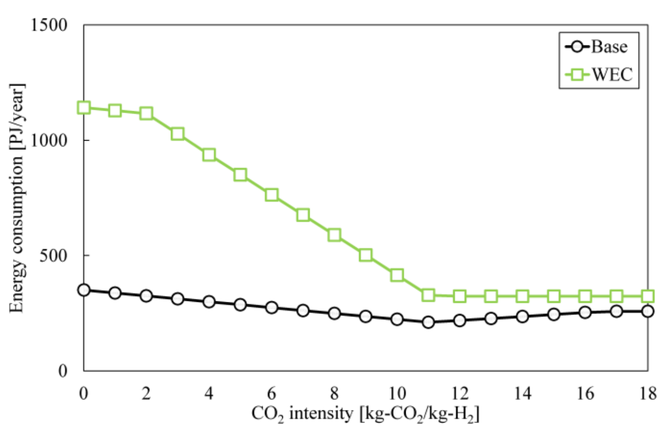


Fig. 4. Energy consumption

3.3 Specific cost of hydrogen production

The specific cost of hydrogen production is presented in Fig. 5. In general terms, specific cost of hydrogen production increases as the CO_2 intensity decreases. This occurs due to the higher energy cost for renewable electricity compared with natural gas; and due to the lower capacity factors for electrolysis using renewable electricity compared with SMR, which requires larger installed capacities to achieved the same hydrogen production.

In the Base scenario, the specific cost of hydrogen production increases from 3.14 to 9.39 USD/kg-H_2 as the CO_2 intensity decreases from 18 to 0 kg-CO_2/kg-H_2. In the WEC scenario, specific cost of hydrogen production remains constant at 4.84 USD/kg-H_2 for CO_2 intensities between 11 and 18 kg-CO_2/kg-H_2, since the optimum configuration of the hydrogen production system is the same. As the CO_2 intensity decreases from 11 to 0 kg-CO_2/kg-H_2, the specific cost of hydrogen production increases from 4.84 to 13.3 USD/kg-H_2. The latter value is 1.4 times the specific cost of hydrogen production for zero emission hydrogen production in the Base scenario.

The Japanese government target for hydrogen supply cost in 2030 was set at 30 JPY/Nm^3 [15], which corresponds to 3.19 USD/kg-H_2. This target seems difficult to achieve in both the scenarios, considering that 1) the specific cost of hydrogen production in the Base scenario is already at 3.14 USD/kg-H_2 for a CO_2 intensity of 18 kg-CO_2/kg-H_2; 2) the specific cost of hydrogen production increases as the CO_2 intensity decreases; and 3) shifting the priority in hydrogen system design from cost minimization to achieving balance between energy use, water use and CO_2 emissions increases the specific cost of hydrogen production. Achieving the government target seems more difficult when the costs associated to hydrogen transport and storage are considered, since the costs estimated in this research correspond only to hydrogen production.

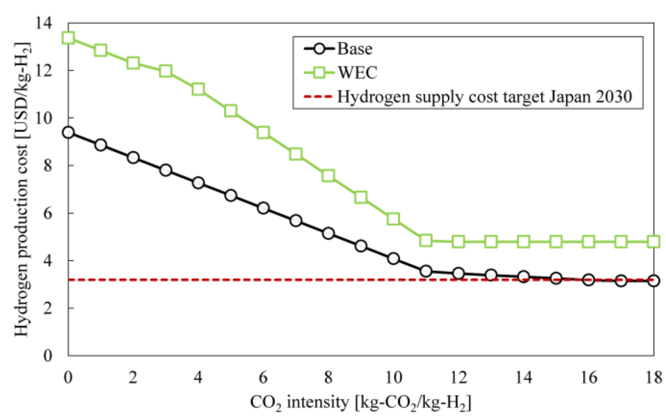


Fig. 5. Specific cost of hydrogen production

3.4 Water consumption

Water consumption is presented in Fig. 6. In general terms, water consumption increases as the CO_2 intensity decreases. This is explained by the higher water consumption in energy carrier production for hydroelectricity and geothermal electricity compared with natural gas; and the higher water consumption in hydrogen production process of electrolysis compared with SMR.

In the Base scenario, water consumption goes from 44.4 to 864 Mm^3-H_2O/year as the CO_2 intensity decreases from 18 to 0 kg-CO_2/kg-H_2. In the WEC scenario, water consumption increase is more moderate, going from 13.2 to 18.0 Mm^3-H_2O/year as the CO_2 intensity decreases from 18 to 3 kg-CO_2/kg-H_2. Since solar PV electricity and wind electricity are not enough to produce all the hydrogen required, geothermal electricity and hydroelectricity are used in electrolysis for CO_2 intensities lower than 3 kg-CO_2/kg-H_2. This causes water consumption to increase from 18.0 to 154 Mm^3-H_2O/year as the CO_2 intensity decreases from 3 to 0 kg-CO_2/kg-H_2. For zero-emission hydrogen production, water consumption in the Base scenario is 5.6 times the value for the WEC scenario.

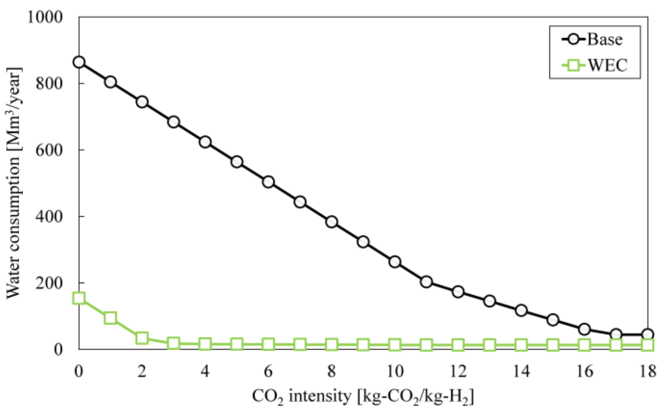


Fig. 6. Water consumption

With the aim of assessing the economic impact of considering the Water-Energy-Carbon nexus on the design of the hydrogen production system, an indicator that quantifies the cost of reducing water consumption in the design of the hydrogen production system is introduced here. The cost of water saved, as defined by Eq. (4). It corresponds to the cost of reducing water consumption in hydrogen production in one unit. This concept is similar to the cost of CO_2 abatement.

$$Cost\ water\ saved = \frac{Cost_{WEC} - Cost_{Base}}{Water_{Base} - Water_{WEC}} \quad (4)$$

Results for the cost of water saved are shown in Fig. 7. The cost of water saved tends to decrease as the CO_2 intensity decreases in the WEC scenario. This is explained by the increase of penetration of hydro electrolysis in hydrogen production in the Base scenario as the CO_2 intensity decreases. It is cheaper to save water for lower CO_2 intensities than for higher CO_2 intensities in the WEC scenario. This can create a synergistic effect where water consumption reduction is pursued simultaneously with CO_2 emissions reduction in the design of the hydrogen production system.

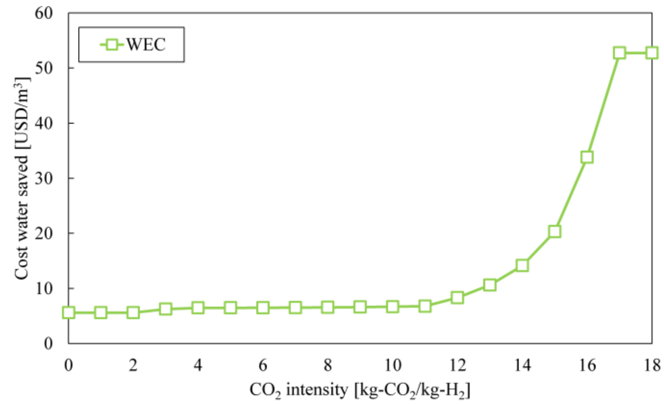


Fig. 7. Cost of saved water

4. CONCLUSIONS

In this research, a static bottom-up LP optimization model that considers simultaneously energy consumption, water consumption, CO_2 emissions and cost was used to analyze the effect of the CO_2 emissions constraint on the optimum design of a hydrogen production system; focusing on Japan in 2030 as case of study. Two scenarios were considered: the Base scenario, focusing on minimizing cost; the WEC scenario, focusing on achieving balance between energy use, water use and CO_2 emissions. Main conclusions are presented below:

1) All natural gas available is utilized to produce hydrogen using SMR for CO_2 intensities higher than 11 kg-CO_2/kg-H_2, complemented with electrolysis since natural gas alone is not enough to produce 1 Mt-H_2/year. As the CO_2 intensity decreases, SMR is replaced by electrolysis using geothermal electricity and hydroelectricity in the Base scenario; and electrolysis using solar PV electricity and wind electricity in the WEC scenario.
2) Installed capacity for electrolyzers increases as the CO_2 intensity decreases; going from 1.33 to 8.45 GW when CO_2 intensity decreases from 18 to 0 kg-CO_2/kg-H_2 in the Base scenario; while in the WEC scenario increases from 8.69 to 30.3 GW. Compared with the Japanese government target of reaching an installed capacity for electrolyzers of 15 GW by 2030, zero-emission hydrogen production is possible in the Base scenario. However, in the WEC scenario

hydrogen production for CO_2 intensities lower than 9 kg-CO_2/kg-H_2 would not be possible.

3) Specific cost increases as the CO_2 intensity decreases; going from 3.14 to 9.39 USD/kg-H_2 as the CO_2 intensity decreases from 18 to 0 kg-CO_2/kg-H_2 in the Base scenario. In the WEC scenario, specific cost of hydrogen production is constant at 4.84 USD/kg-H_2 for CO_2 intensities higher equal or higher than 11 kg-CO_2/kg-H_2; and increases to 13.3 USD/kg-H_2 as the CO_2 intensity decreases to 0 kg-CO_2/kg-H_2. The target of hydrogen supply cost reaching 30 JPY/Nm^3 (3.19 USD/kg-H_2) seems difficult to achieve in the Base and WEC scenarios.
4) Water consumption tends to increase when the CO_2 intensity decreases; going from 44 to 864 Mm^3-H_2O/year as the CO_2 intensity decreases from 18 to 0 kg-CO_2/kg-H_2 in the Base scenario; while in the WEC scenario water consumption increases from 13.2 to 154 Mm^3-H_2O/year. Compared with the Base scenario, it is cheaper to save water for lower CO_2 intensities than for higher CO_2 intensities in the WEC scenario. This is caused by the high penetration of electrolysis using hydroelectricity for low CO_2 intensities in the Base scenario.

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DECLARATION OF INTEREST STATEMENT

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper. All authors read and approved the final manuscript.

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