

Techno-Economic Assessment of the impact of CO₂ Emissions Constraints on the Design of Hydrogen Production Systems[#]

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ABSTRACT

The impact of CO₂ emissions constraints on the optimum configuration of a hydrogen production system and the associated energy flows, material flows and cost was assessed; focusing on Japan as case of study. Two scenarios were considered: Base scenario, focusing on optimizing cost; and WEC+C scenario, focusing on optimizing simultaneously energy use, water use, CO₂ emissions and cost. Results show that all natural gas available is used to produce hydrogen using SMR for CO₂ intensities higher than 11 kg-CO₂/kg-H₂ in both scenarios. As CO₂ intensity decreases, SMR is replaced with electrolysis using hydroelectricity. Levelized cost of hydrogen tends to increase as CO₂ intensity decreases, reaching 9.51 USD/kg-H₂ for a CO₂ intensity of 0 kg-CO₂/kg-H₂ in both scenarios. CO₂ intensity affects energy and material flows. Reducing CO₂ intensity increases water use in the WEC+C scenario as SMR is replaced with electrolysis using hydroelectricity.

Keywords: Hydrogen, Hydrogen Production, Water-Energy-Carbon (WEC) Nexus, Levelized Cost of Hydrogen

NONMENCLATURE

Abbreviations

CTG	Cradle to gate
SMR	Steam methane reforming

Symbols

α	Hydrogen production share
c	Category for evaluation
D_{md}	Annual hydrogen demand
j	Hydrogen production route
Max	Maximum value for the attribute
Min	Minimum value for the attribute
$Prod$	Annual hydrogen production
S	Score
w	Weighting factor
Z	Overall score

1. INTRODUCTION

Adoption of hydrogen in the energy system at a large scale, as part of the strategies to achieve climate change targets, requires the production of hydrogen in different countries at the same scale as fossil fuels are produced today. These countries are likely to have different characteristics regarding availability of fossil fuels, renewable energy and water, ingredients required for the production of hydrogen, that will influence the routes selected for the production of hydrogen.

Hydrogen can be produced through a variety of routes such as coal gasification, steam methane reforming (SMR), methane pyrolysis and water electrolysis; with each route having different characteristics regarding energy use, water use, CO₂ emissions and cost.

Research regarding hydrogen production systems has focused primarily on minimizing costs and/or CO₂ emissions [1,2]. Motivated by fresh water supply concerns associated with climate change [3] and increasing population [4,5], there has been a growing interest in developing solutions for the energy system that have low CO₂ emissions and low water consumption. This has motivated researchers to consider the nexus between energy use, water use and CO₂ emissions (WEC nexus) and cost in hydrogen production [4–6]. However, previous studies have not focused on the impact of CO₂ emissions constraints on energy and material flows associated to hydrogen production.

The objective of this research is to assess the impact of CO₂ emissions constraints on the optimum configuration of a hydrogen production system and the associated energy flows, material flows and cost. Japan was considered as a case of study. The rest of the paper is organized as follows: the formulation of the hydrogen production system model is presented in section 2;

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results and discussion are presented in section 3; and conclusions are presented in section 4.

2. HYDROGEN PRODUCTION SYSTEM MODEL

2.1 Scope of the assessment

The energy system diagram is presented in Fig. 1. Hydrogen production was assessed on a cradle to gate (CTG) basis; including hydrogen production process, energy carrier production and feedstock production.

Hydrogen production using SMR and electrolysis was considered. SMR uses natural gas and water as feedstocks; and natural gas and grid electricity as energy carriers. Electrolysis uses water as feedstock; and electricity as energy carrier. Solar photovoltaic (PV), wind, geothermal, hydro and grid were considered as sources for electricity used in electrolysis.

2.2 Formulation of the optimization model

Linear programming was used to solve the allocation problem between energy carriers, feedstocks and energy conversion technologies to satisfy the hydrogen demand. The model was developed in GAMS and solved using the solver CPLEX. The complete formulation of the model can be found in [6]. A summarized description of the model is presented below.

The model estimates the optimum share of each hydrogen production route on hydrogen production on a one-year basis; optimizing simultaneously energy use, water use, CO₂ emissions and cost (Eqs. (1, 2)).

Similar to Acar and Dincer [7], a normalized indicator (Eq. (3)) is used to perform the simultaneous

optimization of the hydrogen production system in terms of energy use, water use, CO₂ emissions and cost. The normalized indicator represents how each hydrogen production route performs against the top performer in each category.

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

$$\alpha_j = \frac{Prod_j}{Dmd} \quad (2)$$

$$S_{j,c} = \frac{Max_c - Attribute_c}{Max_c - Min_c} \quad (3)$$

The objective function was solved under the following six constraints:

- 1) Non-negativity constraint
- 2) Hydrogen demand satisfaction
- 3) Feedstock availability
- 4) Energy carrier availability
- 5) Feedstock-energy- carrier-hydrogen production technology combinations that are not feasible are excluded.
- 6) CO₂ emissions constraint

2.3 Scenarios for hydrogen production in Japan

In 2020, Japan committed to achieve net zero greenhouse gas emissions by 2050. As part of the ongoing efforts to achieve this goal, the Japanese government set the target to increase hydrogen supply from 2 Mt-H₂/year in 2020 to 3 Mt-H₂/year by 2030 [8]. In 2020, hydrogen was mainly used as feedstock in industrial processes. The net 1 Mt-H₂/year increase between 2020 and 2030 corresponds to hydrogen used

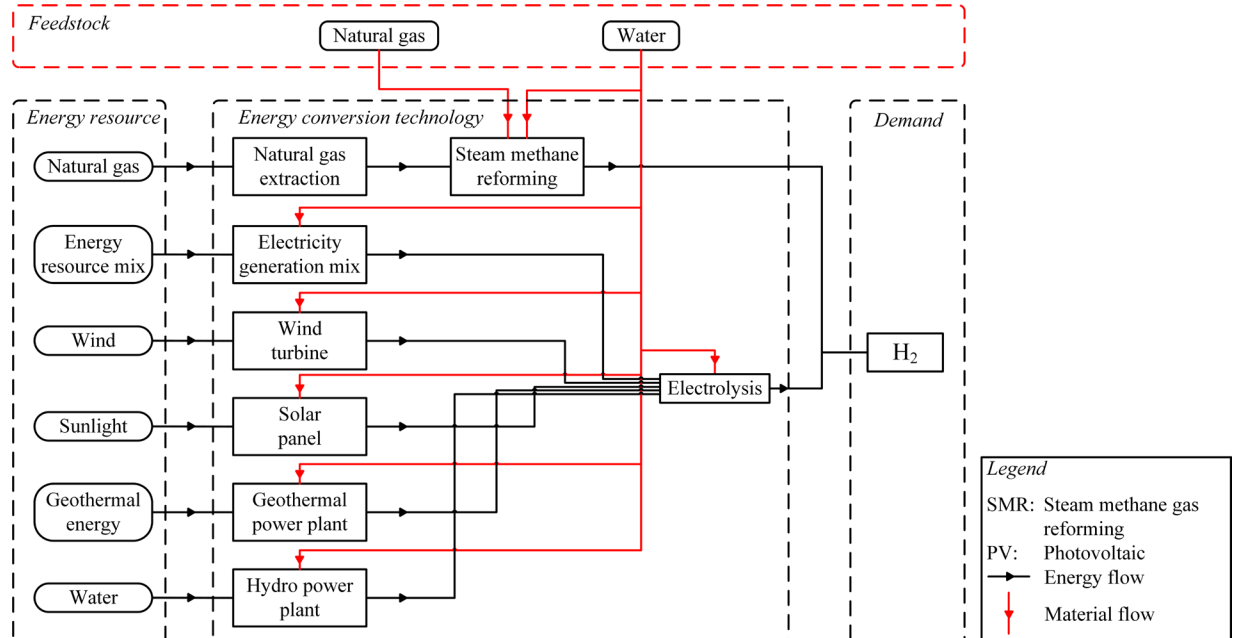


Fig. 1 Energy system diagram

as energy carrier; distributed as 0.8 Mt-H₂/year to achieve 1% of electricity production by co-firing hydrogen or ammonia in thermal power plants, and 0.2 Mt-H₂/year in the transportation sector [9]. In the same direction, the most recent ‘Basic Hydrogen Strategy’ released in June 2023 kept the 1% target for hydrogen and ammonia use in electricity generation, without specifying the target for hydrogen use in the transportation sector [10]. Focusing on hydrogen use as energy carrier in Japan in 2030, this research assumed a hydrogen demand of 1 Mt-H₂/year.

Even though challenges associated with the WEC nexus are global, the characteristics vary depending on each country or region [4]. In the case of Japan, the country is water-rich and fossil fuel-poor. Nevertheless, there are concerns about future fresh water availability due to climate change [11].

Two scenarios were considered: Base scenario and WEC+C scenario. Priorities for hydrogen production system design in each scenario are shown in Table 1. The Base scenario represents the business-as-usual situation, where cost is optimized in the design of the hydrogen production system (weighting coefficient of 1.0 for cost and 0 for energy use, water use and CO₂ emissions). The WEC+C scenario focuses on achieving sustainable development by optimizing simultaneously energy use, water use and CO₂ emissions together with cost (weighting coefficient of 0.25 for energy use, water use, CO₂ emissions and cost).

Table 1 Priorities for hydrogen production system design in each scenario

	Cost	Energy	Water	Carbon
Base	▲▲▲▲			
WEC+C	▲	▲	▲	▲

Only domestic resources were considered for hydrogen production, aiming to improve energy security.

The amount of available water was assumed equal to 10% of industrial water consumption, 1.11 Billion m³-H₂O/year [12]; while the amount of natural gas available was assumed equal to 2.29 Mt-natural gas/year [13]. Feedstock costs were assumed equal to 0.203 USD/m³-H₂O [14] and 0.437 USD/kg-natural gas [15] for water and natural gas, respectively.

Capital costs for SMR and electrolysis were assumed equal to 121 [16] and 800 USD/kW [17], respectively. Capital costs were annualized utilizing a discount rate of 10%. Service lives of 25 and 10 years were assumed for SMR and electrolysis, respectively. Operating and maintenance costs of 0.212 USD/kg-H₂ for SMR, and 0.150 USD/kg-H₂, for electrolysis were used [16,18]. Main characteristics of hydrogen production routes are presented in Table 2.

CO₂ emission factors for natural gas production and water production were assumed equal to 2.29 kg-CO₂/kg-natural gas [19] and 0.453 kg-CO₂/m³-H₂O, respectively. Grid electricity generation emits 0.142 kg-CO₂/MJ [20]; while CO₂ emissions for renewable electricity are zero. Hydrogen production through SMR produces 8.34 kg-CO₂/kg-H₂ [17]; while CO₂ emissions for hydrogen production using electrolysis are zero.

2.4 Main assumptions and limitations

All calculations were performed on a one-year basis, using the Fiscal Year 2017 as base year. Water consumption associated with energy carrier production includes water evaporated and water transpired. Water consumption was limited to ‘operational water consumption’, excluding water embedded in equipment and materials used to fabricate energy conversion technologies and feedstock production technologies. Water purification to meet water purity requirements for electrolysis was not considered.

Table 2 Main characteristics of hydrogen production routes. Built using data from [13,16,17,21–25]

		SMR	Electrolysis				
			Grid	Wind	Solar PV	Geothermal	Hydro
Feedstock consumption [kg/kg-H ₂]	Water	9.09	15.5	15.5	15.5	15.5	15.5
	Natural gas	2.0	-	-	-	-	-
Energy consumption [MJ/kg-H ₂]	Natural gas	46.3	-	-	-	-	-
	Grid electricity	2.1	195	-	-	-	-
	Wind electricity	-	-	195	-	-	-
	Solar electricity	-	-	-	195	-	-
	Geothermal electricity	-	-	-	-	195	-
	Hydroelectricity	-	-	-	-	-	195
Capacity factor [-]		0.90	0.97	0.19	0.12	0.78	0.52
Electricity price [USD/GJ]		35.7	35.7	38.7	52.0	27.0	42.7

3. RESULTS AND DISCUSSION

3.1 Hydrogen production system configuration

The impact of CO₂ emissions constraints on hydrogen production share is shown in Fig. 2. The x axis represents the constraint on CO₂ emissions for hydrogen production expressed in terms of CO₂ emissions per unit H₂ produced, known as CO₂ intensity. As values for CO₂ intensity decrease from 18 to 0 kg-CO₂/kg-H₂, the enforcement of CO₂ emissions constraints necessary to achieve net zero GHG emissions targets is represented.

All natural gas available is used in the production of hydrogen using SMR for CO₂ intensities higher than 11 kg-CO₂/kg-H₂ in both scenarios. Due to its high availability factor, grid electricity is selected in the Base scenario for CO₂ intensities higher than 11 kg-CO₂/kg-H₂; while in the WEC+C scenario electrolysis using hydroelectricity and wind electricity are used. Reducing the CO₂ intensity under 11 kg-CO₂/kg-H₂ replaces SMR with electrolysis using hydroelectricity in both scenarios.

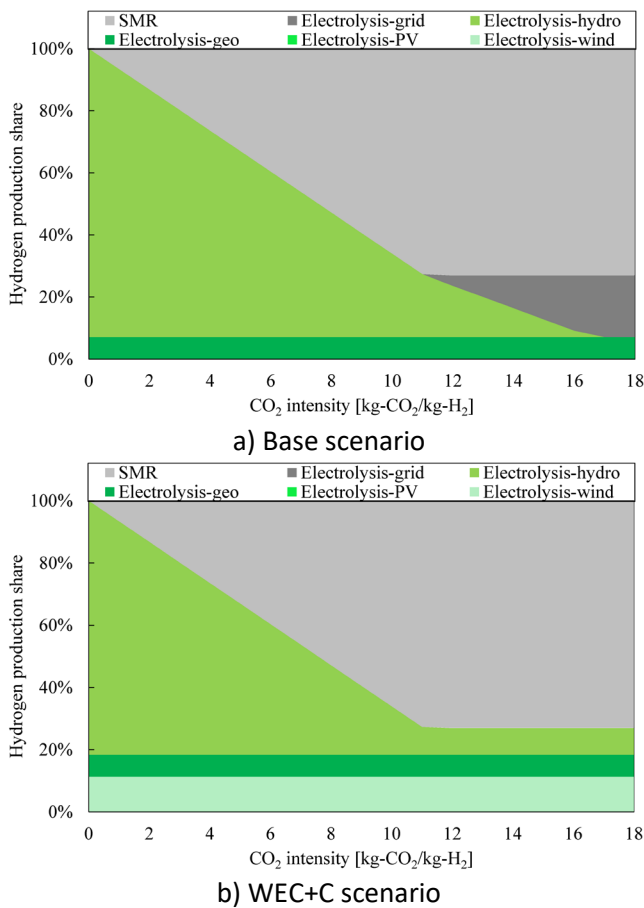


Fig. 2 Hydrogen production share

Installed capacity is shown in Fig. 3. In both scenarios, installed capacity increases as CO₂ intensity

decreases from 18 to 0 kg-CO₂/kg-H₂, driven by penetration of electrolysis using renewable energy, which has lower availability factors and higher energy costs than SMR. The Japanese government targets installing 15 GW of electrolyzers by 2030 [10]. Producing hydrogen using electrolysis with hydro, geothermal and wind electricity makes possible to produce 1 Mt-H₂/year with zero emissions by 2030 with an installed capacity for electrolyzers of 10 GW.

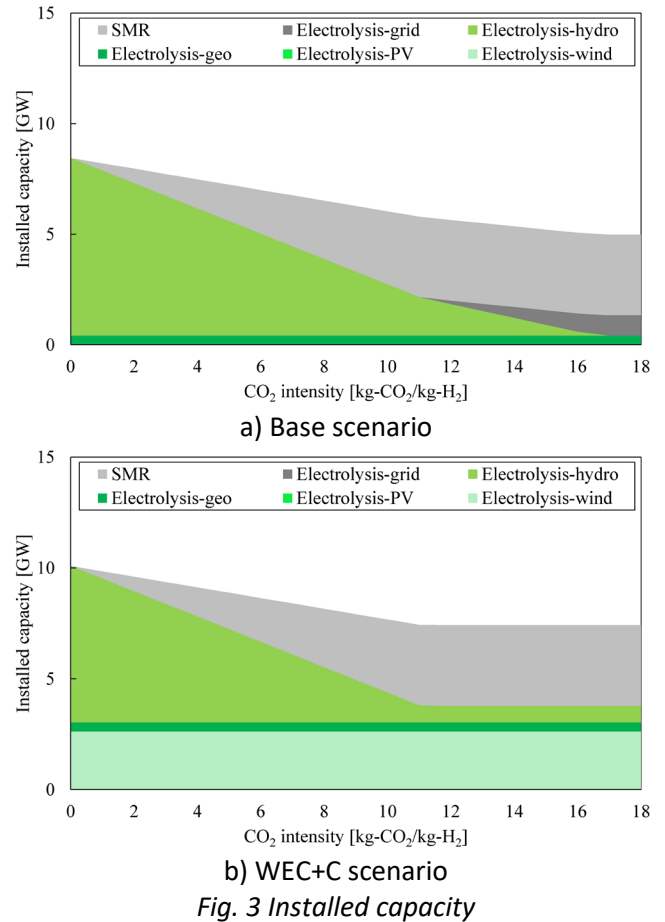


Fig. 3 Installed capacity

3.2 Economic assessment

Levelized cost of hydrogen (LCOH) is presented in Fig. 4. In both scenarios, LCOH tends to increase as CO₂ intensity decreases. In the Base scenario, the increase is moderate for CO₂ intensities between 18 and 11 kg-CO₂/kg-H₂; and becomes steeper for lower CO₂ intensities. In the WEC+C scenario, LCOH remains constant for CO₂ intensities between 18 and 11 kg-CO₂/kg-H₂; and decreases following a trend similar to the Base scenario for lower CO₂ intensities. Energy costs accounts for the largest share of LCOH in both scenarios, followed by capital costs. The share of energy costs in LCOH increases as CO₂ intensity decreases in both

scenarios; reaching 87 and 85% for zero emissions hydrogen in the Base scenario and WEC+C scenario, respectively.

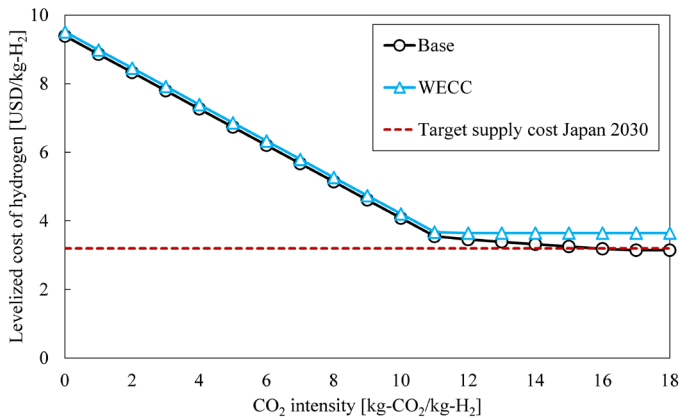


Fig. 4 Levelized cost of hydrogen

3.3 Energy and material flows

CO₂ emissions constraints will affect energy and material flows associated with hydrogen production. For example, energy and material flows for hydrogen

production on a CTG basis for the WEC+C scenario for CO₂ intensities of 18 and 0 kg-CO₂/kg-H₂ are presented in Figs. 5 and 6, respectively. CO₂ intensity reduction causes the shift from SMR to electrolysis using hydroelectricity. This causes a significant increase in water consumption, explained by evaporation losses in dams associated with hydroelectricity generation. In addition, energy consumption increases, due to higher specific energy consumption for electrolysis compared with SMR and energy consumption for energy carrier production for hydroelectricity compared with natural gas.

4. CONCLUSIONS

In this research a linear programming model that optimizes simultaneously energy use, water use, CO₂ emissions and cost was used to estimate the optimum configuration of a hydrogen production system and the associated energy flows, material flows and cost. Main conclusions are presented below:

- 1) All natural gas available is utilized to produce hydrogen using SMR for CO₂ intensities higher than 11 kg-CO₂/kg-H₂ in the Base scenario and WEC+C scenario. As CO₂ intensity decreases,

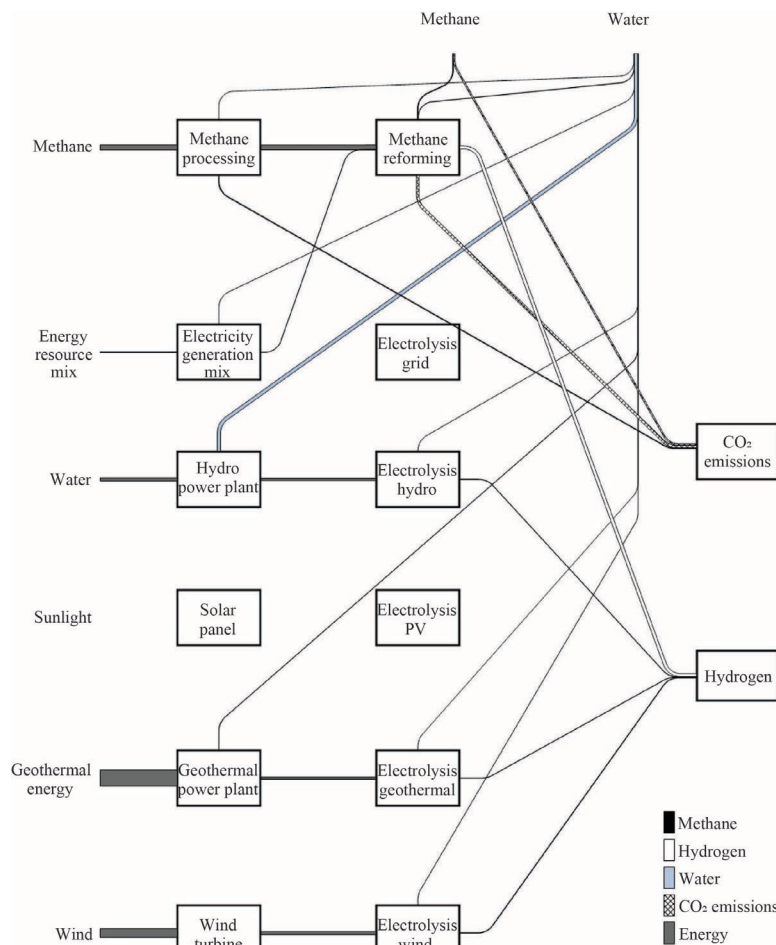


Fig. 5 Energy and material flows in the system for the WEC+C scenario for CO₂ intensity of 18 kg-CO₂/kg-H₂

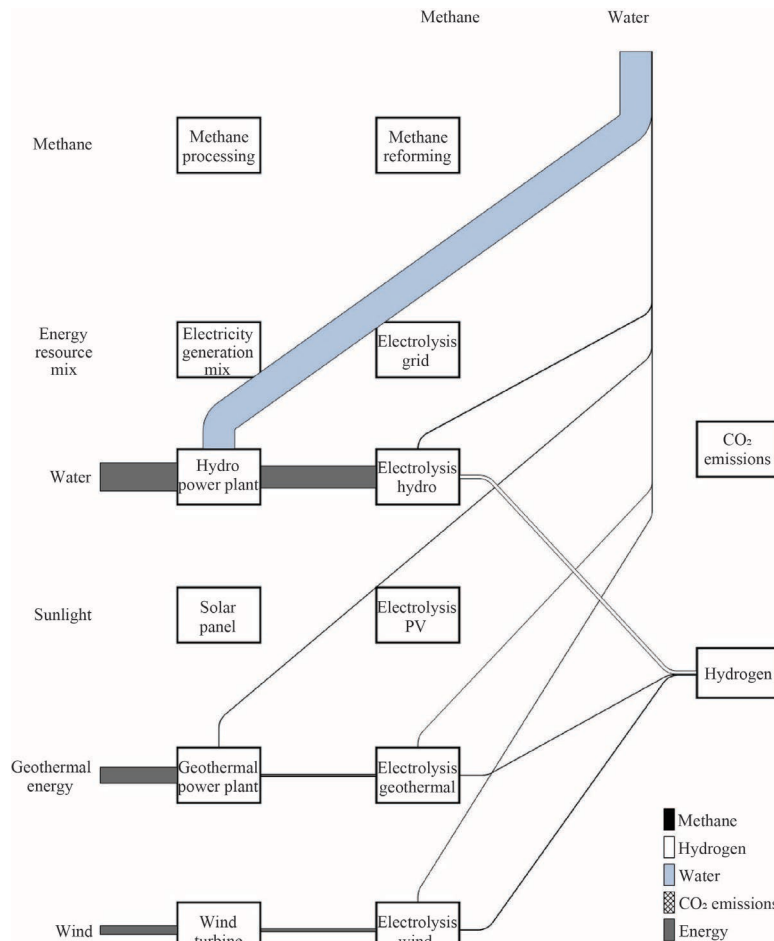


Fig. 6 Energy and material flows in the system for the WEC+C scenario for CO₂ intensity of 0 kg-CO₂/kg-H₂

SMR is replaced by electrolysis using hydroelectricity.

- 2) LCOH tends to increase as CO₂ intensity increases in the Base scenario and WEC+C scenario. LCOH increase becomes steeper for CO₂ intensities lower than 11 kg-CO₂/kg-H₂.
- 3) Reduction of CO₂ intensity affects energy and material flows associated with hydrogen production. In the WEC+C scenario, reducing CO₂ intensity causes an increase of water use, mainly associated to hydroelectricity production.

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