

Article

Regional Assessment of Hydrogen Production and Use in the Intermountain West United States

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Abstract

Given the large natural gas (NG) reserves of the Intermountain West (I-WEST) region in the USA, it can emerge as a leader in hydrogen (H₂) production. Currently, H₂ production via steam methane reforming (SMR) of NG releases carbon dioxide (CO₂) and the natural gas infrastructure has fugitive NG and H₂ losses during production, conversion and transportation. Integrated carbon capture and sequestration (CCS) is a promising approach for producing hydrogen and CO₂ from the SMR process for industrial uses including power, chemicals and fuels. However, the NG losses and regional water availability can be limiting factors for H₂ production. H₂ production assessments are often made at the global scale and neglect regional factors such as abundant gas and limited water in the I-WEST. We demonstrate that a regional SMR process unit sitting near NG wells offers opportunities to significantly reduce fugitive NG losses. We show that regional H₂ production by SMR has a lower emissions profile than widespread natural gas combustion in the I-WEST and reduces the H₂ production cost as well. Replacing the I-WEST transportation sector with H₂ fuel cell vehicles and using 100% H₂-powered electricity can provide substantial reductions in water consumption and fuel costs. This is better than blending H₂ with NG which is more expensive. The captured CO₂ can be effectively used for enhanced oil recovery in I-WEST. Finally, the potential of utilizing produced, brackish and treated impaired water sources is assessed to meet the water needs for H₂ production in the I-WEST.

Keywords: life cycle analysis; fugitive loss; regional hydrogen; water requirement



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1. Introduction

Hydrogen (H₂) is projected to be used significantly across different energy sectors, including the electricity, transportation, and industrial sectors [1–3]. Currently, H₂ is predominantly used in the petroleum and chemical manufacturing industries and for ammonia production [4]. In 2020, 90 million tons of H₂ were produced globally, of which 70 million tons were used to produce ammonia and for refinery operations, with the rest used for methanol and steel production [4]. Similarly, around 10 million tons of H₂ was used in the USA for industrial processes and fertilizer production [5]. H₂ also provides an opportunity to increase the reliability and capacity factor, where it can act as energy storage [2,6]. H₂ can be used with gas turbines, integrated power plants and fuel cells for electricity generation [7–9]. The most prevalent way of producing H₂ is steam methane reforming (SMR) and has been used in industries for decades [10,11]. Recently Digilo et al. [12] proposed gold nanoparticles on poly(2,6-dimethyl-1,4-phenylene oxide) for

formic acid dehydrogenation, while Impemba et al. [13] proposed indium oxide–copper(I) oxide–titanium dioxide composites for solar water splitting for H₂ production.

Numerous life cycle assessments of net carbon dioxide (CO₂) emissions for various H₂ production scenarios have been reported. Howarth and Jacobson [14] concluded that SMR with carbon capture and storage (CCS) modestly reduces lifecycle greenhouse-gas emissions compared to SMR process and can still result in higher net CO₂ emissions than direct natural gas combustion, largely due to methane leakage rates and high energy requirement for SMR process. Bauer et al. [15] concluded that lower CH₄ leakage can significantly lower the carbon footprint for SMR with CCS, and the net emission can potentially be lower than electrolyzer powered by renewable. Additionally, they concluded cost competitiveness of SMR with CCS depends on the expense of mitigating residual emissions and the availability of geological CO₂ storage. Patel et al. [16] compared different NG delivery options for H₂ production and showed that gaseous NG delivery by pipelines has 20% lower CH₄ leakage than liquified NG. The study also highlighted the strong influence of short-lived methane emissions and demonstrated that fossil-based hydrogen pathways remain conditional and assumption-dependent from a climate perspective. Zang et al. [17] carried out a life cycle and cost analysis for H₂ production from different NG basins in the USA with lower fugitive CH₄ emissions than published global assessments [14,15]. The study underscores that regional gas supply characteristics and energy prices critically affect both economics and net emission, suggesting that CCS deployment is not universally cost-effective. Kolb et al. [18] compared the net emission associated with H₂ imports to Germany with domestic H₂ production and concluded that shipping of H₂ can be a significant contributor to net CO₂ emissions. Li et al. [19] optimized SMR CCS configuration with piperazine solvent to reduce the CO₂ capture energy penalty by ~36% and lower the cost of H₂ by ~20%. Al-Khelaiwi et al. [20] emphasized on SMR-CCS short-term economic advantage depends on underlining the need for CCS infrastructure and low-carbon electricity. Most of these studies focused on global greenhouse gas emissions but neglected regional mitigation strategies.

H₂ production is water intensive [21–24]. Olaitan et al. [22] quantified that the fresh-water requirement for H₂ production can vary from 9.2 L/kg_{H₂} for electrolysis powered by wind energy to 105 L/kg_{H₂} for H₂ generated from coal. Simoes et al. [23] assessed the environmental, social, and financial costs of water used for various H₂ production methods. These studies focused on net water requirements and water treatments of impaired water for H₂ generation. Shi et al. [24] calculated the net water impacts of solar-powered H₂ electrolysis for domestic and cross-border and found these to be greatest for China. However, none of these studies have examined the different water quality requirements for various processes used in H₂ production.

The I-WEST region in the USA (which includes New Mexico, Arizona, Colorado, Utah, Montana, and Wyoming) has large NG reserves. The I-WEST region contributes 17.5% of the total energy production of the USA [25], and can become the leading producer of H₂ for local usage and export to other regions [1]. While H₂ is a clean fuel, the CO₂ released from H₂ production SMR and fugitive CH₄ emissions are significant greenhouse gas sources [14,26]. Integrated CCS is a potential path-forward for reducing the emissions generated from SMR processes [27]. The captured CO₂ can also be utilized for enhanced oil recovery with permanent storage, reducing the carbon intensity of oil production by up to 63% compared to conventional methods [28]. CO₂ mixes with oil at the molecular level, reducing its viscosity and enhancing displacement and flow through reservoir rocks, thereby enhancing the oil recovery [29,30].

This study performs a detailed regional life cycle analysis for different scenarios for H₂ production from NG. These scenarios include H₂ production by SMR with and without

CCS and SMR with renewables as heat sources with integrated CCS. The sources for fugitive NG losses are identified, and solutions to reduce these emissions are proposed. A detailed process model for the SMR process was developed and validated to estimate the net energy requirement for hydrogen production. In addition, the water quality and quantity for different processes within the H₂ production industry are determined. A techno-economic analysis (TEA) is conducted to calculate the cost of H₂ production. Finally, based on the NG emissions and water requirements, the net impact on carbon emissions, water requirement and cost resulting from the transition to H₂ as a source of energy for meeting the I-WEST electricity, transportation and industrial sectors needs is estimated.

2. Methodology

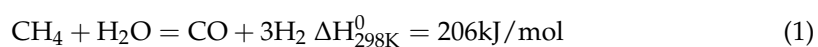
Here, we briefly discuss various H₂ production methods, namely SMR (H_{2,SMR}, grey H₂), SMR with carbon capture (H_{2,SMR+CCS}, blue H₂), and renewable energy-driven H₂ production from NG (blue-green H₂). Natural gas can contain sulfur species (e.g., H₂S and organosulfur odorants such as mercaptans) at ppm levels. Sulfur is a severe poison for Ni-based steam-reforming catalysts; therefore, commercial SMR facilities include a desulfurization section upstream of the reformer. A typical pretreatment train hydrogenates/hydrodesulfurizes organosulfur compounds to H₂S and then removes H₂S in a ZnO guard bed (forming ZnS). In this work, we assume desulfurized, pipeline-quality NG at the reformer inlet; hence sulfur species are not included in natural gas composition used in this study.

A detailed analysis of H_{2,SMR+CCS} is conducted to quantitatively evaluate its potential in reducing regional carbon dioxide emissions. Finally, we present an initial evaluation of H₂ production in the I-WEST region.

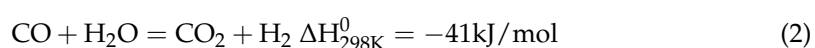
2.1. Steam Methane Reforming

SMR is the dominant commercial route for H₂ production. In conventional SMR commercial production plants, CO₂ generated from a SMR process is released into the environment and the H₂ produced is called “grey H₂”. The SMR production process generates substantial emissions and its carbon footprints are significantly greater than direct NG burning [14].

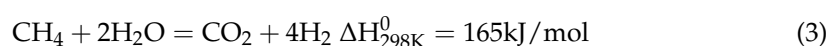
Figure 1a shows the schematic for a traditional SMR process. The NG and steam feed streams are heated to 700–900 °C before flowing into the reformer. The NG is reduced to synthesis gas (syngas):



The resulting syngas product then flows into the water gas shift reactor and here, CO is reacted with more steam to produce more H₂:



The resulting residual syngas mixture then flows into the pressure swing adsorber (PSA) for H₂ purification greater than 99% H₂. The overall reaction can be written as:



Typically, NG is >90% methane (by mass), with heavier hydrocarbons present in low fractions. The typical composition of NG is given in Table S1. The higher hydrocarbons present in NG undergo reforming similar to methane [31], and the reactions are discussed in Supplementary Materials S1.

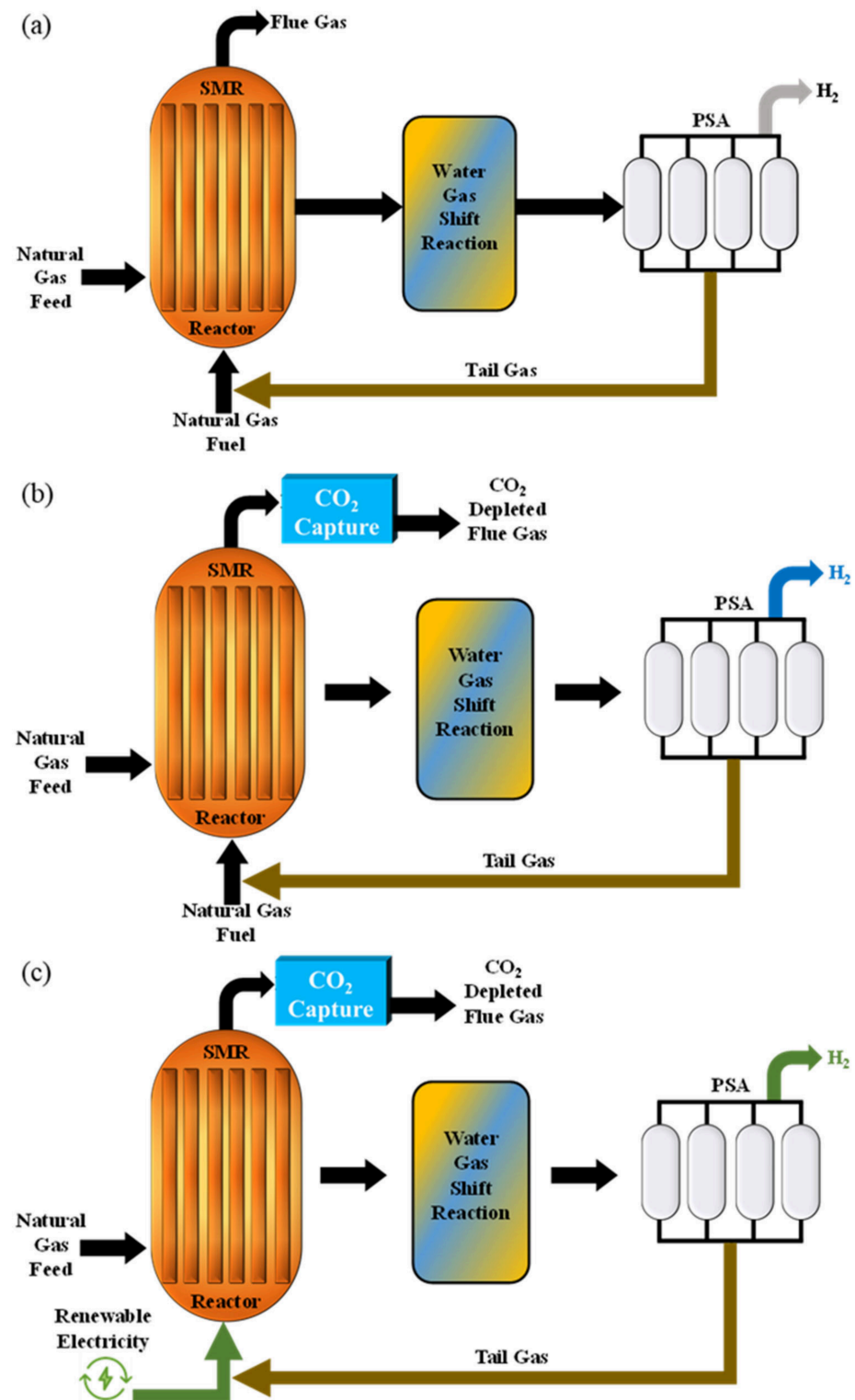


Figure 1. Schematic for different H₂ production process methods as a function of carbon capture and energy source: (a) traditional SMR process (grey H₂), (b) SMR with carbon capture (blue H₂), (c) SMR with carbon capture and energy supplied from renewables (blue-green H₂).

Xu and Froment [32] developed a kinetic model of the SMR process using a Langmuir-Hinshelwood formulation for heterogeneous catalyst. This model is utilized for predicting the SMR reaction kinetics and assumes methane is the only component of NG.

Assuming methane as the most significant component of NG, we therefore use the kinetic model from Xu and Froment [32] as follows:

$$r_1 = \frac{k_1}{(p_{H_2})^{2.5}} \left(p_{CH_4} p_{H_2O} - \frac{(p_{H_2})^3 p_{CO}}{K_1} \right) \frac{1}{\Omega^2} \quad (4)$$

$$r_2 = \frac{k_2}{(p_{H_2})} \left(p_{CO} p_{H_2O} - \frac{p_{H_2} p_{CO_2}}{K_2} \right) \frac{1}{\Omega^2} \quad (5)$$

$$r_3 = \frac{k_3}{(p_{H_2})^{3.5}} \left(p_{CH_4} (p_{H_2O})^2 - \frac{(p_{H_2})^4 p_{CO_2}}{K_3} \right) \frac{1}{\Omega^2} \quad (6)$$

$$\Omega = 1 + \frac{K_{H_2O} p_{H_2O}}{p_{H_2}} + K_{CO} p_{CO} + K_{H_2} p_{H_2} + K_{CH_4} p_{CH_4} \quad (7)$$

where K_{H_2} , K_{CH_4} , and K_{CO} represents the adsorption parameters for H_2 , CH_4 , and CO respectively. K_{H_2O} is the dissociative adsorption parameter for H_2O . K_1 , K_2 , and K_3 represents the equilibrium-based parameters of the reactions. Similarly, k_1 , k_2 , and k_3 represents the kinetic constant parameters of the reactions, respectively. p_{H_2} , p_{CH_4} , p_{H_2O} , p_{CO} , and p_{CO_2} represents the partial pressures of gas species accordingly. Ω represents a dimensionless parameter.

In this work, Equation (5) is also used to model the reaction kinetics of the water gas shift reactor (WGS) process. The results of this model are validated against the previous WGS models in literature to justify the use of these reaction kinetics for the WGS.

We adopt the modeling assumptions of Marin et al. [33] which assumes an axial dispersed plug flow model across the reaction tube. 1D partial differential equation model which assumes negligible radial heat or mass gradients, Peng-Robinson-Stryjek-Vera equation of state for properties of the gas mixture, and the use of Ergun equation for calculating the pressure drop across the reaction tube. The 1D modeling equations are discussed in Table S2.

The SMR model was validated under isothermal, constant-pressure conditions, showing good agreement with Aspen Plus simulation from Thengane et al. [34], with deviations below 2% across key parameters as shown in Table 1. Methane conversion (64.33%) closely matched Aspen Plus predictions (63.29%), and product compositions showed an average deviation of 1.76%. Similarly, the WGS model exhibited strong agreement with Aspen Plus, with CO conversion differing by only 0.15%. Product compositions had an average deviation of 0.57%, confirming high accuracy for both reactor models.

Table 1. Validation of SMR and WGS models.

Steam Methane Reformer Reactor Model Validation [34]			
	Feed	Aspen Plus [34]	This Work
H_2 (mole%)	0	0.4173	0.4237
H_2O (mole%)	0.7623	0.400	0.3949
CO (mole%)	0	0.0453	0.0464
CO_2 (mole%)	0	0.0704	0.0701

Table 1. Cont.

Steam Methane Reformer Reactor Model Validation [34]			
	Feed	Aspen Plus [34]	This Work
CH ₄ (mole%)	0.2377	0.0670	0.0649
Total flow (mol/s)	1.868	2.43	2.44
Temperature (°C)	700	700	700
Enthalpy flow rate (kW)	−325.80	−268.60	−267.64
Pressure (atm)	10	10	10
Conversion (%)		63.29	64.33
Water Gas Shift Reactor Model Validation			
	Feed	Aspen Plus [34]	This work
H ₂ (mole%)	0.4173	0.4591	0.4588
H ₂ O (mole%)	0.400	0.3583	0.3585
CO (mole%)	0.0453	0.0037	0.0038
CO ₂ (mole%)	0.0704	0.1119	0.1119
CH ₄ (mole%)	0.0670	0.0670	0.0670
Total flow (mol/s)	2.43	2.43	2.43
Temperature (°C)	300	300	300
Enthalpy flow rate (kW)	−304.5	−308.5	−308.63
Pressure (atm)	10	10	10
Conversion (%)		91.83	91.69

With operating temperature of 850 °C, pressure of 10 bar, steam to carbon ratio of 3, the SMR conversion efficiency is 95%. The reformed NG undergoes the WGS reaction in two stages: at ca. 350 °C and 200 °C. The reformed gas leaving the SMR reactor is at a high temperature (850 °C) and is cooled before flowing to the WGS reactor. The WGS process conversion efficiency is close to 100% [35], where predominantly all CO is converted to CO₂ and generates additional H₂.

The shifted syngas is cooled to near 40 °C before flowing in the PSA where the H₂ is separated. We have used the model proposed by Ribeiro et al. [36], for H₂ purification (>99.99% purity) over a layered combination of activated carbon and zeolite. Langmuir isotherm adsorption model was used to compute the average adsorbed concentration of each species (q_i) and is given as:

$$\frac{q_i}{q_{i,max}} = a_i \left(1 - \sum_i \frac{q_i}{q_{i,max}} \right)^{a_i} \quad (8)$$

where, $q_{i,max}$ is the saturation adsorbed concentration and a_i is the number of sites occupied by the adsorbate [36]. For the feed quality shown by Equation (7), and operating pressure and temperature of 10 bar and 40 °C, the H₂ recovery ratio calculated is 78%, very close to typical PSA recovery ratio of 80% (R_{H_2}) [37].

To calculate the net energy requirements for the system, we used principle of process integration commonly used to calculate the energy requirement for thermal process [38–40]. Process integration has been commonly used to calculate the energy requirement for SMR process for H₂ production [41,42]. Using similar methodology, we calculated the net energy requirement for hydrogen production. A detailed description is given in Supplementary Materials S1.2.

The flue gas exhaust stream from the SMR process has a high CO₂ concentration, nominally 20 wt.%, that can be readily separated using commercial CO₂ separation technologies such as a monoethanolamine (MEA) absorber and sequestered [43]. In general, CO₂ capture is implemented as post-combustion, pre-combustion, or oxy-fuel/looping schemes, with separation achieved via absorption, adsorption, membranes, cryogenic separation, and looping-based processes [44]. For post-combustion flue gas (dilute CO₂ at near-ambient pressure), chemical absorption (amines and advanced solvent formulations) remains the most mature approach, while adsorption-based processes using solid sorbents (e.g., zeolites/amine-functionalized materials) and membrane-based separations are active development areas [45]. For pre-combustion capture (high-pressure, CO₂-rich shifted gas), physical solvent systems (e.g., Selexol and Rectisol) are established commercial options, and recent reviews summarize performance and techno-economic considerations for these solvents in hydrogen/syngas applications [45,46].

The H₂ produced by this process is known as the blue hydrogen and is abbreviated as SMR_{CCS} [see Figure 1]. We have used the modeling approach proposed by Kim et al. [47] to calculate the thermal energy for carbon capture ($\dot{E}_{CC}$) and is given as:

$$\dot{E}_{CC} = \frac{Q_{sensible} + Q_{reaction} + Q_{latent}}{\dot{m}_{CO_2}} \quad (9)$$

where $Q_{sensible}$ is the sensible heating required across the CO₂ stripper, $Q_{reaction}$ is the energy required for desorption of CO₂, Q_{latent} is the latent heat needed for evaporating water and $\dot{m}_{CO_2}$ is the mass of CO₂ captured. From vapor liquid equilibrium for MEA solution, the loading of CO₂ in MEA can be calculated as a function of partial pressure of CO₂ in the effluent flue gas [48,49]. For a given value of CO₂ loading in rich and lean sample, the operating temperature across the stripper can be calculated and similarly the amount of water evaporated can be estimated [47].

Using NG to provide reformer heat duty produces CO₂ with additional greenhouse gas emissions due to NG leakage. Using renewables as a source of heat can reduce the carbon footprints. We assessed the use of solar photovoltaics (PV) and wind energy for running an electric SMR [50–52], and concentrating solar thermal (CST) as a renewable energy source for the SMR process [53,54]. In an electric SMR, the electrical resistance heating reactor is used to maintain the SMR reactor temperature [52], while heat from CST is transferred to molten salt which is subsequently used for heating the SMR reformer [53]. The renewable energy-integrated SMR process is referred to as SMR_{CCS+RE}.

2.2. Life Cycle Analysis

A cradle-to-grave life cycle analysis (LCA) is performed for H₂ production from SMR. Figure 2 shows the overarching process schematic and the system boundary. The process involved in NG-derived H₂ production includes extraction, processing, and treatment to produce pipeline-grade natural gas. The process also includes, natural gas compression and transportation, H₂ reaction and separation, and H₂ compression. In addition, CO₂ capture, compression, transportation, and sequestration are also required for H₂ production with integrated carbon capture (SMR_{CCS}). The analysis relies on the assumptions listed below in Table 2.

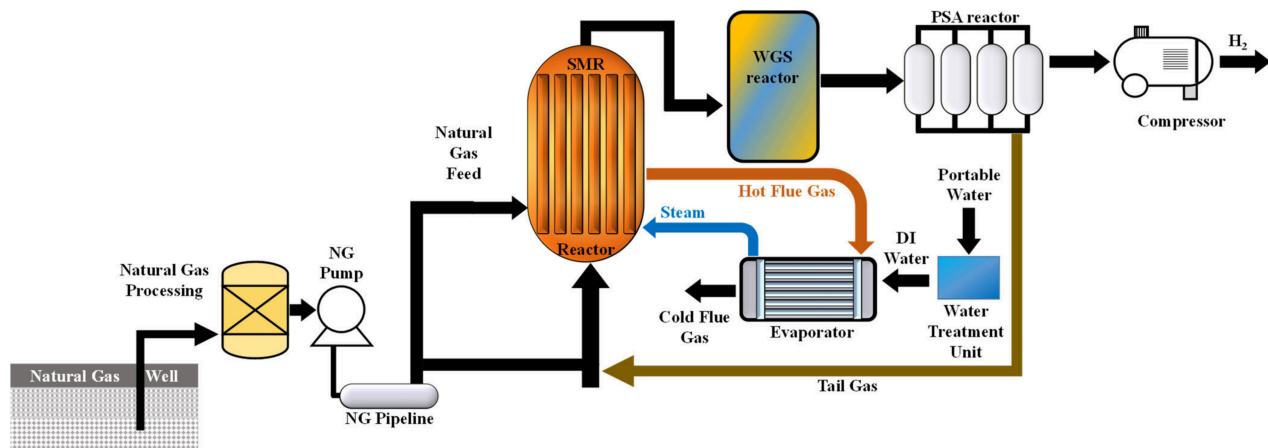


Figure 2. Process schematic for hydrogen production from NG and system boundaries for the LCA.

Table 2. Assumption made for carrying out life-cycle analysis [55].

Parameters	Values	References
NG leakage base case	3.5%	[14]
Emissions from NG extraction and processing	0.328 kgCO ₂ /kg _{NG}	[56]
Compresses NG pressure for pipeline delivery	80 bar	[57]
SMR operating pressure	10 bar	[58]
H ₂ delivery pressure	180 bar	[59]
H ₂ leak from compressor	1%	
CO ₂ capture rate base case	90%	[14]
CO ₂ sequestration pressure	100 bar	[41]
Emissions from Concentrating solar power	10 g/kWh _{th}	[60]
Compressor cooling	Air cooled	[61,62]
Emission for electricity generated from NGCC, (with 3.5% NG leak)	541 g/kWh _e	[56]
Global warming potential for NG with 100 years lifetime	25.8	[see Supplementary Materials S1.2 for details].
NGCC water requirement	0.74 L/kWh _e	[63]
Water required for NG extraction	0.4 L/kg _{NG}	[56]
Deionized water required for carbon capture	0.016 L/kgCO ₂	[64]
Water required for MEA washout	0.1 L/kgCO ₂	[65]
Water required by carbon capture unit process and cooling	2 L/kgCO ₂	[55]
Water required for photovoltaic cleaning	0.4 L/kWh _e	[66,67]

The net CO₂ generated for the standalone SMR process includes the net emissions during NG extraction, NG leakage, emissions from the electricity source used for NG and H₂ compression, water pumping and treatment, H₂ leakage, and CO₂ emissions from the SMR and combustion process, which is provided as:

$$CO_{2, SMR} = \frac{NG_{extract} + NG_{leak} \times GWP_{NG} + CO_{2, elec} [NG_{compress} + H_{2,compress} + water_{pump\&treat}] + H_{2,leak} \times GWP_{H_2} + CO_{2, SMR+Combustion}}{H_{2, production}} \quad (10)$$

The net emissions from NG and H₂ leaks is converted to equivalent CO₂ emissions using respective gases GWP (global warming potential). Energy required for gas (NG, H₂ and CO₂) compression is discussed in Supplementary Materials S2.1. The carbon capture (CC) process requires additional thermal and electrical energy. The thermal energy for carbon capture is supplied via NG combustion and the associated CO₂ emissions are also captures. These net emissions are given as:

$$CO_{2, SMR+CC} = \frac{NG_{extract+CC} + NG_{leak+CC} \times GWP_{NG} + CO_{2, elec} \left[NG_{compress+CC} + H_{2,compress} + water_{pump\&treat} + \dot{E}_{CC} \right] + H_{2,leak} \times GWP_{H_2}}{H_{2, production}} + (1-f) \times CO_{2, SMR+Combustion+CC} \quad (11)$$

where f is the fraction of CO_2 captured.

2.3. Technoeconomic Analysis

To estimate the cost of H_2 produced we have also carried out a techno-economic analysis. The cost H_2 ($C_{H_2, SMR}$) is given as:

$$C_{H_2, SMR} = \frac{FCR \times C_{capital}}{H_{2, production, annual}} + C_{NG} \times m_{NG} + C_{elec} \times \dot{E}_{elec} + C_{water} \times m_{water} + C_{catalyst} + C_{O\&L} \quad (12)$$

where, FCR is fixed charge rate, $C_{capital}$ is the total capital cost of the equipment (including indirect, installation and direct capital cost), C_{NG} is the natural gas cost, C_{elec} is the electricity cost, C_{water} is the water cost, m_{NG} and m_{water} is the mass of NG and water used per kg of H_2 , $C_{catalyst}$ is the catalyst cost and $C_{O\&L}$ is the operation and labor cost.

3. Results

3.1. Process Modeling Result

The parameters and inputs used for process modeling of the system are listed in Table 3. The SMR conversion is obtained as 95%, while WGS conversion ratio was 99.3% and 99.6% for stage 1 and 2. Figure 3 shows the composite curve for the 1 kg of H_2 product. PSA recovery ratio was calculated to 78%. The mass flowrate and the enthalpy values for each stream are listed in Table S5, in Supplementary Materials. Using process integration principle, the net energy required for H_2 production comes out to be 23.9 kWh_{th}/kg H_2 . As can be seen from Figure 3, the heat of hot streams including cooling of SMR syngas, heat from water gas shift reactor and condensate cooling is sufficient to heat the water and NG mixture to 530 °C (inlet temperature for steam and NG into the SMR reactor). The flue gas energy can be utilized for preheating the air, NG and tail gas. By recovering the flue gas energy for pre-heating, it can be cooled to 420 °C. The net cooling required for the SMR and fuel gas is 6.5 kWh_{th}/kg H_2 .

Table 3. Input parameters for SMR.

Parameters	Values	References
Steam to carbon ratio	3	[41]
Operating pressure	10 bar	[41]
Pinch temperature	50 °C	
Inlet temperature for steam and NG into the SMR reactor	530 °C	[68]
Maximum operating temperature inside SMR reactor	850 °C	[68,69]
Heat loss in Reactor	9.8%	[63]
Flue gas outlet temperature leaving the combustion chamber	1000 °C	[62]
WGS 1 operating temperature	350 °C	[41]
WGS 2 operating temperature	200 °C	[41]
PSA operating temperature	40 °C	

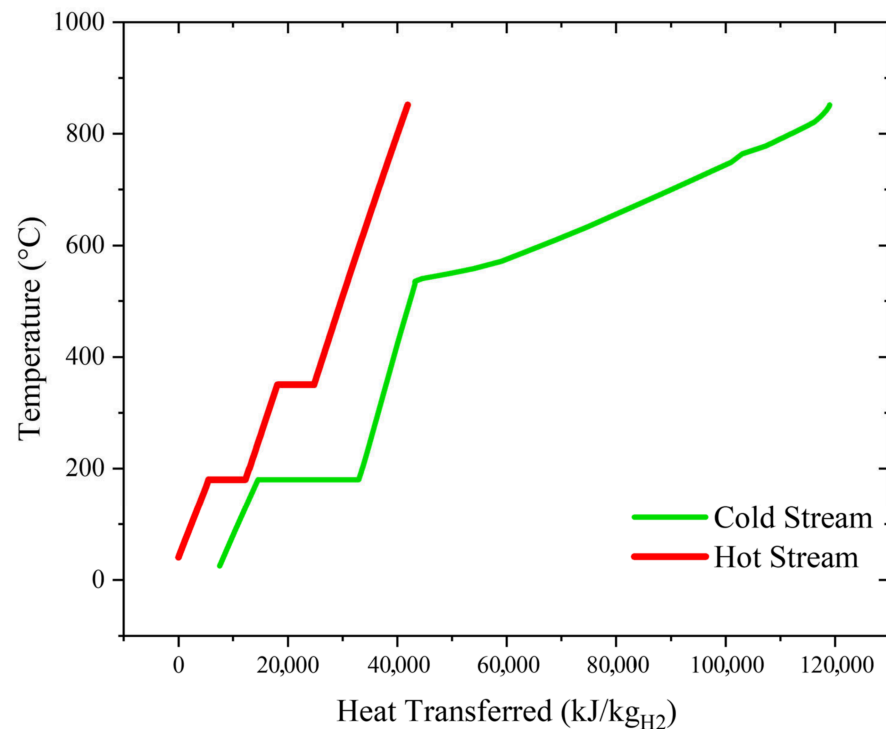


Figure 3. Composite curve for production of 1 kg of the H₂.

The effluent gas leaving the PSA is used as energy source along with additional NG supplied to the combustor unit. The CO₂ concentration leaving the combustion chamber is 19.8% by volume for dry gas (while the wet gas CO₂ concentration is 16.5%). From vapor liquid equilibria for MEA, the rich loading for MEA is calculated to be 54%. For minimum energy consumption, the lean loading for MEA is 20%. The net energy required for carbon capture is calculated to be 0.96 kWh_{th}/kgCO₂. Similarly, we are also trying to capture CO₂ generated due to NG burning to supply heat to carbon capture process. The CO₂ composition for NG flue gas is around 9% (by volume for dry gas) and the energy required to capture CO₂ is 1.02 kWh_{th}/kgCO₂.

3.2. Greenhouse Gas Emissions

Figure 4 show the net CO₂-equivalent emissions breakdown for H₂ production estimated over a 100-year timescale with a GWP of 25.8 for different production scenarios. For H₂ production from SMR without carbon capture, the major contributor to CO₂ emissions (approximately 63%) is the NG reforming as well as combustion of NG to provide heat for the reformer. NG leaks contribute 21% of the total CO₂ emissions, NG extraction contributes 8%, H₂ compression is 5% and NG compression is 3%. The other minor contributors are H₂ leaks and the electrical energy required for pumping and running the cooling system (<0.1% combined). The net calculated CO₂ emission for H₂ production using SMR is 16.4 kgCO₂/kgH₂. It may be noted that hydrogen leakage contributes only 0.5% when a GWP value of 8 is assumed. However, recent literature reports H₂ GWP values in the range of 11–12, which would increase the contribution of H₂ leakage to approximately 0.7%, while the net CO₂ emissions increase by only about 0.2%.

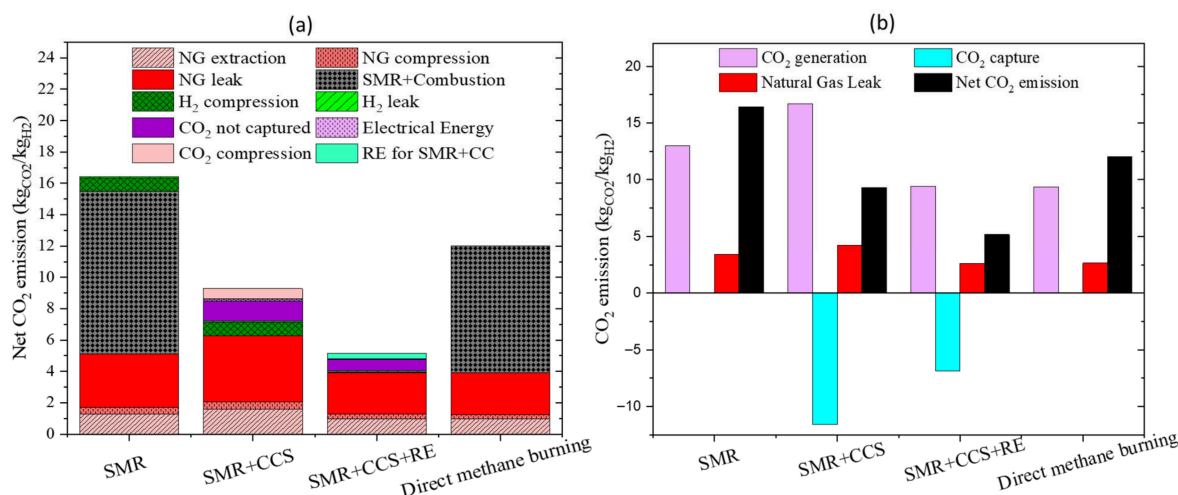


Figure 4. (a) CO₂ net emissions source breakdown for H₂ production and (b) calculated net CO₂ generation, capture, NG leakage, and net CO₂ emissions. Plot of carbon emission and captured CO₂. NG losses are fixed at 3.5%, SMR heating requirements of 23.9 kWh_{th}/kg_{H2}, carbon capture efficiency and energy consumption 90% and 0.96 kWh_{th}/kg_{CO2}. To generate 1 kg of H₂, SMR, SMR_{CCS}, and SMR_{CCS+RE} need 4, 4.9, and 2.6 kg of NG, respectively. A detailed energy balance for different scenarios is discussed in Supplementary Materials S2.2 and net emissions is discussed in Supplementary Materials S3.

For SMR_{CCS}, NG required increases by 21% in comparison to the SMR base case, to supply more energy for the CO₂ capture from the tail gases. Therefore, the CO₂ generation increases by 27% [see Figure 4b] relative to SMR without carbon capture. For 90% CO₂ capture from the flue gas, around 11.6 kg_{CO2}/kg_{H2} can be captured and the net CO₂ emissions for SMR_{CCS} production reduces to 9.8 kg_{CO2}/kg_{H2} (around 43% lower than SMR). For SMR_{CCS} the major CO₂ emissions contributor is NG leakage (45%, see Figure 4). Therefore, to further reduce the CO₂ emissions for SMR_{CCS}, NG usage should be minimized, and leaks should be restricted.

By using renewables, including solar or wind (both in abundance in the Intermountain-West of the U.S.) as the energy source for both the SMR and CO₂ capture units, the net CO₂ release are lowered by 70% to 5.1 kg_{CO2}/kg_{H2}. Similarly, for SMR_{CCS+RE} the major CO₂ emissions contributors are the NG fugitive emissions (51%), followed by NG extraction, H₂ compression, and CO₂ not captured.

H₂ combustion generates 120 MJ_{th} of heat per kg, and 2.55 kg of NG is required to generate the same quantity of heat energy. Compared to the SMR processes with or without carbon capture, direct combustion of NG will generate around 12 kg_{CO2}/kg_{H2-eq}. Therefore, carbon capture from SMR gives a marginal reduction in net CO₂ emission of 22% compared to direct burning of CO₂.

The main drivers of the net CO₂ release are the NG leaks and thermal energy required for the reformer. In Supplementary Materials Section S4, a comprehensive sensitivity analysis was conducted to evaluate how key parameters influence the overall CO₂ footprints of H₂ production. For the SMR-CCS process, methane leakage from the NG supply chain was identified as a critical factor. Reducing the leakage rate from the assumed 3.5% to 1% can lead to a substantial decrease of approximately 50% in CO₂-equivalent emissions, highlighting the sensitivity of the system to upstream methane emissions. Similarly, improvements in the efficiency of the conventional SMR process can significantly lower CO₂ emissions, with potential reductions of up to 40% compared to baseline scenarios. Furthermore, increasing the carbon capture efficiency within the SMR-CCS system contributes to an additional reduction of around 10% in CO₂ emissions, demonstrating the complementary

role of capture technology in mitigating the climate impact of blue hydrogen. This analysis underscores that both upstream methane management and process optimization are crucial levers for minimizing the carbon intensity of hydrogen production.

3.3. Regional Hydrogen

Here, we quantitatively assess the benefits of regional H_2 production by SMR, SMR_{CCS} , and SMR_{CCS+RE} and compare them with direct NG combustion. As discussed in Section 3.1, NG leaks contribute 21%, 45% and 51% of the CO_2 -equivalent emissions over a 100-year timescale for SMR, SMR_{CCS} and SMR_{CCS+RE} , respectively. Figure 5 shows the major contributors for NG leakage. Gas compressors account for largest NG leaks (45%). In reciprocating units, leaks occur at the rod-packing system, whereas centrifugal compressors commonly leak from wet seals. Storage and pipeline NG leakage accounts for 27% due to gas diffusion from the valves and pipes. Drilling and extraction account for 28% of the NG emissions, including flared gas and pipeline leakage [70,71].

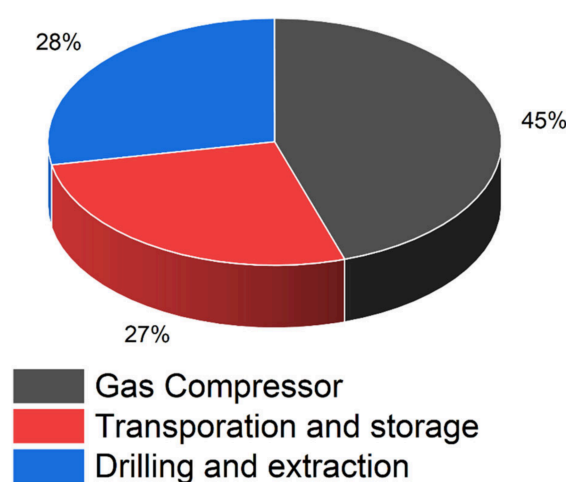


Figure 5. Fugitive emissions from natural gas [64,65].

To generate 1 kg of H_2 , SMR, SMR_{CCS} , and SMR_{CCS+RE} need 4, 4.9, and 3 kg of NG, respectively. From the stoichiometry alone, 1 kg of H_2 requires 2 kg of NG. The additional NG is required due to the external energy required for the SMR process. However, due to the incomplete conversion in SMR, lower H_2 recovery from the PSA, and energy losses, the NG consumption increases significantly. Due to higher NG requirements, the NG leaks significantly contribute to the net carbon emissions for H_2 production.

One possible solution to mitigate NG leaks is regional H_2 production plants near abundant gas supplies and fossil reservoirs. Rather than compressing the NG and transporting it to distant SMR facilities, hydrogen can be locally produced via the siting of SMR plants close to NG production sites. It may also facilitate CO_2 sequestration due to the proximity of the geological reservoirs and will reduce CO_2 transportation costs. Even so, the volumetric energy density of H_2 is three times smaller relative to NG ($11.5 \text{ MJ } H_{2,STP}/m^3$ compared to $35.5 \text{ MJ } CH_{4,STP}/m^3$). This increases the pumping-related energy required from 4% for NG to 15% for H_2 . In addition, as H_2 is a much lighter fluid relative to CH_4 , it is estimated to have $1.3\times$ to $3\times$ more leakage [72]. In our studies, we considered a hydrogen leakage of about 2.5 times of NG. Furthermore, H_2 has an indirect global warming potential of 8 over 100 years [72].

Regional H_2 production with carbon capture reduces CO_2 emissions by 31% compared to non-regional SMR_{CCS} [see Figure 6a]. This reduction is primarily due to NG leakage during compression, as the compression duty in the regional case is minimal because of the lower outlet pressure of 10 bar. In addition, NG transportation is not required, which

further reduces NG leakage. Although parasitic H_2 leakage increases slightly, the combined effect is a net CO_2 emission reduction of 2.9 kg. As a result, siting SMR near NG sites can lower CO_2 emissions. Furthermore, due to proximity to NG resources and geological reservoirs, regional H_2 production requires a more compact infrastructure, resulting in lower leakage compared to a centralized H_2 production approach. Even with a higher GWP of 12 for H_2 , the net CO_2 emissions for regional H_2 production with regional SMR_{CCS} are only 1.5% higher compared to a GWP of 8.

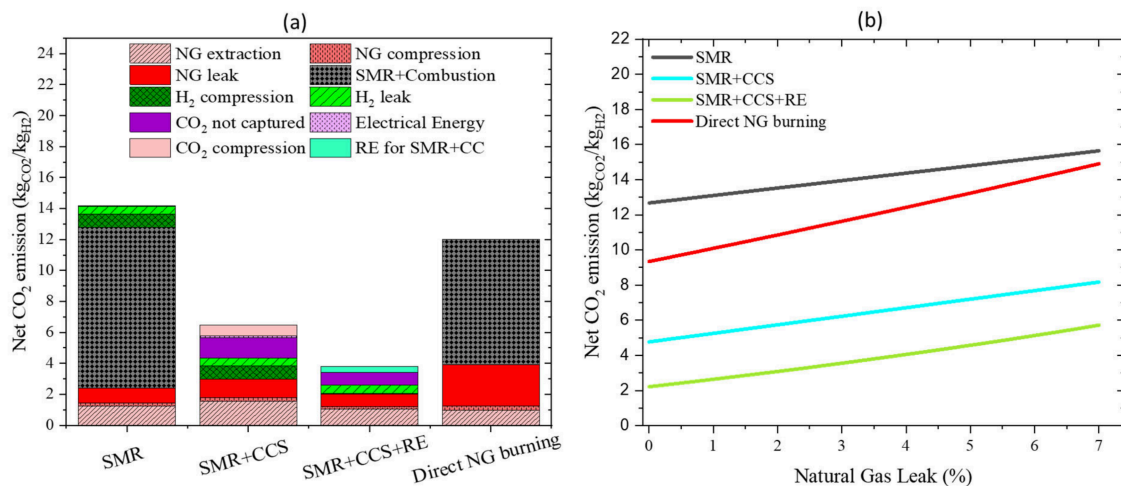


Figure 6. (a) CO_2 net emission source breakdown for regional hydrogen production. Plot of carbon emission and captured CO_2 . NG leakage is fixed at 3.5%, SMR heating energy consumption of $24.1 \text{ kWh}_{th}/\text{kg}_{H_2}$, carbon capture efficiency of 90%. (b) Net CO_2 emissions for regional H_2 productions as a function of NG leakage, while the SMR heating energy requirement and carbon capture efficiency are kept constant at $24.1 \text{ kWh}_{th}/\text{kg}_{H_2}$, and 90%.

3.4. Water Usage

Water is a scarce resource in the I-WEST region that is needed in SMR as a feedstock for cooling and CO_2 capture. Here, we evaluate both the quality and quantity needed for our regional H_2 economy. Figure 7 shows the water requirements for different H_2 generation process schemes per kg H_2 production. We note that various processes used in H_2 production require different water qualities. For example, SMR and carbon capture units require deionized (DI) quality water. The use of DI water prevents salt deposition on the process equipment. Here, we have used a reverse osmosis (RO) system to generate DI water from potable water sources. Typically, a RO system operates with an 80% recovery ratio, i.e., 80% of the DI water is generated from the potable water source and the rest is rejected as waste [73]. The SMR process needs around 5.7 L of potable water to generate 4.5 L of DI water, which is later utilized for 1 kg H_2 production. It may be noted that any unused water leaving the WGS reactor is condensed and recycled. All H_2 generation processes require electricity from pumping, water purification, compression, cooling towers, and carbon capture systems. For electricity produced from a natural gas combined cycle (NGCC) power plant, the net potable water required is around $0.74 \text{ L}/\text{kWh}_e$ [74]. Water is predominantly required to cool the power cycle. The net potable water required to supply electrical energy for SMR is $1.8 \text{ L}/\text{kg}_{H_2}$, and with carbon capture it increases to $2.4 \text{ L}/\text{kg}_{H_2}$. The renewable energy source needs around $0.4 \text{ L}/\text{kWh}_e$ of potable water for photovoltaic panel cleaning [66,67]. The CST mirror cleaning would require around $0.2 \text{ L}/\text{kWh}_{th}$ for mirror cleaning. The net potable water required to generate electricity and thermal energy for SMR with carbon capture powered with renewable energy is around $5.5 \text{ L}/\text{kg}_{H_2}$. NG extraction also requires water and can use impaired water sources like brackish water with

salt concentrations up to 5000 ppm. The net water required for NG extraction is 1.8 L/kg_{H₂} for SMR_{CCS}.

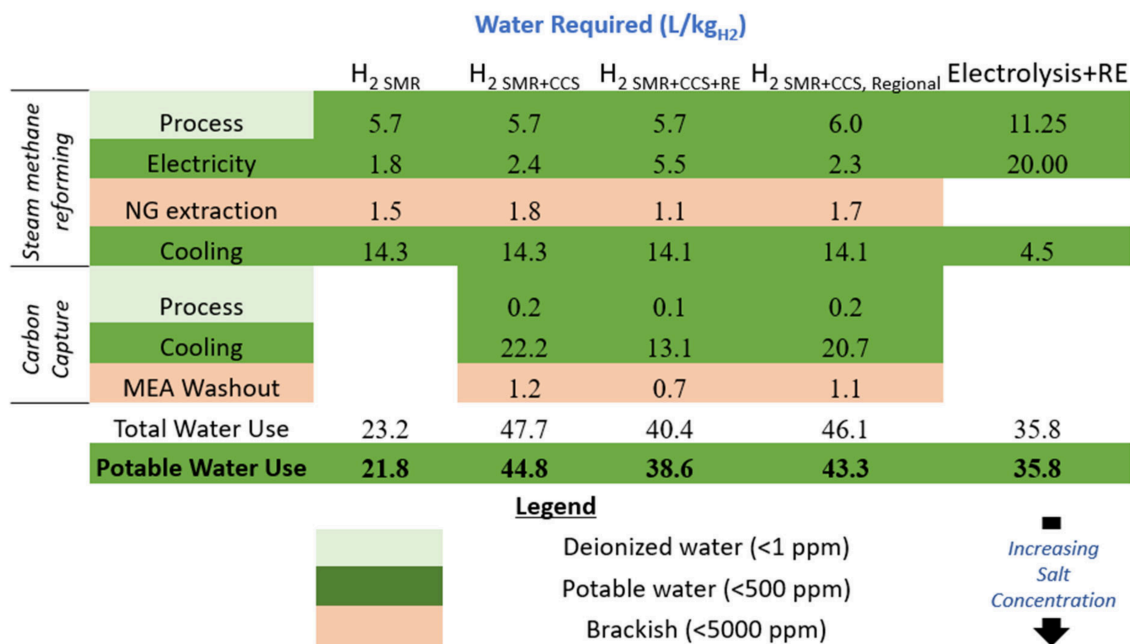


Figure 7. Water requirement for different H₂ production processes. The water required for mining, NG extraction and panel cooling are taken from [67,75,76].

It may be noted instead of using potable water, brackish water could also be used as a feed for generating DI water; however, depending on the feed concentration of brackish water the energy demand could be in the range 0.5–2 kWh_e/m³ and the recovery ratio will further go down. However, with use of brackish water, the potable water use will reduce to 6.6 and 29 L/kg_{H₂} for SMR and SMR_{CCS}, while the total water usage will increase to 14.4 and 38.5 L/kg_{H₂}.

MEA solutions (30% wt.) demand DI water, while cooling (including flue gas and MEA cooling) requires potable water. The flue gas leaving the carbon capture unit carries MEA that needs to be washed (dissolved) in water [55,56]. Since brackish water contains only salt, it can be used to remove MEA from flue gas during the MEA washout. The SMR_{CCS} process requires an additional 22.4 L/kg_{H₂} of potable water for the carbon capture process and 1.2 L/kg_{H₂} of brackish water for the MEA washout.

The total potable water required for the SMR_{CCS} is 44.8 L/kg_{H₂}. In comparison, the H₂ generated from water electrolysis powered with photovoltaics would need around 35.8 L/kg_{H₂} of potable water.

It is worth noting that I-WEST is an oil and gas producer, has massive produced and brackish water resources [77]. However, potable water can be scarce. In the carbon capture and power cycle, cooling is the major contributor to the net potable water demand. Supplementary Materials S5 shows the results for the use of the produced water or brackish water as cooling water sources. The net potable water demand can be reduced to 5.9 L/kg_{H₂} for SMR with carbon capture and regional SMR with carbon capture [see Figure S4]. Note that the pumping power required for the system will increase due to a significant increase in the produced water demand for once through cooling. The overall increase in net CO₂ emissions is around 3.3% for regional H₂ with carbon capture.

The other approach to reduce the cooling water demand is using an air cooler for cooling the power cycle, carbon capture unit and SMR process cooling. The net effect is a reduction in total water consumption to 8.9 and 9 L/kg_{H₂} for SMR_{CCS}, and regional SMR_{CCS},

respectively [see Figure S5] while the net potable water demand reduces to 5.9 L/kg_{H₂}. Compared to the electrolysis process, the net potable water demand for regional H₂ production reduces by 81% with air cooling. With air cooling, the electricity requirement increases slightly for H₂ production, resulting in a net increase in net CO₂ emissions by 3.1%, while the net water requirement can be reduced by 84.4%.

Thermal management and cooling represent major challenges in hydrogen energy systems due to their high energy and water requirements. These challenges arise not only during hydrogen production but also in end-use technologies such as fuel cells, where effective heat dissipation is critical for performance. Recent advances in thermal management solutions, such as novel liquid-cooled plate designs, have shown potential to improve efficiency while reducing the overall cooling burden [78].

3.5. Techno-Economic Analysis Results

Table 4 lists the input parameters used for TEA. Figure 8a shows the production cost for different H₂ processes. The H₂ cost is cheapest for standalone SMR and is 1.73 \$/kg_{H₂}. The major cost is the cost of NG, followed by capital cost, O&M cost and electricity cost. Water and catalyst cost are marginal. With carbon capture the capital cost almost doubles, resulting to increase in H₂ cost to 2.9 \$/kg_{H₂}. For SMR powered with renewable energy, the lower capacity factor increases the capital cost, and the price increases to 3.22 \$/kg_{H₂}. Regional H₂ cost is slightly cheaper compared to SMR_{CC} due to lower electricity consumption. If the CO₂ sequestration credit of 85 \$/tonne_{CO₂} is included, the cost of H₂ reduces to 1.88, 2.6 and 1.79 \$/kg_{H₂} for SMR_{CC}, SMR powered with renewable and regional H₂. With air cooler, the regional H₂ will increase merely by 0.4%.

Table 4. Input parameters for TEA.

Parameters	Values	References
H ₂ capital cost (M\$/tonne _{H₂} /day)	2150	[79]
Carbon capture capital cost (M\$), (<i>Size_{CC}</i> is carbon capture system size in tonne/day)	$421 \times \left(\frac{Size_{CC}}{5142}\right)^{0.8}$	[64]
FCR	0.07	[77]
NG price (\$/kg)	0.18	[80]
Electricity price (\$/kWh _e)	0.08	[80]
Water Price (\$/m ³)	2	[81]
H ₂ catalyst replacement cost (\$/kg _{H₂})	0.021	[79]
H ₂ O&M cost (\$/kg _{H₂})	0.26	[79]
Carbon capture material cost (\$/tonne _{CO₂})	4.1	[64]
Carbon capture O&M cost (\$/tonne _{CO₂})	9	[64]
CO ₂ sequestration and monitoring cost (\$/tonne _{CO₂})	9.1	[64]
Current CO ₂ permanent sequestration and storage credit (\$/tonne _{CO₂})	85	[82]
H ₂ production size (tonne _{H₂} /day)	5	
Capacity factor	85%	[77]
Current electrolyzer H ₂ cost (\$/kg _{H₂})	6.3	[79]
Current clean H ₂ tax benefit (\$/kg _{H₂})	3	[83]
Future electrolyzer H ₂ cost (\$/kg _{H₂})	3.1	

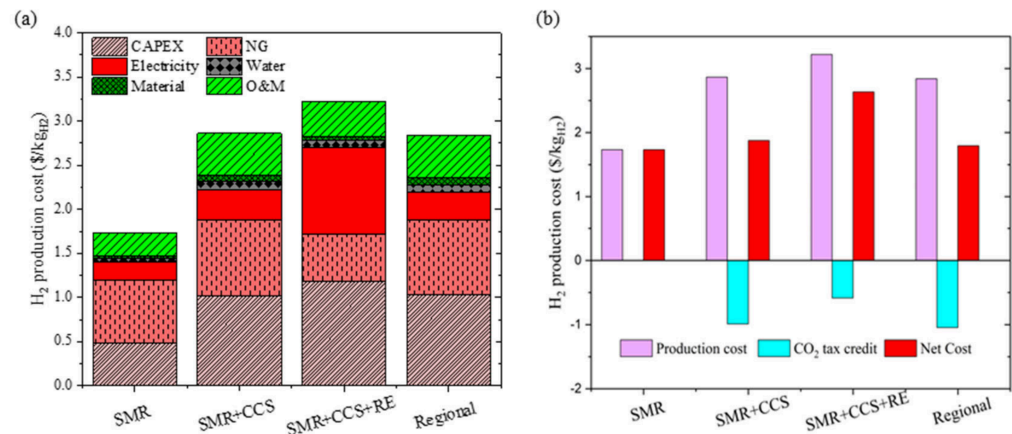


Figure 8. (a) H₂ production cost bifurcation, (b) Effect of CO₂ tax credit on H₂ production cost.

4. Case Study

We have considered the case study of the I-WEST region, situated on the rocky mountain range and contributing 17.5% of the total energy production in the USA [25], for decarbonizing regional transportation, electricity generation and fuel production.

4.1. Transportation

The primary drivers of transportation energy in I-WEST include gasoline (63%) and diesel (32.2%), with a total net energy content of ca. 419 TWh_{th}/year [see Figure 9a] [84]. The major contributor to transportation in I-WEST is Arizona, followed by Colorado, Utah, New Mexico, Wyoming, and Montana, and is 32%, 23.4%, 15.2%, 14.8%, 7.6% and 7.1%, respectively. The net CO₂ emissions from the transportation sector are 139.86 million-tonne/year [see Figure 9b]. The overall water usage for the total fuel production is 248 million m³/year, of which 67.5% is required by gasoline and 32.3% by diesel. NG-specific water consumption is 90% lower than gasoline and diesel [see Figure 9b].

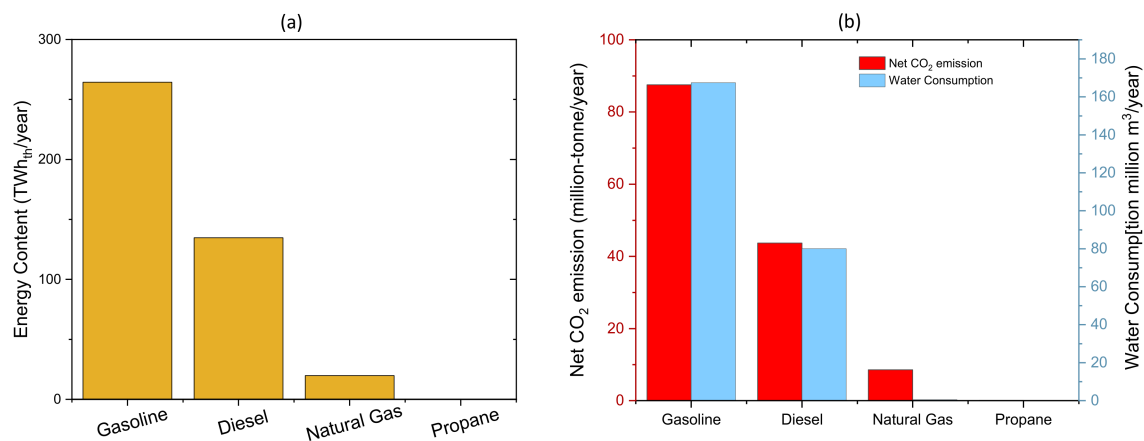


Figure 9. (a) Net energy content, (b) CO₂ emissions and overall water use to produce hydrocarbon fuel for transportation in the I-WEST [75,84,85]. The net CO₂ emissions for gasoline, diesel are 4.1 kgCO₂/kg_{gasoline} and 4.08 kgCO₂/kg_{diesel}, respectively [86], while for NG is 5.7 kgCO₂/kg_{NG} [calculated from Figure 4]. Water consumption for extraction and processing of: gasoline is 0.65 and 5 L/L_{gasoline} [75,87], diesel is 0.3 and 5 L/L_{diesel} [75,87], and NG is 0.004 and 0.34 L/kg_{NG} [56].

We can reduce the net CO₂ emissions by displacing gasoline and diesel combustion in transportation with H₂ fuel cells. The conversion efficiency for internal combustion engines using gasoline is only 19%, diesel is 31% and NG is 17% [88] while the H₂ fuel cell efficiency varies from 40% to 60% [89]. Supposing a mean efficiency of about

50% for an H₂ fuel cell vehicle, the overall H₂ required for the transportation demand is 5.72 million-tonne/year. The effect of shifting away from hydrocarbon fuels to H₂ fuel cells is shown in Figure 10a. For the current scenario with 3.5% NG leaks, replacing the existing hydrocarbon fuel source with H_{2,SMR+CCS} could lower the CO₂ emissions by 56%, while regional H_{2,SMR+CCS} could lower the net CO₂ emissions by 71%. While transitioning to H₂ fuel-cell vehicles with H₂ generated from SMR_{CCS} the net water requirement increases by 10% to 274 million m³/year relative to current water demand for the transportation sector. Water electrolysis powered with RE has a net water requirement of 230 million m³/year [Figure 10c]. In addition to the total water requirement, the water quality is also a key parameter since electrolysis and SMR need deionized water, and is generated by the reverse osmosis of freshwater (<500 ppm total dissolved salts, TDS) with 80% recovery. For mining and NG extraction, brackish water (<5000 ppm, TDS) can be used. Moving towards H_{2,SMR+CCS}, and regional H_{2,SMR+CCS} for transportation with the current state of the art will help in reducing the CO₂ emissions by 62–74%, while the water requirement is almost the same. Transitioning from hydrocarbon to H₂ fuel source is significantly cheaper, with a potential saving in fueling cost by 75% with regional H₂ [Figure 10e]. Similarly with use of H₂ generated from electrolysis the net reduction in fuel cost is 60%. For current scenario, CO₂ sequestration credit of 85 \$/ton_{CO2} is assumed while for electrolyzer a credit of 3 \$/kg_{H2} is used. For a current cost of H₂ from electrolyzer is around 6.3 \$/kg_{H2}, and with H₂ credit it reduces to 3.3 \$/kg_{H2}.

In the second example, we evaluate a futuristic case of SMR-H₂ process where the NG leak is decreased to 1%, which is justified by compact infrastructure with increased efficiency of the SMR process. Since the leading driver of NG emissions are leaks, a potential solution is placing the compressors inside boxes to capture all the leaked NG for use as an energy source for compressor pumping. Efforts are also being utilized for lowering emissions using advanced natural gas storage designs with pipeline materials selection. Deploying these advanced designs with process intensification will reduce the energy required in the SMR to 10.4 kWh_{th}/kg_{H2} [see Figure S2 for details]. These cutting edge improvements can also increase capture efficiency to 97% and potential future increases of efficiency to 60% of H₂ fuel cell vehicles [89]. By utilizing the advanced SMR-H₂ process, the transition to H_{2,SMR+CCS}, and regional H_{2,SMR+CCS}, can further reduce the net CO₂ emission by 86%, and 87% respectively [see Figure 10b]. In addition, the overall water required can also reduce [Figure 10d]. Therefore, H_{2,SMR+CCS}, and regional H_{2,SMR+CCS} can be critical in reducing the net CO₂ emissions provided technological advancements reduce both CH₄ leakage and SMR energy consumption. To reduce the water requirement, air cooling is used and with an optimized SMR process, the net water requirement can be reduced by 85%, for both H_{2,SMR+CCS}, and regional H_{2,SMR+CCS}. The net saving in fueling cost is around 78% regional H₂ and 68% with electrolyzer. For future scenarios the cost of H₂ for SMR, SMR+CCS, SMR+RE, regional SMR+CC and electrolyzer is calculated to be 1.5, 2.5, 3, 2.4 and 3.1 \$/kg_{H2}. For future scenarios the carbon credit and hydrogen credit are not considered.

It may be noted that constant average efficiency of 50% and 60% for hydrogen fuel cell vehicles for current and future scenario provides a transparent basis for system-level comparison. In real-world operation, vehicle efficiency is dynamic and incorporating real-time traffic information into energy management frameworks can further enhance vehicle efficiency [90].

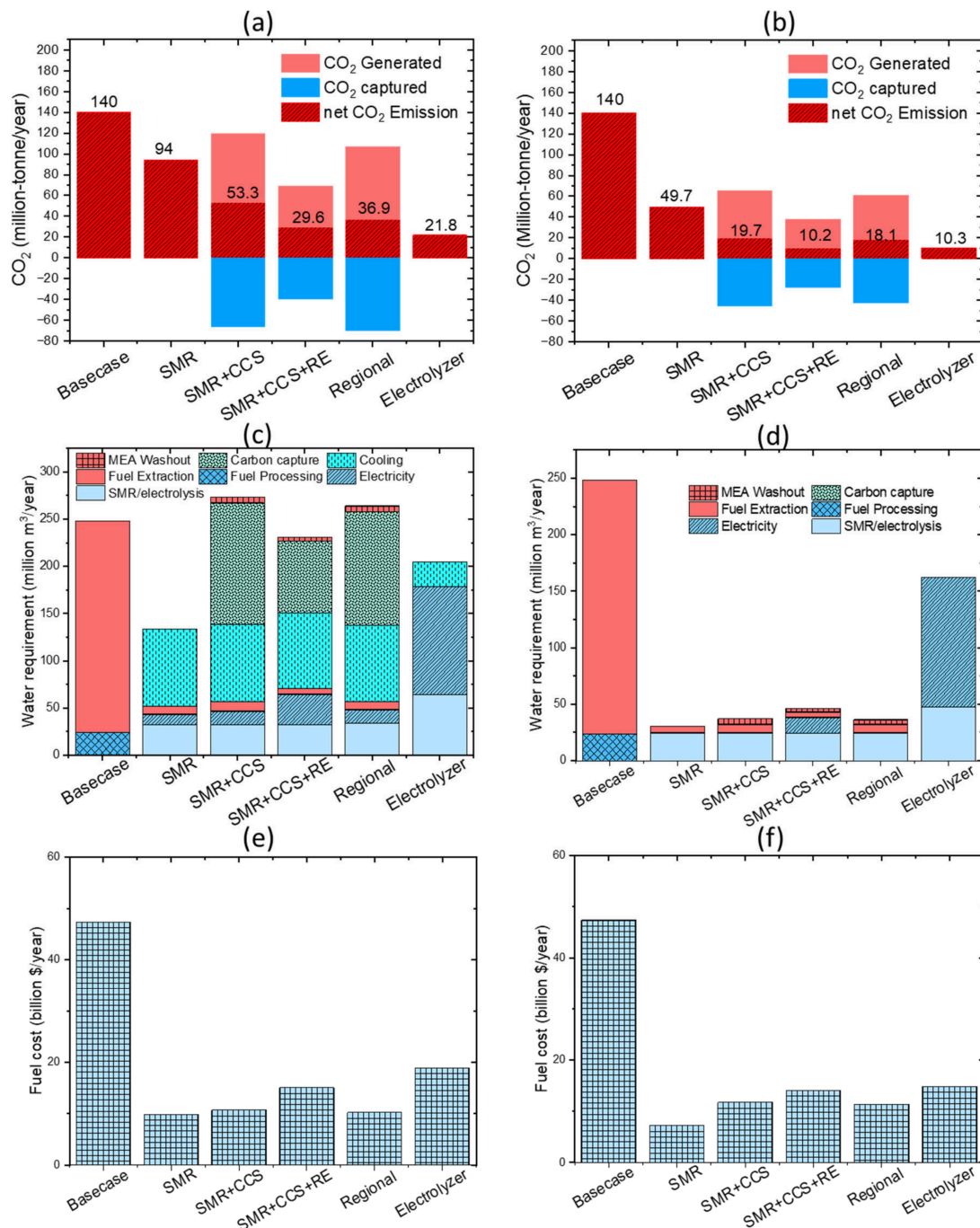


Figure 10. Role of H₂,SMR+CCS, H₂,SMR+CCS+RE and regional H₂,SMR+CCS in decarbonizing the transportation sector for I-WEST for (a,b) present and future scenario, (c,d) the net water consumption for use of H₂ for transportation and (e,f) fuel cost incurred with different H₂ for present and future scenario. For current scenario (NG leak of 3.5%, heating energy of 24.1 kWh/kg, carbon capture efficiency of 90%, fuel cell efficiency of 50%, electrolysis energy requirement of 50 kWh_e/kgH₂ [91] and electrolysis net CO₂ emissions of 3.8 kgCO₂/kgH₂ [92]). For future H₂ production (NG leak of 1%, heating energy of 10.3 kWh/kgH₂, carbon capture efficiency of 97%, fuel cell efficiency of 60% and electrolysis energy requirement of 25 kWh_e/kgH₂ [91] and net CO₂ emissions of 1.8 kgCO₂/kgH₂ [92]). Note that SMR/electrolysis, cooling, processing, and cleaning require freshwater with <500 ppm salt concentration, while mining and MEA washout could utilize brackish water with <5000 ppm salt concentration.

It also may be noted that currently over 80% of the world CO₂ injection is taking place in Permian basin, located in New Mexico and Texas [93]. Just of the many oil and

gas operators are currently storing around 6.5 million-tons of CO₂ per year. The CO₂ captured from transportation sector can be used directly for enhanced oil recovery in Permian basin [93].

4.2. Electricity Generation

Figure 11a shows electricity requirement for the I-WEST region, indicating a yearly production of 315 TWh_e. Coal accounts for 37.7% contribution, NG power plant is 12.7%, NGCC is 12.7%, wind energy 13.5%, nuclear energy 10.1%, hydro energy 6.1%, solar energy is 4.5%, along with modest contributions from petroleum, geothermal and biomass (combined for 0.7%) is also included. The net annual CO₂ emissions from electricity plants is 171 million tons/year, see Figure 11b. Due to the lower efficiency of a coal power plant (33%), the net CO₂ emissions are highest at 69.6%. NGCC contributes 17.5%, while the NGCC contributes 10.7% of the total CO₂ emissions. The net water required for electricity generation is 766 million m³/year [see Figure 11b]. Due to the evaporation of water from the surface of the reservoir surface, hydropower contributes 42% of the total water use, followed by coal 36%, nuclear at 9.6%, NG at 6.4%, and NGCC at 3.9%.

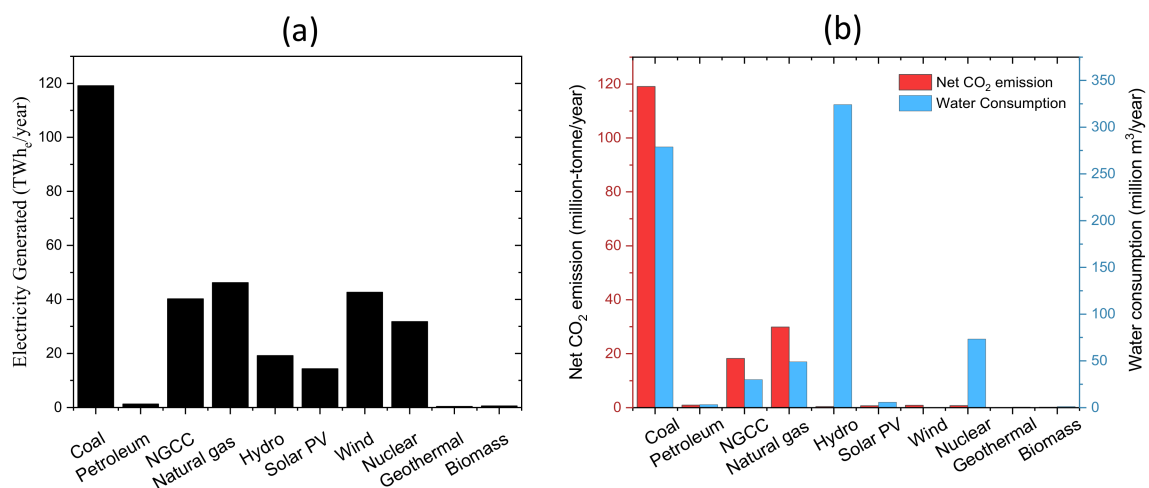


Figure 11. (a) Net electricity production and (b) net CO₂ emissions and water requirements for different energy sources in the I-WEST. The specific CO₂ emissions from coal, petroleum, NG, NGCC, hydropower, solar PV, wind, nuclear, geothermal and biomass are assumed to be 1000, 735, 453, 647, 20, 25, 122 and 300 kg/MWh_e, respectively [56,60,94–98]. The net water usage of a coal power plant is 250 L/tonne_{coal} for coal mining [99] and 2250 L/kWh_e electricity production [100], petroleum requires 0.65 and 5 L/L_{Petroleum} for processing and extraction [75,87] while petroleum power cycle cooling requires 1060 L/MWh_e (updated from [56]), NG and NGCC require 954 and 654 L/MWh_e (updated from [56]), hydropower requires 16,850 L/kWh_e [100], photovoltaic requires 400 L/MWh_e for panel cleaning, [66,67], nuclear power requires 137, 294 and 1875 L/MWh_e (for mining, fuel processing and cooling) [101], geothermal requires 1730 L/MWh_e [100], and biomass requires 2075 L/MWh_e [100].

Figure 12a illustrates the potential pathways towards lowering the CO₂ emissions from electric power generation in the I-WEST. The first potential pathway involves replacing the entire coal-fired units, NG units, and remaining hydrocarbon plants with a NGCC. With the NGCC operating at peak efficiencies (60%), net CO₂ emissions could be lowered by 45% (based on a mean NG leakage of 3.5%), while the net water requirement is reduced by 27% [Figure 10c]. Another approach can be blending the NG with 30% H₂ (by volume) [102,103], as the current NGCC operation is limited to 30% H₂. By blending with 30% regional H_{2,SMR+CCS} while running it as a combined cycle, can reduce the CO₂ emissions by 45%. Similarly, the water requirement reduces by 23.6%, with blended 30% regional H_{2,SMR+CCS}. It may be noted that the potential benefit of 30% H₂ blending with NG is marginal, and it is

better to replace all hydrocarbon power production with NGCC. In addition, the cost of electricity generation also increases marginally due to use of H₂ [see Figure 10e].

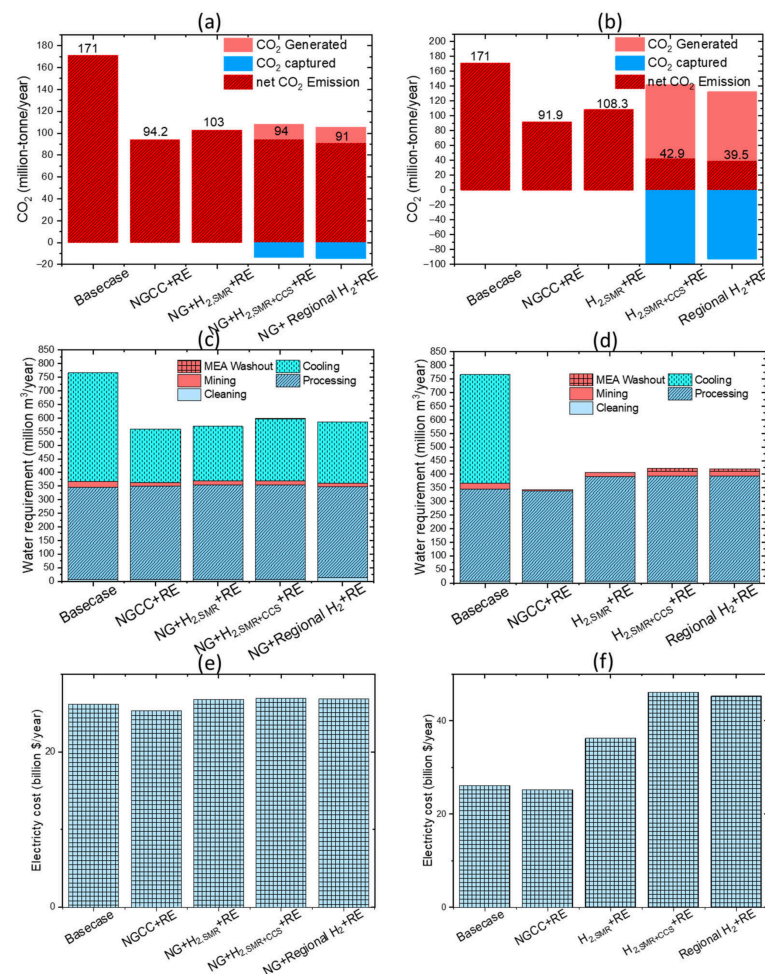


Figure 12. Role of blending 30% by volume H_{2,SMR+CCS}, H_{2,SMR+CCS+RE} and regional H_{2,SMR+CCS} in decarbonizing the electricity sector for I-WEST for (a,b) present and future scenario, (c,d) the net water consumption for use of H₂ for transportation and (e,f) electricity cost different H₂ as energy source for present and future scenario. For current scenario (NG leak of 3.5%, heating energy of 24.1 kWh/kg, carbon capture efficiency of 90% and fuel cell efficiency of 50%). For future H₂ production (NG leak of 1%, heating energy of 10.3 kWh/kg_{H₂}, carbon capture efficiency of 97% and fuel cell efficiency of 60%). Note that SMR/electrolysis, cooling, processing, and cleaning require freshwater with <500 ppm salt concentration, while mining and MEA washout could utilize brackish water with <5000 ppm salt concentration.

As emerging high-efficiency turbines advances, NGCC might be able to operate with 100% H₂ [104]. Moreover, with less NG leaks, energy-efficient SMR, with improved carbon capture, the net CO₂ emissions can be lowered by 77% with regional H_{2,SMR+CCS} [see Figure 10b]. With the use of 100% pure H_{2,SMR+CCS} the amount of carbon capture increases to 100 million-tonne/year. Also, air cooling can reduce the cooling water requirements to zero, thereby the net water requirements can be reduced by 45% for regional H_{2,SMR+CCS} [see Figure 10d]. The major contributor to water requirements is hydropower, requiring around 324 million m³/year of freshwater. However, with use of regional H₂, the cost of electricity generation increases by 73%, and this is predominantly due to higher H₂ cost compared to NG [see Figure 10f].

4.3. Hydrogen Replacement Fuel for Natural Gas in the I-WEST Region

Figure 13a illustrate the overall natural gas capacity in the I-WEST region is about 1894 TWh_{th}/year [25], corresponding to 143 million tons/year of NG. In the I-WEST region, New Mexico is the major contributor to NG production at 40.2%. It may be noted that Arizona does not produce NG. If we have to convert all the NG to regional H_{2,SMR+CCS}, around 30 million-tonne/year of H₂ can be produced [see Figure 13b], (for current SMR with 3.5% NG leak). However, for the future scenario (1% NG leak), 40 million-tons/year of regional H_{2,SMR+CCS} can be produced respectively. Notably, net H₂ production varies significantly as the net NG demand varies with H₂ process [see Section 3.3].

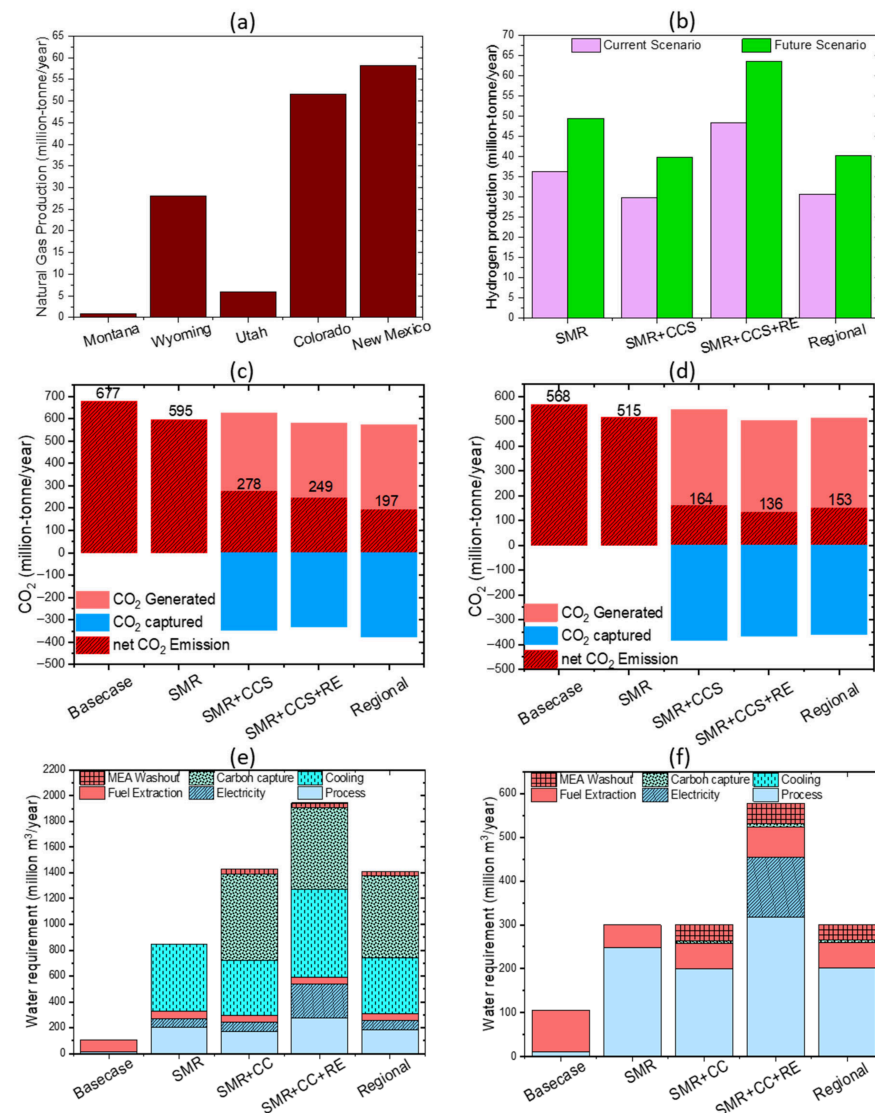


Figure 13. (a) annual NG output, (b) estimated H₂ output based on yearly NG production for near-term and long-term scenarios, (c) impact on CO₂ emissions during the shift from NG to hydrogen in the near-term (d) long-term scenario, and (e) net water demand to transition towards different hydrogen production based on the current scenario and (f) future scenario. The current scenario assumes 3.5% NG leak, 24.1 kWh_{th}/kg_{H₂} SMR heating required with a CO₂ capture efficiency of 90%. The future scenario assumes 1% NG leak, 10.3 kWh_{th}/kg_{H₂} heating required with a CO₂ capture efficiency of 97%. It may be noted MEA washout and fuel extraction require brackish quality water with total salt concentration <5000 ppm, while the process, cooling and carbon capture require fresh water with salt concentration <500 ppm.

Figure 13c,d show the net CO₂ generated while producing H₂ from NG. For the base case of NG production with a 3.5% NG leak, the net CO₂ emissions is 676 million-tonne/year. With H_{2,SMR+CCS+RE} and regional H_{2,SMR+CCS} can help in reducing the CO₂ emissions by 63%, and 70%, respectively. Notably, the net reduction in CO₂ emissions with H_{2,SMR+CCS+RE} is lower due to the 60% higher H₂ production than regional H_{2,SMR+CCS}. With a future scenario of 1% NG leak, the net reduction in CO₂ emission can be 73% for regional H_{2,SMR+CCS}.

Figure 13e,f show the water use for different cases under a base case of 105 million m³/year. The net rise in overall water use in comparison with the base case is by a factor of 19 and 14 for H_{2,SMR+CCS+RE}, and regional H_{2,SMR+CCS}, respectively. As already explained, the major contributor to water demand is cooling water, which is required for electricity, systems, and carbon capture. Using an air cooler, for future scenarios, net water demand can be reduced by 70% compared to the current scenario [see Figure 13f].

5. Conclusions

Our life cycle analysis demonstrates that regional H₂ can be important in decarbonizing the energy sector of the I-WEST region. Numerous studies presented in the literature have compared different hydrogen production scenarios from a large-scale perspective and neglected the advantages of regional resource availability. Our study quantifies the primary drivers of carbon footprints when making hydrogen. Although NG leaks remain the dominant factor in adopting H₂ energy, the other dominant factor is still the specific energy usage for H₂ processes.

To highlight the practical relevance of H₂ in achieving a low-emissions energy sector, we have considered substituting fossil fuels currently used in the transportation and electrical power generation sectors with H₂ in the I-WEST region. I-WEST transportation contributes to 140 million-tons/year of CO₂ and requires 248 million m³/year of water. For the base case scenario, the regional H₂ with carbon management can lower the overall CO₂ emissions by 74%, and the fuel cost for transportation can be reduced by 76%. Replacing all fossil fuel powered electricity production with the natural gas combined cycle can reduce CO₂ emissions by 45%. However, H₂ blending with natural gas does not give a significant improvement in CO₂ reduction relative to converting all NG to NGCC plants. However, future scenarios using 100% hydrogen for electricity generation can result in an 77% reduction in CO₂ emissions, but the electricity cost will increase by 73%. Using regional H₂ in the I-WEST transportation and electricity sectors can potentially reduce the net CO₂ emission by 87%, and water consumption by 55% in the future. However, this would need a 50.5% increase in natural gas production.

Making hydrogen requires substantial amounts of water, especially when potable water is the source. Future research will focus on developing an adoption curve for these H₂ production technologies. In addition, other H₂ production processes, including autothermal reforming, partial oxidation, biomass reforming, and electrolysis, will be assessed in detail, together with the industry standard SMR process.

Our future work will focus on dynamic modeling with detailed control schemes to optimize hydrogen production. Additionally, we plan to extend the current analysis of transportation to supply-chain models that incorporate dynamic, traffic-informed vehicle energy management strategies.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/cleantechnol8030077/s1>. Figure S1. Composite curve for steam methane reformer process; Figure S2. Composite curve for steam methane reformer process with pinch temperature of 10 °C; Figure S3. (a) Net CO₂ emission as a function of NG leakage while the SMR energy requirement, carbon capture efficiency and heating energy requirement are kept constant

at $24.1 \text{ kWh}_{\text{th}}/\text{kg}_{\text{H}_2}$ and 90%. (b) Net CO_2 emission as a function of SMR energy requirement, while the NG leakage and carbon capture efficiency are kept constant at 3.5% and 90%. (c) Net CO_2 emission as a function of carbon capture efficiency and NG leak, while the SMR heating energy requirement is kept constant at $24.1 \text{ kWh}_{\text{th}}/\text{kg}_{\text{H}_2}$ and (d) Comparison between the performance of $\text{H}_{2,\text{SMR}+\text{CCS}}$ and $\text{H}_{2,\text{SMR}+\text{CCS}+\text{RE}}$ powered with different renewable energy including solar photovoltaics, wind energy, concentrating solar thermal and battery powered Renewable energy. NG leak, carbon capture efficiency and energy requirement are kept constant at 3.5%, and 90%; Figure S4. Water requirement for different H_2 production process, with cooling water supplied from produced water; Figure S5. Water requirement for different H_2 production process, with air cooling for electricity, SMR and carbon capture; Table S1. Typical pipeline composition of NG flowing through an interstate pipeline; Table S2. Mass, energy, and momentum balance equations of the SMR and WGS models; Table S3. Global warming potential for different constituent of natural gas; Table S3. Global warming potential for different constituent of natural gas; Table S4. Compressor energy required for natural gas; Table S5. Stream flow data for the SMR process; Table S6. Net energy consumption for H_2 production; Table S7. Net energy consumption for H_2 production with optimized scenario; Table S8. Life cycle analysis for H_2 production for 3.5% NG leak, 1% H_2 leak from compressor while the SMR energy heating energy requirement of $24.1 \text{ kWh}_{\text{th}}/\text{kg}_{\text{H}_2}$; Table S9. Operating parameters for different renewable energy sources. References [41,55,60,61,63,70,71,77,105–110] are cited in the Supplementary Materials.

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Nomenclature

a	Site occupied by the adsorbate in PSA
C_{pg}	Gas mixture heat capacity ($\text{J kg}^{-1}\text{K}^{-1}$)
C_i	Concentration of gas component i (mol m^{-3})
CCS	Carbon capture and sequestration
CH_4	Methane
C_2H_6	Ethane
C_3H_8	Propane
C_4H_{10}	Butane
CO	Carbon Monoxide
CO_2	Carbon Dioxide
DI	Deionized
D_L	Axial mass dispersion constant (m^2s^{-1})
d_p	Particle diameter (m)
E	Energy required

$h_{out,s}$	Isentropic enthalpy
h_{in}	Inlet enthalpy
H ₂ O	Water
I-WEST	Intermountain West USA
H ₂	Hydrogen
$\dot{m}$	Mass flowrate
MEA	Monoethanolamine
N ₂	Nitrogen
NG	Natural gas
NGCC	Natural gas combined cycle
q	Saturation concentration
Q	Heat transferred
PSA	Pressure swing adsorption
P	Pressure
RE	Renewable Energy
RO	Reverse osmosis
r_j	Reaction rate of reaction j ($\text{mol kg}_{\text{cat}}^{-1}\text{s}^{-1}$)
S	Steam to methane ratio
SMR	Steam Methane reforming
T	Temperature
T_w	Wall temperature
t	Time
TEA	Techno-economic Analysis
u_z	Interstitial velocity (ms^{-1})
U	Solid thermal conductivity ($\text{Wm}^{-1}\text{K}^{-1}$)
$\dot{w}_{\text{comp}}$	Compressor work
WGS	Water gas shift
x	SMR conversion efficiency
$\eta_{\text{isen, comp}}$	Isentropic efficiency of compressor
z	Reactor axial length
ϵ_b	Bed porosity
ρ_s	Catalyst density (kgm^{-3})
ρ_g	Gas mixture density (kgm^{-3})
ν_{ij}	Stoichiometry coefficient of reaction j component i
η_j	Effectiveness factor of reaction j
λ	Effectiveness thermal conductivity ($\text{Wm}^{-1}\text{K}^{-1}$)
ΔH_r	Heat of reaction (Jmol^{-1})
μ	Gas mixture viscosity ($\text{Pa}\cdot\text{s}$)

References

- Chen, F.; Ma, Z.; Nasrabadi, H.; Chen, B.; Mehana, M.Z.S.; Van Wijk, J. Capacity assessment and cost analysis of geologic storage of hydrogen: A case study in Intermountain-West Region USA. *Int. J. Hydrogen Energy* **2023**, *48*, 9008–9022. [CrossRef]
- Erdener, B.C.; Sergi, B.; Guerra, O.J.; Chueca, A.L.; Pambour, K.; Brancucci, C.; Hodge, B.M. A review of technical and regulatory limits for hydrogen blending in natural gas pipelines. *Int. J. Hydrogen Energy* **2023**, *48*, 5595–5617. [CrossRef]
- Dawood, F.; Anda, M.; Shafiullah, G.M. Hydrogen production for energy: An overview. *Int. J. Hydrogen Energy* **2020**, *45*, 3847–3869. [CrossRef]
- Ajanovic, A.; Sayer, M.; Haas, R. The economics and the environmental benignity of different colors of hydrogen. *Int. J. Hydrogen Energy* **2022**, *47*, 24136–24154. [CrossRef]
- Epstein, P. Hydrogens Present and Future in the us Energy Sector, New York. 2021. Available online: <https://www.aoshearman.com/en/insights/hydrogens-present-and-future-in-the-us-energy-sector> (accessed on 24 April 2024).
- Turner, J.A. A Realizable Renewable Energy Future. *Science* **1999**, *285*, 687–689. [CrossRef]
- Meziane, S.; Bentebbiche, A. Numerical study of blended fuel natural gas-hydrogen combustion in rich/quench/lean combustor of a micro gas turbine. *Int. J. Hydrogen Energy* **2019**, *44*, 15610–15621. [CrossRef]

8. Pocha, C.K.R.; Chia, W.Y.; Silvanir; Kurniawan, T.A.; Khoo, K.S.; Chew, K.W. Thermochemical conversion of different biomass feedstocks into hydrogen for power plant electricity generation. *Fuel* **2023**, *340*, 127472. [CrossRef]
9. Welder, L.; Stenzel, P.; Ebersbach, N.; Markewitz, P.; Robinus, M.; Emonts, B.; Stolten, D. Design and evaluation of hydrogen electricity reconversion pathways in national energy systems using spatially and temporally resolved energy system optimization. *Int. J. Hydrogen Energy* **2019**, *44*, 9594–9607. [CrossRef]
10. Zhang, Y.; Cheng, X.; Zhao, J.; Yang, F.; Cheng, F. Effect of Particle Size on Simultaneous Calcination and Sulfation of Limestone. *Int. J. Energy A Clean. Environ.* **2023**, *24*, 163–175. [CrossRef]
11. Zapantis, A. Blue Hydrogen, n.d. Available online: <https://www.globalccsinstitute.com/wp-content/uploads/2021/04/Circular-Carbon-Economy-series-Blue-Hydrogen.pdf> (accessed on 2 April 2024).
12. Diglio, M.; Contento, I.; Impemba, S.; Berretti, E.; Della Sala, P.; Oliva, G.; Naddeo, V.; Caporali, S.; Primo, A.; Talotta, C.; et al. Hydrogen production from formic acid decomposition promoted by gold nanoparticles supported on a porous polymer matrix. *Energy Fuels* **2025**, *39*, 14320–14329. [CrossRef]
13. Impemba, S.; Provinciali, G.; Filippi, J.; Caporali, S.; Muzzi, B.; Casini, A.; Caporali, M. Tightly Interfaced Cu₂O with In₂O₃ to Promote Hydrogen Evolution in Presence of Biomass-Derived Alcohols. *ChemNanoMat* **2024**, *10*, e202400459. [CrossRef]
14. Howarth, R.W.; Jacobson, M.Z. How green is blue hydrogen? *Energy Sci. Eng.* **2021**, *9*, 1676–1687. [CrossRef]
15. Bauer, C.; Treyer, K.; Antonini, C.; Bergerson, J.; Gazzani, M.; Gencer, E.; Gibbins, J.; Mazzotti, M.; McCoy, S.T.; McKenna, R.; et al. On the climate impacts of blue hydrogen production. *Sustain. Energy Fuels* **2022**, *6*, 66–75. [CrossRef]
16. Patel, G.H.; Havukainen, J.; Horttanainen, M.; Soukka, R.; Tuomaala, M. Climate change performance of hydrogen production based on life cycle assessment. *Green. Chem.* **2024**, *26*, 992–1006. [CrossRef]
17. Zang, G.; Graham, E.J.; Mallapragada, D. H₂ production through natural gas reforming and carbon capture: A techno-economic and life cycle analysis comparison. *Int. J. Hydrogen Energy* **2024**, *49*, 1288–1303. [CrossRef]
18. Kolb, S.; Müller, J.; Luna-Jaspe, N.; Karl, J. Renewable hydrogen imports for the German energy transition—A comparative life cycle assessment. *J. Clean. Prod.* **2022**, *373*, 133289. [CrossRef]
19. Li, Y.; Ren, J.; Ma, H.; Campbell, A.N. Technical and economic performance assessment of blue hydrogen production using new configuration through modelling and simulation. *Int. J. Greenh. Gas. Control* **2024**, *134*, 104112. [CrossRef]
20. Mehmeti, A.; Angelis-Dimakis, A.; Arampatzis, G.; McPhail, S.J.; Ulgiati, S. Life cycle assessment and water footprint of hydrogen production methods: From conventional to emerging technologies. *Environments* **2018**, *5*, 24. [CrossRef]
21. Al-Khelaiwi, M.S.; Al-Masaabi, T.A.; Farag, H.; Rehman, S. Evaluation of Green and Blue Hydrogen Production Potential in Saudi Arabia. *Energy Convers. Manag. X* **2024**, *24*, 100742. [CrossRef]
22. Olaitan, D.; Bertagni, M.; Porporato, A. The water footprint of hydrogen production. *Sci. Total Environ.* **2024**, *927*, 172384. [CrossRef] [PubMed]
23. Simoes, S.G.; Catarino, J.; Picado, A.; Lopes, T.F.; di Berardino, S.; Amorim, F.; Gírio, F.; Rangel, C.M.; de Leão, T.P. Water availability and water usage solutions for electrolysis in hydrogen production. *J. Clean. Prod.* **2021**, *315*, 128124. [CrossRef]
24. Shi, X.; Liao, X.; Li, Y. Quantification of fresh water consumption and scarcity footprints of hydrogen from water electrolysis: A methodology framework. *Renew. Energy* **2020**, *154*, 786–796. [CrossRef]
25. EIA. State Profiles and Energy Estimates. 2024. Available online: <https://www.eia.gov/state/data.php?sid=NM> (accessed on 16 January 2024).
26. Romano, M.C.; Antonini, C.; Bardow, A.; Bertsch, V.; Brandon, N.P.; Brouwer, J.; Campanari, S.; Crema, L.; Dodds, P.E.; Gardarsdottir, S.; et al. Comment on “How green is blue hydrogen?”. *Energy Sci. Eng.* **2022**, *10*, 1944–1954. [CrossRef]
27. Longden, T.; Beck, F.J.; Jotzo, F.; Andrews, R.; Prasad, M. Clean’ hydrogen?—Comparing the emissions and costs of fossil fuel versus renewable electricity based hydrogen. *Appl. Energy* **2022**, *306*, 118145. [CrossRef]
28. Karacan, C.Ö.; Brennan, S.T.; Buursink, M.L.; Freeman, P.A.; Lohr, C.D.; Merrill, M.D.; Olea, R.A.; Warwick, P.D. A residual oil zone (ROZ) assessment methodology with application to the central basin platform (Permian Basin, USA) for enhanced oil recovery (EOR) and long-term geologic CO₂ storage. *Geoenergy Sci. Eng.* **2023**, *230*, 212275. [CrossRef]
29. Olalotiti-Lawal, F.; Onishi, T.; Datta-Gupta, A.; Fujita, Y.; Watanabe, D.; Hagiwara, K. Model calibration and optimization of a post-combustion CO₂ WAG pilot in a mature oil field. *Fuel* **2019**, *255*, 115810. [CrossRef]
30. Zhang, R.; Datta-Gupta, A.; Park, J.; Nunna, K.; Briz, E.; Gordillo, R.; Chen, H. Multi-stage three-phase and compositional history matching: Field application to CO₂ enhanced oil recovery in the Permian Basin, Texas. *Fuel* **2025**, *387*, 134339. [CrossRef]
31. Anzelmo, B.; Wilcox, J.; Liguori, S. Hydrogen production via natural gas steam reforming in a Pd-Au membrane reactor. Comparison between methane and natural gas steam reforming reactions. *J. Memb. Sci.* **2018**, *568*, 113–120. [CrossRef]
32. Xu, J.; Froment, G.F. Methane steam reforming, methanation and water-gas shift: I. Intrinsic kinetics. *AIChE J.* **1989**, *35*, 88–96. [CrossRef]
33. Marín, P.; Patiño, Y.; Díez, F.V.; Ordóñez, S. Modelling of hydrogen perm-selective membrane reactors for catalytic methane steam reforming. *Int. J. Hydrogen Energy* **2012**, *37*, 18433–18445. [CrossRef]

34. Thengane, S.K.; Hoadley, A.; Bhattacharya, S.; Mitra, S.; Bandyopadhyay, S. Exergy efficiency improvement in hydrogen production process by recovery of chemical energy versus thermal energy. *Clean. Technol. Environ. Policy* **2016**, *18*, 1391–1404. [CrossRef]
35. Minette, F.; de Almeida, L.C.; Ratan, S.; De Wilde, J. Pressure drop and heat transfer of ZoneFlow™ structured catalytic reactors and reference pellets for Steam Methane Reforming. *Chem. Eng. J.* **2021**, *417*, 128080. [CrossRef]
36. Tabrizi, F.F.; Mousavi, S.A.H.S.; Atashi, H. Thermodynamic analysis of steam reforming of methane with statistical approaches. *Energy Convers. Manag.* **2015**, *103*, 1065–1077. [CrossRef]
37. Moon, D.K.; Lee, D.G.; Lee, C.H. H₂ pressure swing adsorption for high pressure syngas from an integrated gasification combined cycle with a carbon capture process. *Appl. Energy* **2016**, *183*, 760–774. [CrossRef]
38. Sharan, P.; Bandyopadhyay, S. Integration of multiple effect evaporators with background process. *Chem. Eng. Trans.* **2015**, *45*, 1591–1596. [CrossRef]
39. Bandyopadhyay, S.; Sahu, G.C. Modified problem table algorithm for energy targeting. *Ind. Eng. Chem. Res.* **2010**, *49*, 11557–11563. [CrossRef]
40. Sharan, P.; Bandyopadhyay, S. Integration of thermo-vapor compressor with multiple-effect evaporator. *Appl. Energy* **2016**, *184*, 560–573. [CrossRef]
41. Song, C.; Liu, Q.; Ji, N.; Kansha, Y.; Tsutsumi, A. Optimization of steam methane reforming coupled with pressure swing adsorption hydrogen production process by heat integration. *Appl. Energy* **2015**, *154*, 392–401. [CrossRef]
42. Peng, X.D. Analysis of the thermal efficiency limit of the steam methane reforming process. *Ind. Eng. Chem. Res.* **2012**, *51*, 16385–16392. [CrossRef]
43. Biermann, M.; Normann, F.; Johnsson, F.; Hoballah, R.; Onarheim, K. Capture of CO₂ from Steam Reformer Flue Gases Using Monoethanolamine: Pilot Plant Validation and Process Design for Partial Capture. *Ind. Eng. Chem. Res.* **2022**, *61*, 14305–14323. [CrossRef]
44. Nema, A.; Kumar, A.; Warudkar, V. An in-depth critical review of different carbon capture techniques: Assessing their effectiveness and role in reducing climate change emissions. *Energy Convers. Manag.* **2025**, *323*, 119244. [CrossRef]
45. Akinmoladun, A.; Tomomewo, O.S. Advances and future perspectives in post-combustion carbon capture technology using chemical absorption process: A review. *Carbon Capture Sci. Technol.* **2025**, *16*, 100461. [CrossRef]
46. Smith, K.H.; Ashkanani, H.E.; Morsi, B.I.; Siefert, N.S. Physical solvents and techno-economic analysis for pre-combustion CO₂ capture: A review. *Int. J. Greenh. Gas. Control* **2022**, *118*, 103694. [CrossRef]
47. Kim, H.; Hwang, S.J.; Lee, K.S. Novel shortcut estimation method for regeneration energy of amine solvents in an absorption-based carbon capture process. *Environ. Sci. Technol.* **2015**, *49*, 1478–1485. [CrossRef] [PubMed]
48. Puxty, G.; Maeder, M. A simple chemical model to represent CO₂-amine-H₂O vapour-liquid-equilibria. *Int. J. Greenh. Gas. Control* **2013**, *17*, 215–224. [CrossRef]
49. Aronu, U.E.; Lauritsen, K.G.; Grimstvedt, A.; Mejdell, T. Impact of heat stable salts on equilibrium CO₂ absorption. *Energy Procedia* **2014**, *63*, 1781–1794. [CrossRef]
50. Ambrosetti, M.; Beretta, A.; Groppi, G.; Tronconi, E. A Numerical Investigation of Electrically-Heated Methane Steam Reforming Over Structured Catalysts. *Front. Chem. Eng.* **2021**, *3*, 747636. [CrossRef]
51. From, T.N.; Partoon, B.; Rautenbach, M.; Østberg, M.; Bentien, A.; Aasberg-Petersen, K.; Mortensen, P.M. Electrified steam methane reforming of biogas for sustainable syngas manufacturing and next-generation of plant design: A pilot plant study. *Chem. Eng. J.* **2024**, *479*, 147205. [CrossRef]
52. Wismann, S.T.; Engbaek, J.S.; Vendelbo, S.B.; Bendixen, F.B.; Eriksen, W.L.; Aasberg-Petersen, K.; Frandsen, C.; Chorkendorff, I.; Mortensen, P.M. Electrified Methane Reforming: A Compact Approach to Greener Industrial Hydrogen Production n.d. Available online: <https://www.science.org> (accessed on 24 April 2024).
53. Shagdar, E.; Lougou, B.G.; Shuai, Y.; Ganbold, E.; Chinonso, O.P.; Tan, H. Process analysis of solar steam reforming of methane for producing low-carbon hydrogen. *RSC Adv.* **2020**, *10*, 12582–12597. [CrossRef]
54. Gunawan, A.; Singh, A.K. A solar thermal sorption-enhanced steam methane reforming (SE-SMR) approach and its performance assessment. *Sustain. Energy Technol. Assess.* **2022**, *52*, 102036. [CrossRef]
55. Florida Power & Light Company. Natural Gas Specs Sheet. 2004. Available online: https://www.naesb.org/pdf2/wgq_bps100605w2.pdf (accessed on 24 April 2024).
56. Laurenzi, I.J.; Jersey, G.R. Life cycle greenhouse gas emissions and freshwater consumption of marcellus shale gas. *Environ. Sci. Technol.* **2013**, *47*, 4896–4903. [CrossRef]
57. Boms, A.; Aka, N.; Godwin, C.; Jacob, E.; Emmanuel, O. Estimating Pressure Drop in Natural Gas Pipeline: (A Case Study of Rumuji-Bonny NLNG Pipeline). *Int. J. Sci. Eng. Res.* **2017**, *8*, 822–830.
58. Chen, J.; Song, W.; Xu, D. Compact Steam-Methane Reforming for the Production of Hydrogen in Continuous Flow Microreactor Systems. *ACS Omega* **2019**, *4*, 15600–15614. [CrossRef]

59. Hydrogen and Fuel Cell Technologies Office. Gaseous Hydrogen Delivery. 2023. Available online: <https://www.energy.gov/cmei/fuels/2023-hydrogen-and-fuel-cell-technologies-office-webinar-archives> (accessed on 24 April 2024).
60. Life Cycle Greenhouse Gas Emissions from Concentrating Solar Power (Fact Sheet), NREL (National Renewable Energy Laboratory), (n.d.). Available online: https://www.google.com/url?sa=t&rct=j&q=&esrc=s&source=web&cd=&ved=2ahUKEwiNqviHgsf6AhVtjokEHf5nCMUQFnoECAYQAQ&url=https://www.nrel.gov/docs/fy13osti/56416.pdf&usg=AOvVaw2EZQxNcLYAn_pJZdql-cRr (accessed on 3 October 2022).
61. Sharan, P.; Neises, T.; McTigue, J.; Turchi, C. Cogeneration using multi-effect distillation and a solar-powered supercritical carbon dioxide Brayton cycle. *Desalination* **2019**, *459*, 20–33. [CrossRef]
62. Sharan, P.; Neises, T.; Turchi, C. Thermal desalination via supercritical CO₂ Brayton cycle: Optimal system design and techno-economic analysis without reduction in cycle efficiency. *Appl. Therm. Eng.* **2019**, *152*, 499–514. [CrossRef]
63. Aili, A.; Zhao, D.; Tan, G.; Yin, X.; Yang, R. Reduction of water consumption in thermal power plants with radiative sky cooling. *Appl. Energy* **2021**, *302*, 117515. [CrossRef]
64. Panja, P.; McPherson, B.; Deo, M. Techno-Economic Analysis of Amine-based CO₂ Capture Technology: Hunter Plant Case Study. *Carbon Capture Sci. Technol.* **2022**, *3*, 100041. [CrossRef]
65. Liu, F.; Qi, Z.; Fang, M.; Wang, T.; Yi, N. Evaluation on water balance and amine emission in CO₂ capture. *Int. J. Greenh. Gas. Control.* **2021**, *112*, 103487. [CrossRef]
66. Meldrum, J.; Nettles-Anderson, S.; Heath, G.; Macknick, J. Life cycle water use for electricity generation: A review and harmonization of literature estimates. *Environ. Res. Lett.* **2013**, *8*, 015031. [CrossRef]
67. Sinha, P.; Meader, A.; De Wild-Scholten, M. Life cycle water usage in CdTe photovoltaics. *IEEE J. Photovolt.* **2013**, *3*, 429–432. [CrossRef]
68. Tran, A.; Aguirre, A.; Durand, H.; Crose, M.; Christofides, P.D. CFD modeling of a industrial-scale steam methane reforming furnace. *Chem. Eng. Sci.* **2017**, *171*, 576–598. [CrossRef]
69. Tutar, M.; Üstün, C.E.; Campillo-Robles, J.M.; Fuente, R.; Cibrián, S.; Arzua, I.; Fernández, A.; López, G.A. Optimized CFD modelling and validation of radiation section of an industrial top-fired steam methane reforming furnace. *Comput. Chem. Eng.* **2021**, *155*, 107504. [CrossRef]
70. Spath, P.L.; Mann, M.K. *Life Cycle Assessment of Hydrogen Production via Natural Gas Steam Reforming*; Technical Report No. NREL/TP-570-27637; National Renewable Energy Lab: Golden, CO, USA, 2000.
71. Kirchgessner, D.A.; Lott, R.A.; Cowgill, R.M.; Harrison, M.R.; Shires, T.M. Estimate of Methane Emissions from the U.S. Natural Gas Industry. *Chemosphere* **1997**, *35*, 1365–1390. [CrossRef]
72. Ocko, I.B.; Hamburg, S.P. Climate consequences of hydrogen emissions. *Atmos. Chem. Phys.* **2022**, *22*, 9349–9368. [CrossRef]
73. Sharan, P.; Yoon, T.J.; Jaffe, S.M.; Ju, T.; Currier, R.P.; Findikoglu, A.T. Can capacitive deionization outperform reverse osmosis for brackish water desalination? *Clean. Eng. Technol.* **2021**, *3*, 100102. [CrossRef]
74. Ali, S.W.M.; Vahedi, N.; Romero, C.; Oztekin, A. An optimization for water requirement in natural gas combined cycle power plants equipped with once-through and hybrid cooling systems and carbon capture unit. *Water-Energy Nexus* **2020**, *3*, 117–134. [CrossRef]
75. Wu, M.; Mintz, M.; Wang, M.; Arora, S. Water consumption in the production of ethanol and petroleum gasoline. *Environ. Manag.* **2009**, *44*, 981–997. [CrossRef]
76. Macknick, J.; Newmark, R.; Heath, G.; Hallett, K.C. A Review of Operational Water Consumption and Withdrawal Factors for Electricity Generating Technologies. 2011. Available online: <http://www.osti.gov/bridge> (accessed on 24 April 2024).
77. Sharan, P.; Thengane, S.K.; Yoon, T.J.; Lewis, J.C.; Singh, R.; Currier, R.P.; Findikoglu, A.T. A novel approach for produced water treatment: Supercritical water oxidation and desalination. *Desalination* **2022**, *532*, 115716–115727. [CrossRef]
78. Qi, W.; Lan, P.; Yang, J.; Chen, Y.; Zhang, Y.; Wang, G.; Peng, F.; Hong, J. Multi-U-Style micro-channel in liquid cooling plate for thermal management of power batteries. *Appl. Therm. Eng.* **2024**, *256*, 123984. [CrossRef]
79. Lee, S.; Kim, H.S.; Park, J.; Kang, B.M.; Cho, C.H.; Lim, H.; Won, W. Scenario-based techno-economic analysis of steam methane reforming process for hydrogen production. *Appl. Sci.* **2021**, *11*, 6021. [CrossRef]
80. EIA. Natural Gas Prices. Available online: https://www.eia.gov/dnav/ng/ng_pri_sum_dcu_nus_m.htm (accessed on 24 April 2024).
81. Yoon, T.J.; Sharan, P.; Craddock, E.P.; Lewis, J.C.; Matteson, J.A.; Seong, J.G.; Singh, R.P.; Maerzke, K.A.; Currier, R.P.; Findikoglu, A.T. Selective recovery of critical materials in zero-liquid discharge supercritical water desalination. *Desalination* **2022**, *537*, 115849. [CrossRef]
82. Bright, M. A The Inflation Reduction Act Creates a Whole New Market for Carbon Capture. Clean Air Task Force. 2022. Available online: <https://www.catf.us/2022/08/the-inflation-reduction-act-creates-a-whole-new-market-for-carbon-capture/> (accessed on 24 April 2024).
83. Ding, Y.; Baldino, C.; Zhou, Y. Understanding the Proposed Guidance for the Inflation Reduction Act’s Section 45V Clean Hydrogen Production Tax Credit n.d. Available online: <https://theicct.org/publication/proposed-guidance-for-the-inflation-reduction-act-45v-clean-hydrogen-tax-credit-mar29/> (accessed on 28 August 2024).

84. DOE. Alternative Fuels Data Center: State Information. Available online: <https://afdc.energy.gov/states> (accessed on 20 October 2022).
85. Magnuson, M.L.; Julie, P.E.; Valdez, M.; Lawler, C.R.; Nelson, M.; Petronis, L. New Mexico Water Use by Categories. 2015. Available online: <https://mainstreamnm.org/wp-content/uploads/2024/01/2015-Water-Use-and-Conservation-Report.pdf> (accessed on 20 October 2024).
86. Wang, M.; Han, J.; Elgowainy, A. The Life-Cycle Analysis of Petroleum Fuels and Biofuels with GREET. 2016. Available online: https://ww2.arb.ca.gov/sites/default/files/classic/fuels/lcfs/lcfs_meetings/12132016wang.pdf (accessed on 20 October 2024).
87. Sun, P.; Elgowainy, A.; Wang, M.; Han, J.; Henderson, R.J. Estimation of U.S. refinery water consumption and allocation to refinery products. *Fuel* **2018**, *221*, 542–557. [\[CrossRef\]](#)
88. Albatayneh, A.; Assaf, M.N.; Alterman, D.; Jaradat, M. Comparison of the Overall Energy Efficiency for Internal Combustion Engine Vehicles and Electric Vehicles. *Environ. Clim. Technol.* **2020**, *24*, 669–680. [\[CrossRef\]](#)
89. Cigolotti, V.; Genovese, M.; Fragiaco, P. Comprehensive review on fuel cell technology for stationary applications as sustainable and efficient poly-generation energy systems. *Energies* **2021**, *14*, 4963. [\[CrossRef\]](#)
90. Zhang, Y.; Xu, S.; Song, Y.; Qi, W.; Guo, Q.; Li, X.; Kong, L.; Chen, J. Real-Time Global Optimal Energy Management Strategy for Connected PHEVs Based on Traffic Flow Information. *IEEE Trans. Intell. Transp. Syst.* **2024**, *25*, 20032–20042. [\[CrossRef\]](#)
91. Aulakh, D.J.S.; Boulama, K.G.; Pharoah, J.G. On the reduction of electric energy consumption in electrolysis: A thermodynamic study. *Int. J. Hydrogen Energy* **2021**, *46*, 17084–17096. [\[CrossRef\]](#)
92. Weidner, T.; Tulus, V.; Guillén-Gosálbez, G. Environmental sustainability assessment of large-scale hydrogen production using prospective life cycle analysis. *Int. J. Hydrogen Energy* **2023**, *48*, 8310–8327. [\[CrossRef\]](#)
93. Duncan, I. CO₂ Enhanced Oil Recovery: A Key Bridge to Large Scale CO₂ Sequestration n.d. Available online: <https://naturalresources.house.gov/uploadedfiles/duncantestimony06.12.08.pdf> (accessed on 31 October 2025).
94. EIA. Carbon Dioxide Emissions Coefficients. 2024. Available online: https://www.eia.gov/environment/emissions/co2_vol_mass.php (accessed on 24 April 2024).
95. Schlömer, S.; Bruckner, T.; Fulton, L.; Austria, E.H.; McKinnon, A.U.; Perczyk, D.; Roy, J.; Schaeffer, R.; Hänsel, G.; de Jager, D.; et al. Annex III: Technology-specific Cost and Performance Parameters. In *Climate Change 2014: Mitigation of Climate Change*; Cambridge University Press: Cambridge, UK, 2014; pp. 1329–1356. Available online: https://www.ipcc.ch/site/assets/uploads/2018/02/ipcc_wg3_ar5_annex-iii.pdf (accessed on 24 April 2024).
96. Pomponi, F.; Hart, J. The greenhouse gas emissions of nuclear energy—Life cycle assessment of a European pressurised reactor. *Appl. Energy* **2021**, *290*, 116743. [\[CrossRef\]](#)
97. Fridriksson, T.; Merino, A.M.; Orucu, A.Y.; Audinet, P. *Greenhouse Gas Emissions from Geothermal Power Production*; World Bank: Washington, DC, USA, 2016. [\[CrossRef\]](#)
98. Beagle, E.; Belmont, E. Comparative life cycle assessment of biomass utilization for electricity generation in the European Union and the United States. *Energy Policy* **2019**, *128*, 267–275. [\[CrossRef\]](#)
99. Moon, E. Why Do Coal Mines Need so Much Water? 2017. Available online: <https://phys.org/news/2017-04-coal.html> (accessed on 24 April 2024).
100. Macknick, J.; Newmark, R.; Heath, G.; Hallett, K.C. Operational water consumption and withdrawal factors for electricity generating technologies: A review of existing literature. *Environ. Res. Lett.* **2012**, *7*, 045802. [\[CrossRef\]](#)
101. UCSUSA. How It Works: Water for Nuclear. 2013. Available online: <https://www.ucsusa.org/resources/water-nuclear#sources> (accessed on 24 April 2024).
102. Zeng, G.; Xu, Z.; Zhang, Z.; Bai, H. Natural gas-hydrogen hybrid combustion retrofit method and practice for F-class heavy-duty combustion engines. *Eng. Res. Express* **2023**, *5*, 035061. [\[CrossRef\]](#)
103. EPA. Hydrogen in Combustion Turbine Electric Generating Units Technical Support Document New Source Performance Standards for Greenhouse Gas Emissions from New, Modified, and Reconstructed Fossil Fuel-Fired Electric Generating Units; Emission Guidelines for Greenhouse Gas Emissions from Existing Fossil Fuel-Fired Electric Generating Units; and Repeal of the Affordable Clean. 2023. Available online: <https://www.eia.gov/todayinenergy/detail.php?id=24612> (accessed on 24 April 2024).
104. Blending Hydrogen into Natural Gas Pipeline Networks. Nature Portfolio. Available online: <https://www.nature.com/articles/d42473-020-00545-7> (accessed on 27 November 2023).
105. Hodnebrog, Ø.; Dalsøren, S.B.; Myhre, G. Lifetimes, direct and indirect radiative forcing, and global warming potentials of ethane (C₂H₆), propane (C₃H₈), and butane (C₄H₁₀). *Atmos. Sci. Lett.* **2018**, *19*, e804. [\[CrossRef\]](#)
106. Skytt, T.; Nielsen, S.N.; Jonsson, B.G. Global warming potential and absolute global temperature change potential from carbon dioxide and methane fluxes as indicators of regional sustainability—A case study of Jämtland, Sweden. *Ecol. Indic.* **2020**, *110*, 105831. [\[CrossRef\]](#)
107. Sharan, P.; McTigue, J.; Yoon, T.J.; Currier, R.; Findikoglu, A.T. Energy efficient supercritical water desalination using a high-temperature heat pump: A zero liquid discharge desalination. *Desalination* **2021**, *506*, 115020. [\[CrossRef\]](#)
108. Bernardo, G.; Araújo, T.; da Silva Lopes, T.; Sousa, J.; Mendes, A. Recent advances in membrane technologies for hydrogen purification. *Int. J. Hydrogen Energy* **2020**, *45*, 7313–7338. [\[CrossRef\]](#)

109. Jasper, F.B.; Späthe, J.; Baumann, M.; Peters, J.F.; Ruhland, J.; Weil, M. Life cycle assessment (LCA) of a battery home storage system based on primary data. *J. Clean. Prod.* **2022**, *366*, 132899. [[CrossRef](#)]
110. Hiremath, M.; Derendorf, K.; Vogt, T. Comparative life cycle assessment of battery storage systems for stationary applications. *Environ. Sci. Technol.* **2015**, *49*, 4825–4833. [[CrossRef](#)]

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