ENERGY earthshots

HYDROGEN SHOT TECHNOLOGY ASSESSMENT

THERMAL CONVERSION APPROACHES

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EXECUTIVE SUMMARY

In June 2021, the United States (U.S.) Department of Energy (DOE) announced the first of a series of Department-wide Energy Earthshots™ designed to accelerate breakthroughs of more abundant, affordable, and reliable clean energy solutions within the decade. The Hydrogen Shot™ seeks to reduce the cost of clean hydrogen production to $1 per 1 kilogram in 1 decade ("1 1 1"). As part of this initiative, DOE is developing in-depth technology assessments of three general approaches to clean hydrogen production: thermal conversion (covered in this report); electrolysis; and advanced pathways.

Today, thermal conversion of fossil fuels, primarily steam methane reforming (SMR), represents the predominant, lowest cost method of hydrogen production. However, this production method, and others like it, emits around 10 kg of CO_2 equivalents per kg of H_2 produced on a life cycle basis. Carbon capture has been demonstrated on reforming pathways and the combination of the two is commercially ready. But to meet the Hydrogen Shot™ goal, most thermal conversion pathways with a thorough carbon management strategy will need to achieve costs lower than what has been currently modeled.

Based on screening-level analyses conducted by the U.S. DOE's National Energy Technology Laboratory (NETL), this report shows that technology advancements may reduce modeled costs from $1.64/kg H_2 to $1.40/kg H_2 for SMR with CCS, and from $1.60/kg H_2 to $1.33/kg H_2 for ATR with CCS (2020$). These cost reductions may be achieved through process intensification and the integration of lower technology readiness level CO_2 capture techniques. In addition, the report shows that hydrogen project developers must also consider factors such as plant scale, market scenarios, plant site location, optimization of CO_2 transport and storage infrastructure, by-product sales, CO_2 valuation, and integration with other energy systems to achieve the Hydrogen Shot™.

INTRODUCTION

Hydrogen Shot

The Hydrogen Shot™ is the first Energy Earthshot launched under the U.S. Department of Energy's (DOE's) Energy Earthshots™ Initiative, which will accelerate breakthroughs of more abundant, affordable, and reliable clean energy solutions within the decade. Achieving the Energy Earthshots will help America tackle the toughest remaining barriers to addressing the climate crisis, and more quickly reach the Biden–Harris Administration's goal of net-zero carbon emissions by 2050 while creating good-paying union jobs and growing the economy.

The Hydrogen Shot is a key aspect of the national strategy for clean hydrogen, as laid out in the *U.S. National Clean Hydrogen Strategy and Roadmap* [1]. The three pillars of this strategy—target high-impact end uses, reduce the cost of clean hydrogen, and focus on regional networks— are being pursued through a

The first Energy Earthshot, launched June 7, 2021— Hydrogen Shot—seeks to reduce the cost of clean hydrogen by 80% to **$1** per **1 kilogram** in **1 decade** ("**1 1 1**").

whole-of-government approach, coordinated under the Hydrogen Interagency Task Force [2]. Along with historic investments funded through the Bipartisan Infrastructure Law (e.g., the Regional Clean Hydrogen Hubs) and strong incentives for clean hydrogen production and investment in the Inflation Reduction Act, efforts conducted under the Hydrogen Shot are helping to advance clean hydrogen technologies and ensure progress toward national decarbonization goals. Industries are beginning to implement clean H_2 to reduce emissions, yet many hurdles remain to deploying it at scale. Currently, H_2 from clean and renewable energy can cost over $5 per kilogram. Achieving the Hydrogen Shot's 80% cost reduction goal can unlock new markets for H_2, including steel manufacturing, clean ammonia, energy storage, and heavy-duty trucks. This would create more clean energy jobs, reduce greenhouse gas emissions, and position America to compete in the clean energy market on a global scale. These efforts would ensure that environmental protection and benefits for local communities are a priority.

Impact

The Hydrogen Shot goal is aligned with the priorities for affordable clean H_2 articulated in the *National Strategy and Roadmap*. If the Hydrogen Shot goals are achieved, scenarios show opportunities for the production of 50 million metric tons of clean hydrogen in the United States annually. The *National Strategy and Roadmap* also shows the potential for a 10% reduction in carbon dioxide emissions by 2050. In addition, industry estimates in the *Road Map to a US Hydrogen Economy* [3] identify the potential for $140 billion in revenues and 700,000 jobs by 2030. The Hydrogen Shot will catalyze innovation in all clean H_2 production pathways, providing incentives to diverse regions across the country.

Clean Hydrogen Technology Pathways

In pursuit of its goals, the Hydrogen Shot focuses on the research, development, demonstration, and deployment of multiple technology pathways with the potential to achieve affordable clean H_2 production in the near- and longer-terms, leveraging different regional resources across the nation. These technology pathways fall broadly in three main categories:

- **Electrolysis:**
  The *electrolysis pathways* are based on commercial and near-commercial technologies for splitting water (H_2O) into H_2 and oxygen, which can be powered by low-carbon energy sources such as wind, solar, and nuclear to produce clean H_2. Examples include low-temperature electrolyzers using liquid alkaline solutions or proton-exchange-membranes as ionic conductors; and higher-temperature solid-oxide electrolyzers with the potential for higher electricity to H_2 conversion efficiency. Hydrogen Shot strategic priorities for the *electrolysis pathways* include reducing cost of integrated electrolyzer systems (e.g., stacks and balance of plant) at giga-watt scales; optimizing integration of electrolyzer systems with renewable and/or nuclear power to leverage low-cost onsite electricity; and facilitating expanded production capacity.

- **Thermal Conversion:**
  Thermal conversion processes use heat as a primary energy source to drive chemical reactions that convert carbon-based feedstocks into H_2 and other byproducts. Examples include reforming, gasification, and pyrolysis processes. Carbon capture, utilization, and storage is typically used in conjunction with thermal conversion to reduce the carbon footprint of the H_2 produced. Hydrogen Shot strategic priorities in the *thermal conversion pathways* include improving the performance and cost of integrated systems for natural gas reforming with carbon capture and storage (CCS) to achieve emissions targets; and development of diverse options such as gasification of waste feedstocks with CCS and pyrolysis of natural gas into H_2 and solid carbon to meet cost and emission goals.

- **Advanced Pathways:**
  As part of the longer-term vision, clean H_2 can also be produced through a variety of new and *advanced pathways* requiring little or no electricity inputs. Examples include photoelectrochemical and thermochemical processes for direct solar H_2O splitting that do not require electricity, and biological processes that can convert biomass or waste streams into H_2 with value-added co-products (such as purified H_2O). Additionally, advanced hybrid approaches combining electrochemical, thermochemical, pyrolytic, and/or photoelectrochemical processes producing clean H_2 from H_2O, biomass, or wastes could are being explored; and other interesting options, such as geological H_2, are being investigated. Hydrogen Shot strategic priorities in the *advanced pathways* include high-risk/high-reward research and development that develops fundamental scientific understanding transferable to the other pathways.

Technology Screening Assessment vs. Commercial Liftoff

This document provides a technology screening assessment of the *thermal conversion pathways* for clean H_2 production covered by the Hydrogen Shot. Other documents will provide

technology assessments of the *electrolysis pathways* and the *advanced pathways.* Consistent with methodologies adopted in all of DOE's Energy Earthshots, these assessments are intended to track status and research, development, and demonstration (RD&D) improvements relative to a decadal performance target specifically tied to National clean energy goals. As such, a technoeconomic framework has been adopted in this report referencing a static technology performance baseline separate from fluctuating economic factors such as inflation. Specifically for the Hydrogen Shot, technology baselines for the various clean H_2 production pathway costs were established using a 2020-year dollar basis; and status and projected cost reductions compared to the baselines are reported in the same 2020-year dollar basis to emphasize the impact of RD&D on technology advancement and facilitate comparison between pathways, separate from consideration of macroeconomic factors. It is also important to note that costs presented in this report are modeled costs and do not represent the cost of any particular H_2 producer. Since there is no legal mandate to produce low carbon H_2 in the United States, many of the technologies explored in this report are not commercially practiced but are commercially ready and are incorporated into commercial development plans for new H_2 plants around the world.

In contrast, DOE, through its **Pathways to Commercial Liftoff Initiative,** also tracks year-over-year changes in the commercial deployment status and prospects of different clean energy technologies reflective of the present economy-wide realities, including inflation and supply chain factors; these views are intended specifically to help create situational awareness for industry stakeholders and investors who have the potential to accelerate deployment. The **Pathways to Commercial Liftoff: Clean Hydrogen Report** [4] addresses technologies in the thermal conversion pathways, as well as the other Hydrogen Shot pathways; however, the technoeconomic framework in that report is slightly different, and considers available costs in current-year dollars as well as the impacts of various incentives. While cost projections presented in this Technology Screening Assessment document are related to various cost scenarios in the Commercial Liftoff report, interpretation of results relative to specific thermal conversion technologies must account for the different objectives of each document, as well as the different technoeconomic frameworks employed.

This **Hydrogen Shot Technology Screening Assessment of Thermal Conversion Approaches** presents a snapshot of various thermal conversion pathways for clean H_2 production, including technology status and envisioned approaches for achieving the Hydrogen Shot goals through RD&D advances. The *Hydrogen Shot Technology Assessments* of diverse production pathways and the *Pathways to Commercial Liftoff: Clean Hydrogen Report* will be updated periodically by the DOE to reflect progress reported by stakeholders from industry, academia, and the national labs.

THERMAL CONVERSION OVERVIEW

Thermal conversion can be defined as a process that uses heat as the energy source to drive chemical reactions that convert carbon-based feedstocks into other fuels and chemical energy carriers, and it includes processes such as reforming, gasification, and pyrolysis. Thermal conversion of fossil fuels is the most widespread and lowest-cost method of hydrogen (H_2) production today. In 2020, more than 75 percent of H_2 was produced via dedicated fossil fuel thermal conversion globally compared to just 1 percent from water electrolysis, with the balance produced as a by-product in refineries [5]. Decarbonization of future thermal conversion processes are critical options for successfully achieving the Department of Energy (DOE) Energy Earthshots™ Hydrogen Shot™ goal of reducing the cost of clean H_2 to $1 per 1 kilogram (kg) in 1 decade, or by 2031 [6].

Under the 2021 Bipartisan Infrastructure Law (BIL), the DOE must establish an initial standard for the carbon intensity of clean H_2 production in consultation with the Environmental Protection Agency (EPA) while considering input from industry and other stakeholders. The BIL allows for the initial standard to be adjusted downward over time. The BIL defines the term "clean hydrogen" to mean "hydrogen produced with a carbon intensity equal to or less than 2 kg [carbon dioxide] equivalents … produced at the site of production per kg of hydrogen produced" [7]. In June 2023, the DOE produced an initial Clean Hydrogen Production Standard (CHPS) of 4 kg CO_2 equivalents per kg of H_2 that incorporates stakeholder feedback. The CHPS accounts for "well-to-gate" lifecycle greenhouse gas (GHG) emissions in addition to those produced at the site of production [8]. Thermal conversion technologies can meet the BIL definition of clean H_2 with the implementation of carbon management methods such as carbon capture and storage (CCS); however, doing so requires process design and project development approaches that minimize both scope 1 and scope 2 greenhouse gas (GHG) emissions.

As noted above, several thermal conversion technologies of interest are already commercial or nearly commercial which means that these process systems do not face fundamental research, development, and demonstration (RD&D) challenges. These technologies include steam methane reforming (SMR) of natural gas (NG), autothermal reforming (ATR) of NG, partial oxidation (POX) of NG, gasification of solid fuels such as coal and biomass, and plasma pyrolysis of NG. Advanced thermal conversion technologies are those facing fundamental RD&D challenges prior to commercialization and include gasification of waste materials such as municipal solid waste (MSW), and plastic waste; thermal and catalytic pyrolysis of NG, solid fuels, and waste; chemical looping concepts involving NG and solid fuels; catalytic POX; catalytic gasification; dry reforming of methane (DRM); oxidative DRM; advanced SMR and ATR concepts; in situ H_2 generation, and others.

In this initial screening, current and target performance and cost of several of the aforementioned thermal conversion technologies are explored. Additionally, factors outside of the scope of the plant such as feedstock price assumptions, by-product sales, etc. were considered; however, the levelized cost of hydrogen (LCOH) results for these technologies are only a preliminary screening assessment. It should be noted that the screening results presented were determined independently and are not endorsed by individual vendors.

Exhibit 1 shows a summary of the thermal conversion technologies discussed in this report and their similarities and differences in terms of whether they are commercial or advanced, the feedstock(s) used, potential by-products, and how carbon emissions are controlled.

Exhibit 1. Summary table of thermal conversion technologies discussed

Technology	Commercial or Advanced	Feedstock(s)	Potential By-Products	Carbon Emissions Control[1,2]
Steam Methane Reforming	Commercial	Natural Gas	n/a	Pre-/post-combustion CO_2 removal
Autothermal Reforming			Argon	Pre-combustion CO_2 removal
Partial Oxidation			Argon	Pre-combustion CO_2 removal
Plasma Pyrolysis			Carbon Black	Sequestration in solid carbon product
Gasification		Coal and/or Biomass	Argon, Slag, and/or Sulfur	Pre-combustion CO_2 removal
Chemical Looping	Advanced	Natural Gas	Argon	CO_2 separated via chemical looping process
Dry Reforming of Methane			Argon	Pre-/post-combustion CO_2 removal
In Situ Reforming			Argon	CO_2 trapped in situ

[1] Pre-combustion CO_2 removal involves separation of CO_2 in process streams, generally at high pressures and concentrations, prior to combustion of the stream.
[2] Post-combustion CO_2 removal involves separation of CO_2 in combustion product streams generally at low pressure and concentrations

REFORMING OF NATURAL GAS WITH CARBON CAPTURE

Introduction

NG SMR, ATR, and POX are considered commercial, state-of-the-art H_2 production technologies. The majority of current global merchant, high-purity H_2 production is produced via SMR of NG without carbon dioxide (CO_2) capture; this method is currently the cheapest way to produce H_2, aided by technology advancements since its introduction nearly 100 years ago [9]. Adding CO_2 capture to this technology can result in a clean and relatively low-cost H_2 product.

Exhibit 2 shows operating and planned NG-based H_2 production facilities with CCS. To date, market conditions have limited capture rates to approximately 60%. A handful of H_2 production facilities are currently operating with CCS at CO_2 capture rates less than 60 percent. Several others with CO_2 capture rates above 90 percent are in the planning stages targeting initial operation in the mid- to late-2020s [10] [11] [12] [13] [14] [15] [16]. Nevertheless, these projects demonstrate that NG-based H_2 production with CO_2 capture is commercially available and a preferred method of clean H_2 production by industry.

Exhibit 2. List of operating and planned projects for NG reforming technologies with CCS

Project Name	Location	Status	H_2 Production (MMSCFD)	H_2 Production Technology	CO_2 Capture Technology	Overall CO_2 Capture Rate (%)
Air Products Port Arthur	United States	Operating	200	SMR	VSA	60
Air Liquide Port Jerome	France	Operating	45	SMR	Membranes, CRYOCAP™	60
Shell Quest	Canada	Operating	191	SMR	ADIP-X	50
H-Vision	Netherlands	Under Development	636	ATR	Rectisol™	88
HyNet	United Kingdom	Under Development	90	ATR	TBD	97.2
H21	United Kingdom	Under Development	2,900 from 9 units	ATR	aMDEA	94.2
Acorn	Scotland	Under Development	48	ATR	Amine	98.7
H2Teesside	United Kingdom	Under Development	250	TBD	TBD	98
Air Products Alberta	Canada	Under Development	>623	ATR	TBD	95
Air Products Louisiana	United States	Under Development	>750	ATR/POX	TBD	95

The reforming process involves the reaction of methane (CH_4) from NG with oxygen (O_2)—added via steam, gaseous O_2 from air, or both—to form syngas, or a mixture primarily consisting of carbon monoxide (CO) and H_2. The water-gas shift (WGS) reaction, $H_2O + CO \leftrightarrow CO_2 + H_2$; $\Delta H^o_{rxn} = -41.2 \ kilojoule$ (kJ)/mole (mol), is utilized to further improve H_2 yield and convert CO into CO_2. The CO_2 is captured from syngas and/or flue gas streams and H_2 is purified into the final product.

Exhibit 3 shows a block flow diagram (BFD) of an example SMR process with CO_2 capture. Natural gas feed is first desulfurized and then sent to a pre-reformer where it is mixed with process steam. The pre-reformer serves the primary purpose of reforming higher hydrocarbons in the feed, which reduces carbon deposition on downstream catalysts, reducing the load on the primary reforming, and improving product recovery. The mixture is then reacted over a nickel-based catalyst contained inside a system of tubes according to following simplified chemical equation: $CH_4 + H_2O \leftrightarrow CO + 3H_2$; $\Delta H^o_{rxn} = 205.8$ kJ/mol. The resulting syngas is cooled and

sent through a series of shift reactors that both increase H_2 production and convert CO to CO_2 for capturing. CO_2 is removed from the syngas through a pre-combustion CO_2 capture process. Finally, high-purity (99.90 vol.%) H_2 product suitable for multiple applications (e.g., ammonia manufacturing, thermal power generation) is generated via a pressure swing adsorber (PSA) unit. Further purification would be required for proton-exchange membrane (PEM) applications. The PSA off-gas is used as a fuel gas, along with a sufficient quantity of supplemental NG, to provide external heat to the catalyst tubes to drive the primary reforming reaction. Heat is recovered from the resulting flue gas, and it is then sent through a post-combustion CO_2 capture system, which increases the overall capture rate of the process. The CO_2 streams are dried and compressed into a CO_2 product.

Exhibit 3. BFD of SMR plant with CO_2 capture
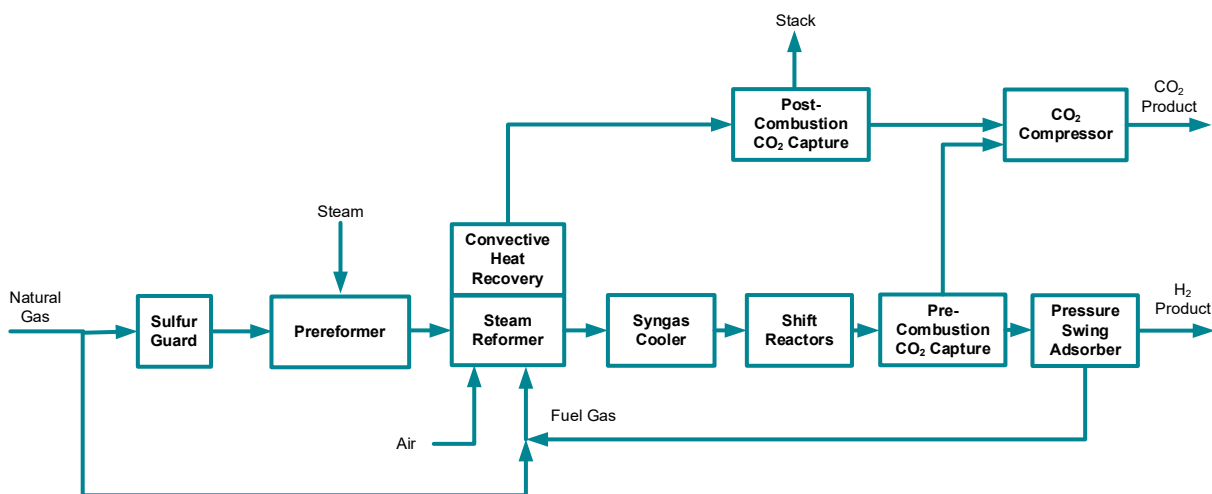
Exhibit 4 shows a BFD of an example ATR process with CO_2 capture. The ATR flowsheet is similar to the SMR flowsheet with a few key differences. Within the primary reformer, unlike in the SMR case, the heat-generating partial oxidation reaction, $CH_4 + \frac{1}{2}O_2 \leftrightarrow CO + 2H_2$; $\Delta H^o_{rxn} = -36.0 \text{ kJ/mol}$ provides heat to drive the SMR reaction, $CH_4 + H_2O \leftrightarrow CO + 3H_2$; $\Delta H^o_{rxn} = 205.8 \text{ kJ/mol}$. High-purity O_2, which is typically supplied by an air separation unit (ASU), is fed to the primary reformer for the partial oxidation reaction. This also creates a synergy where H_2 is used for the manufacture of ammonia (NH_3) requiring purified nitrogen (N_2), a potential byproduct of the ASU. The downstream syngas cleanup processes are identical to the SMR flowsheet. Another difference is the fate of the PSA off-gas. Most of this gas, enough to generate sufficient heat for other plant processes, is combusted in the fired heater, and the rest is recycled prior to the pre-combustion CO_2 capture unit to improve CO_2 capture and H_2 recovery. The mostly-decarbonized flue gas from the fired heater is sent to the exhaust stack.

Exhibit 4. BFD of ATR plant with CO_2 capture
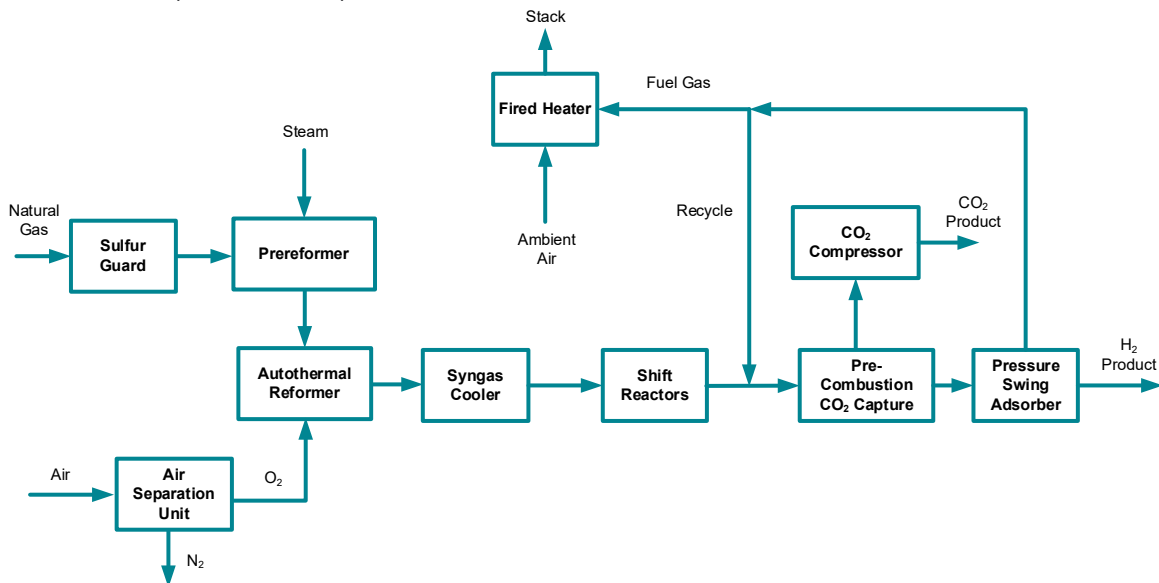
Exhibit 5 shows the BFD of a POX process with CO_2 capture. The POX flowsheet is similar to the ATR flowsheet with some key simplifications. The POX reactor is non-catalytic, requires no steam, and utilizes the following heat-generating reaction for H_2 production: $CH_4 + \frac{1}{2}O_2 \leftrightarrow CO + 2H_2$; $\Delta H^o_{rxn} = -36.0 \text{ kJ/mol}$. These characteristics eliminate the need for dedicated reformer steam generation and feed pretreatment; however, a downside is that the H_2 yield for POX systems is inherently lower based on the reaction stoichiometry [17]. The downstream syngas cleanup processes are identical to the ATR flowsheet, except that the fate of the PSA off-gas may be better suited for internal power generation. A full techno-economic analysis (TEA) has not been conducted for the POX technology, so only performance results from literature are available and cost reduction pathways are primarily qualitative.

Exhibit 5. BFD of POX plant with CO_2 capture
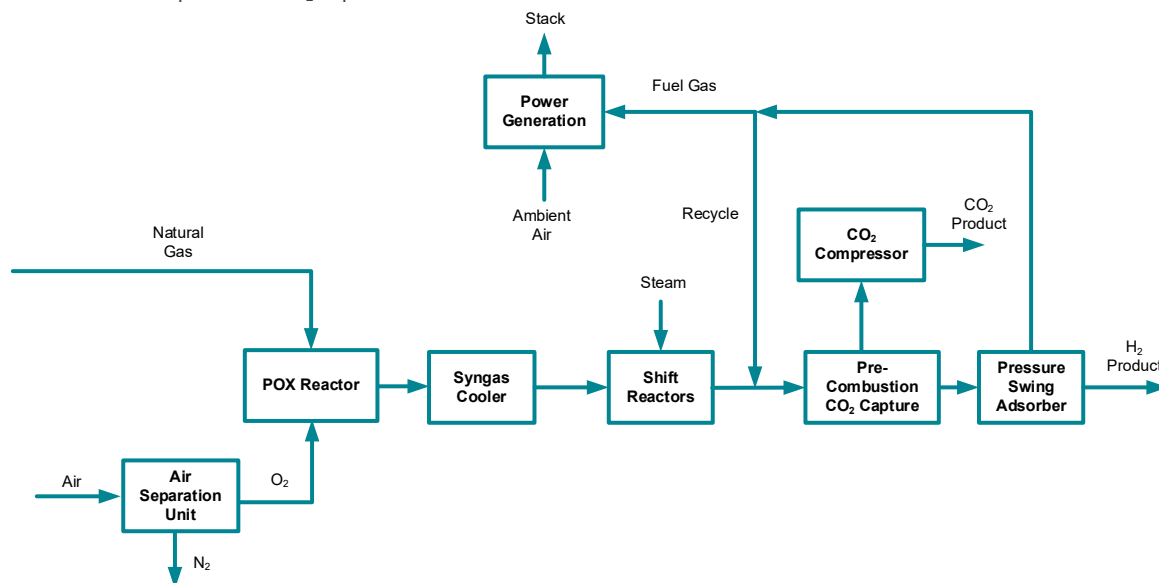
Baseline Performance and Cost

Baseline performance and cost for SMR and ATR plants with CCS have been estimated and reported [9]. Exhibit 6 provides performance results. The ATR with CCS case has a plant capacity approximately 1.4 times greater than the SMR with CCS case, as the SMR with CCS case has been limited to a single-reactor capacity of 200 million standard cubic feet per day (MMSCFD) H_2. The SMR with CCS has a slightly higher CO_2 capture rate, approximately 1.7 percentage points higher, than the ATR with CCS case. The net power output represents the difference between the gross power output and the parasitic power requirements of the plant for items such as blowers, compressors, and pumps. These power requirements are hereafter referred to as auxiliary power load. Since the example reforming cases do not produce any power, the net power output is simply the negative of the total auxiliary load.

Exhibit 6. Baseline performance results for SMR and ATR plants with CCS

Parameter	SMR with CCS	ATR with CCS
H_2 Production Rate (kg/hr)	20,125	27,500
CO_2 Capture Rate (%)	96.2	94.5
Total Gross Power (MWe)	0	0
Total Auxiliaries (MWe)	41	110
Net Power Output (MWe)	-41	-110
Natural Gas Flow Rate (kg/hr)	75,472	96,930
HHV Cold Gas Efficiency (%)	72.1	75.7
HHV Effective Thermal Efficiency (%)	68.4	67.9
Raw Water Consumption (L/kg H_2)	24.2	24.3
CO_2 Exhaust Stack Emissions (kg CO_2/kg H_2)	0.38	0.51
Molar Steam:Carbon Ratio	2.56	1.57
Mass H_2:NG Yield	0.27	0.28

The imported power for the ATR with CCS plant is more than double that of the SMR with CCS plant, almost entirely due to the high auxiliary load of the ASU. While this represents a significant increase in operating cost, that increase is offset by capital cost reductions in the autothermal reactor and CO_2 capture units.

The cold gas efficiency (CGE), defined as the ratio of the heat content (British thermal unit [Btu]/hour [hr]) of the H_2 product to the heat content (Btu/hr) of the NG feedstock expressed as a percentage, is 72.1 percent (higher heating value [HHV]) for the SMR with CCS plant and 75.7 percent (HHV) for the ATR with CCS plant. The effective thermal efficiency (ETE), raw water consumption, and mass H_2:NG yield are similar for the two reforming plants. The ETE is defined as the ratio of the H_2 product heat content plus net power in equivalent units (Btu/hr) to the NG heat content (Btu/hr).

The performance assumptions for the CO_2 capture units were the same for all cases studied. The reason that the SMR with CCS case achieved a 1.7 percentage point higher CO_2 capture

rate is that it employed both pre-combustion CO_2 capture and post-combustion CO_2 capture whereas the ATR with CCS case only employed pre-combustion CO_2 capture.

Limited information is available publicly for baseline performance of POX with CCS. According to industrial H_2 technology suppliers, POX systems have a 6–9 percent greater NG consumption for equivalent H_2 production, compared to ATR systems, resulting in an estimated mass H_2:NG yield of 0.26. Suppliers claim an overall CO_2 capture rate of 98–99 percent for POX systems; however, this may come at the expense of lower-purity H_2 product [17]. Further analysis of POX systems is required to fully assess the performance on a comparable basis with the baseline SMR and ATR cases.

The cost results of the SMR with CCS and ATR with CCS plants are summarized in Exhibit 7. The baseline SMR with CCS plant has a LCOH of $1.69/kg H_2 and the ATR with CCS plant has a LCOH of $1.64/kg H_2. Approximately 50 percent of the LCOH is attributed to the cost of the NG fuel. The SMR with CCS plant has higher capital costs, contributing to 20 percent of the LCOH, due primarily to the post-combustion CO_2 capture system and lack of economies of scale compared to the ATR plant, which has capital costs that make up 17 percent of the LCOH. On the other hand, the ATR with CCS plant has higher variable costs, making up 22 percent of the LCOH, primarily due to the ASU which contributes significantly to the grid electricity needed to be purchased for the plant. To compare, the SMR with CCS plant's variable costs account for 15 percent of its LCOH. CO_2 transport and storage (T&S) costs make up about 6 percent of the LCOH for both reforming plants. A H_2 pressure credit considers a scenario in which the H_2 compressor, which is needed to compress the H_2 product to a pipeline-ready pressure of 925 pounds per square inch gauge (psig), is not included in the flowsheet, resulting in a slight reduction of both the capital cost and variable costs of reforming plants. Including the pressure credit results in a 3 percent reduction in the LCOH, which is about $0.04/kg H_2. The baseline LCOH does not include a H_2 pressure credit; however, the cost reduction pathways start with the lower LCOH values for SMR and ATR that include the credit.

Exhibit 7. Baseline LCOH results for SMR and ATR plants with CCS

Cost Component	SMR with CCS (2020$/kg H_2)	ATR with CCS (2020$/kg H_2)
Capital	0.34	0.27
Fixed O&M	0.15	0.12
Variable O&M	0.25	0.37
Fuel	0.85	0.80
CO_2 T&S	0.10	0.09
Total (including CO_2 T&S)	**1.69**	**1.64**
H_2 Pressure Credit	-0.04	-0.04
Total (including H_2 Pressure Credit)	**1.64**	**1.60**

The left chart in Exhibit 8 is a bar graph representation of the data in Exhibit 7 and the right chart is a donut chart that breaks down the capital costs by cost account for the SMR with CCS plant. The error bars on the left chart represent the potential LCOH range relative to the

maximum and minimum capital cost uncertainty ranges. The largest contributor to the capital cost is the post-combustion CO_2 capture system, which makes up about 35 percent. The next-largest contributor is the balance of plant (BOP), which is a miscellaneous category that includes costs for capital such as instrumentation and control, buildings and structures, NG pipeline and start-up systems. The reformer and accessories account for 14 percent of the total capital cost, and this account includes costs for the primary reformer, syngas coolers, performer, and sulfur guard bed. Equipment for CO_2 compression and drying makes up 11 percent of costs.

Exhibit 8. Breakdown of SMR with CCS baseline LCOH by cost component (left) and capital costs (right)
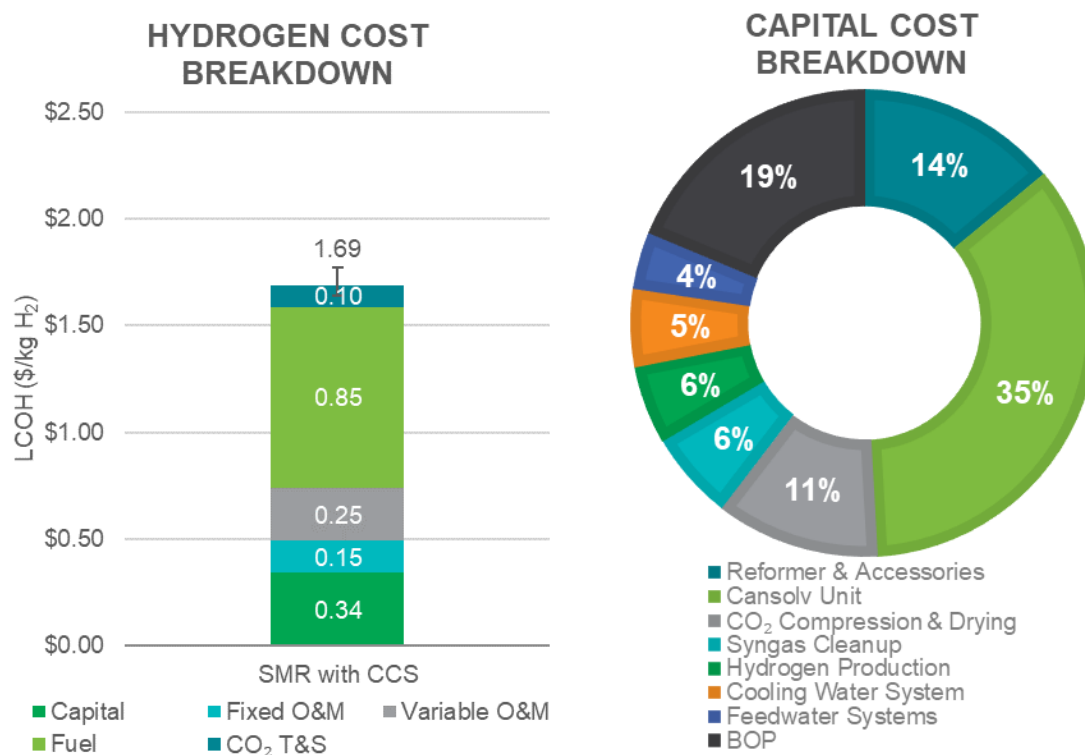
The left chart in Exhibit 9 is a bar graph representation of the data in Exhibit 7 and the right chart is a donut chart that breaks down the capital costs by cost account for the ATR with CCS plant. The error bars on the right chart represent the potential LCOH range relative to the maximum and minimum capital cost uncertainty ranges. The capital cost breakdown is similar to the SMR with CCS case, except that the portion of capital costs designated for the post-combustion CO_2 capture system is essentially replaced by that of the ASU, which makes up 37 percent of the total capital costs. The next-highest contributors are the BOP, which makes up 20 percent, and the CO_2 compression and drying equipment, which makes up 11 percent of costs. The reformer and accessories costs only make up 6 percent of the total capital cost, and this can be attributed to the simpler design and construction of the single-vessel ATR, compared to the SMR. The syngas cleanup account includes costs for the recycle compressor, pre-combustion CO_2 capture unit, and WGS reactors.

Exhibit 9. Breakdown of ATR with CCS baseline LCOH by cost component (left) and capital costs (right)
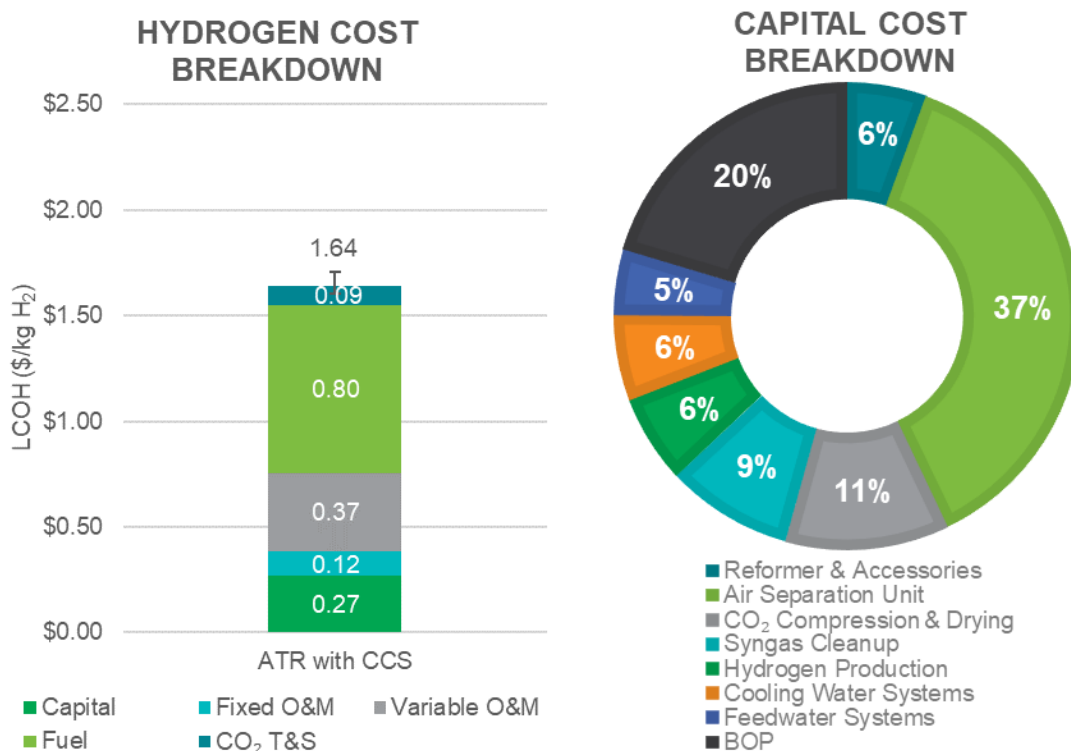
The baseline POX is claimed to have lower operating costs, due to a reduction of required power import and no reformer catalyst replacement, and lower capital costs, due to minimal feed gas pretreatment, compared to ATR [17]. However, due to the lower H_2:NG yield, it will have higher fuel costs compared to SMR and ATR plants at equivalent H_2 production rates. Further analysis of POX systems is required to fully assess the cost on a comparable basis with the baseline SMR and ATR cases presented here.

CO_2 Transport and Storage

The cost of CO_2 T&S varies based on geologic, geographic, and CO_2 capture rate variations between the scenarios in the TEAs and the H_2 production pathways considered in the analysis. A modeling tool has been developed to estimate state-specific T&S costs for pipeline and storage infrastructure that is either dedicated to a single source or shared among many sources. When comparing dedicated T&S costs with shared infrastructure T&S costs, model calculations indicated that shared high-capacity trunkline and storage hub infrastructure can reduce state-specific T&S costs for SMR by 9 percent up to 48 percent, which is equivalent to a LCOH reduction as small as $0.01/kg H_2 in the state of Florida to as large as $0.21/kg H_2 in Montana. Similarly, high-capacity shared infrastructure can lower state-specific ATR T&S costs from nearly 0 percent to 55 percent, which is equivalent to a LCOH reduction ranging from $0.01/kg H_2 in Illinois to $0.33/kg H_2 in Washington. Exhibit 10 and Exhibit 11 demonstrate SMR and ATR T&S cost reduction percentages by state, respectively. Lower percentage savings from shared infrastructure reflect a U.S. state's close proximity to high-quality storage reservoirs, since these states will have low dedicated T&S costs to begin with, and therefore, these states do not benefit as much from the economies of scale provided by shared high-capacity T&S infrastructure.

Exhibit 10. ATR CO_2 T&S cost reduction percentage, by state, from dedicated T&S infrastructure to shared high-capacity T&S infrastructure
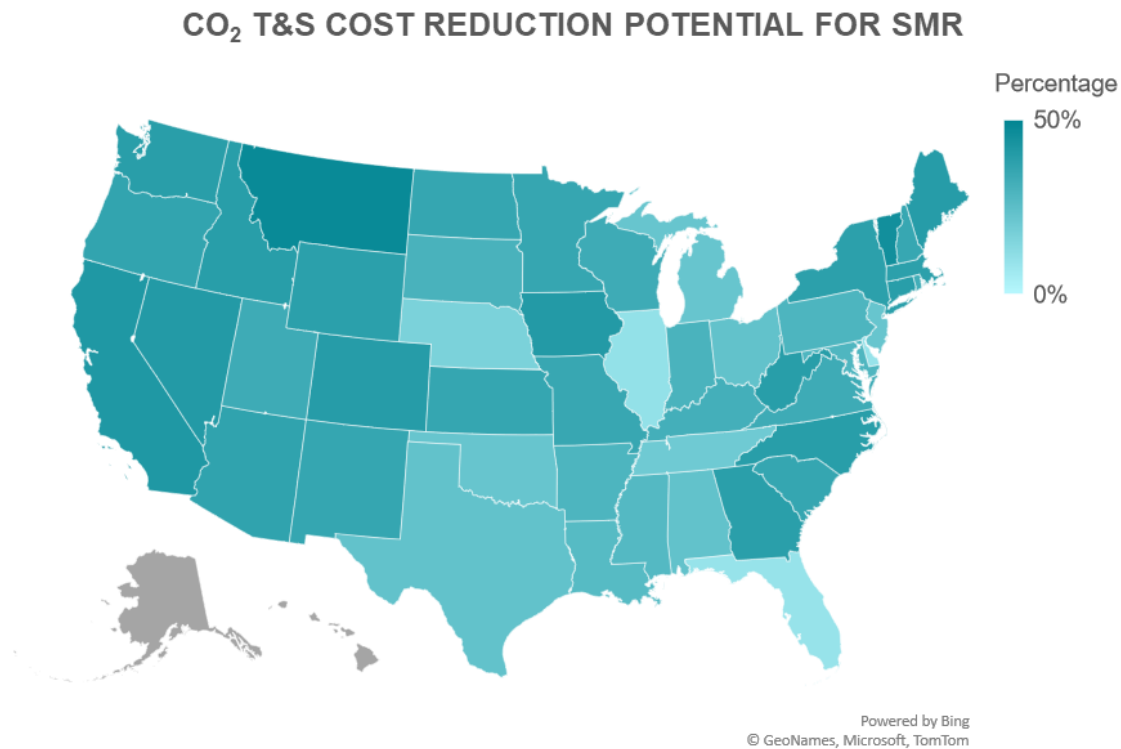

Exhibit 11. SMR CO_2 T&S cost reduction percentage, by state, from dedicated T&S infrastructure to shared high-capacity T&S infrastructure
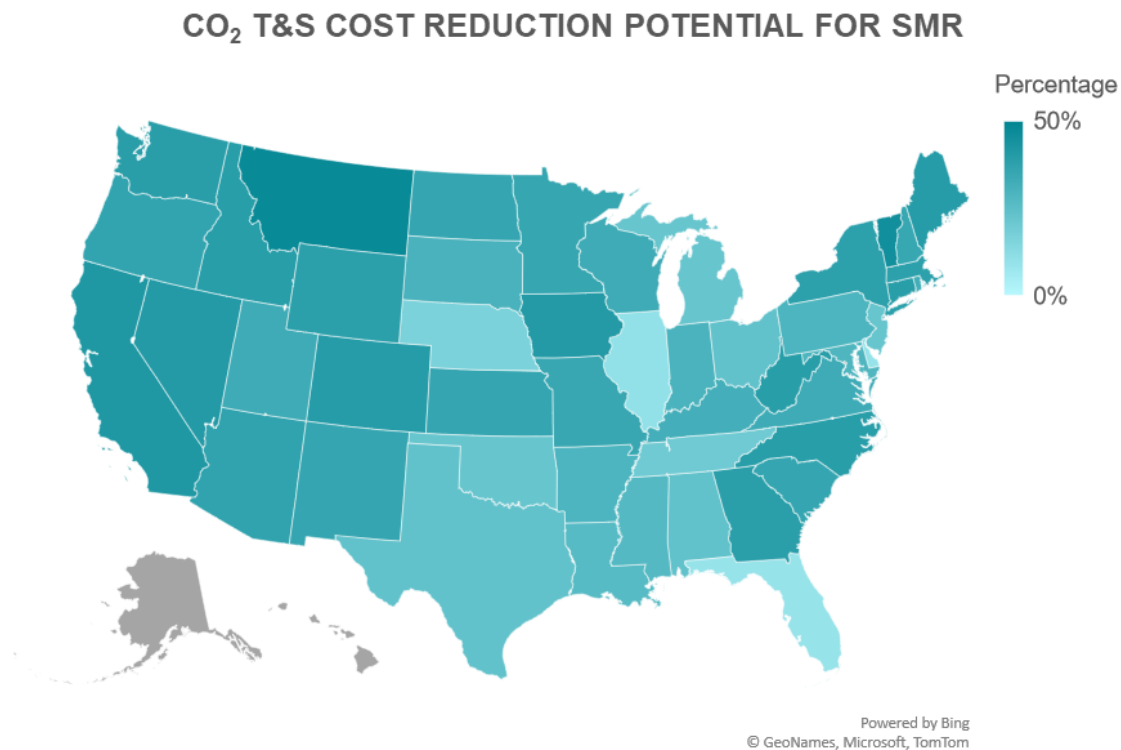
Additional T&S cost reductions can be generated by site selection; however, each case is geographically unique and therefore site selection analysis is difficult to automate. As mentioned previously, fuel costs for the SMR and ATR with CCS baselines account for about 50% of the LCOH. Therefore, the state with the lowest NG fuel price, Missouri, was selected as an example candidate for siting SMR and ATR facility projects. Additional detail on the site selection methodology is provided in the Appendix. To demonstrate CO_2 T&S cost optimization in Missouri (MO), four T&S scenarios were evaluated (shown in Exhibit 13), which varied the location of the H_2 production facility, the CO_2 transport pipeline length and type, and the CO_2 storage project location and type. The locations of the H_2 production facility and the CO_2 storage facility site in the different scenarios are shown in Exhibit 12. The first-year break-even cost of transporting and storing CO_2 for each scenario are provided in Exhibit 14. The costs are expressed as 2020 dollars per kg H_2 produced for either the SMR or ATR technologies, and assume a regional dip (i.e., relatively flat) geologic structural regime. T&S cost waterfalls of SMR-based technologies and ATR-based technologies are presented in Exhibit 15, and demonstrate that a high-capacity (5.0 metric tons per annum [tpa]) shared CO_2 trunkline is the most impactful T&S cost reduction option as shown in the MO-3 T&S scenario.

Exhibit 12. Map of T&S scenarios in Missouri
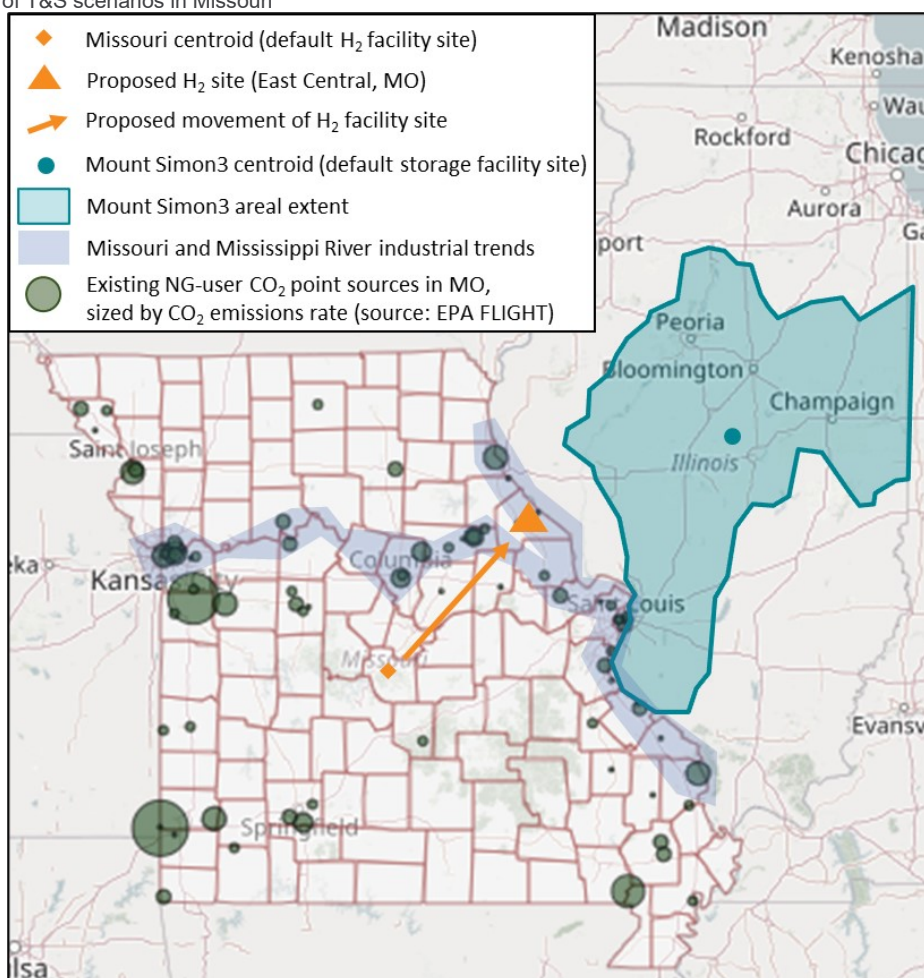
Missouri CO_2 point sources base map source: EPA Facility Level Information on GreenHouse gases Tool (FLIGHT) [18]

Exhibit 13. CO_2 T&S cost optimization options for SMR or ATR

T&S Scenario	Hydrogen Project Location	CO_2 Pipeline Transport	CO_2 Storage Operation	Storage Location Formation Centroid
MO-1	MO geographic centroid (default)	Dedicated (200 miles [mi])	Dedicated	Mount Simon3, Illinois (IL)
MO-2	Relocation to East Central MO emissions cluster	Dedicated (150 mi)	Dedicated	Mount Simon3, IL
MO-3	East Central MO	Trunkline (150 mi)	Dedicated	Mount Simon3, IL
MO-4	East Central MO	Trunkline (150 mi)	Storage Hub	Mount Simon3, IL

Exhibit 14. T&S scenarios demonstrating user-option impacts on SMR and ATR LCOH reduction in Missouri

T&S Scenario	SMR T&S Cost Contribution to LCOH			ATR T&S Cost Contribution to LCOH		
	Transport Cost ($/kg H_2)	Storage Cost ($/kg H_2)	Total Cost ($/kg H_2)	Transport Cost ($/kg H_2)	Storage Cost ($/kg H_2)	Total Cost ($/kg H_2)
MO-1	0.134	0.072	0.205	0.106	0.059	0.165
MO-2	0.101	0.072	0.173	0.079	0.059	0.138
MO-3	0.046	0.072	0.119	0.040	0.059	0.099
MO-4	0.043	0.047	0.091	0.038	0.044	0.082

Exhibit 15. T&S cost waterfalls for Missouri SMR (left) and ATR (right) technologies
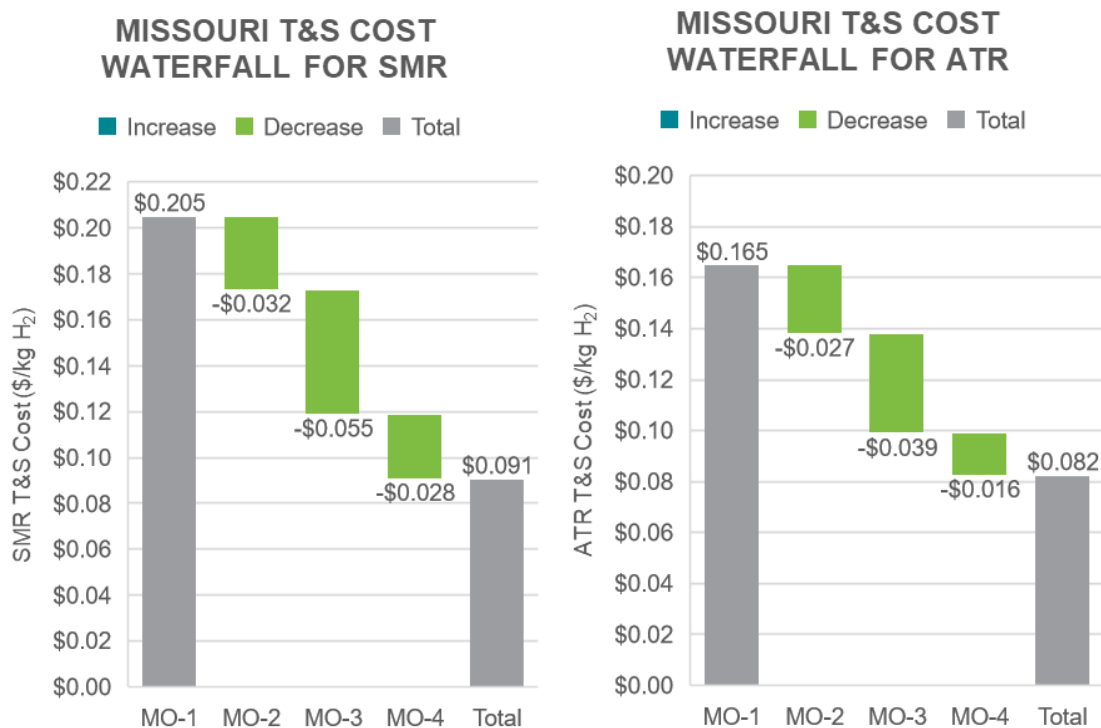
Emissions and LCA Discussion

Life cycle analysis (LCA) models were created for the baseline technologies of SMR without CCS, and SMR and ATR with CCS plants, as shown in Exhibit 16. The SMR without CCS plant is modeled two ways: one that considers excess steam in the system and one that does not. Using an LCA technique called displacement, fossil energy avoided in producing excess steam is included as a credit for the case that considers steam displacement. Results are presented as global warming potential (GWP) in units of kg CO_2 equivalent (CO_2e)/kg H_2. Further description of LCA methodology and impact assessment can be found in the Appendix.

Exhibit 16. LCA results for reforming technologies
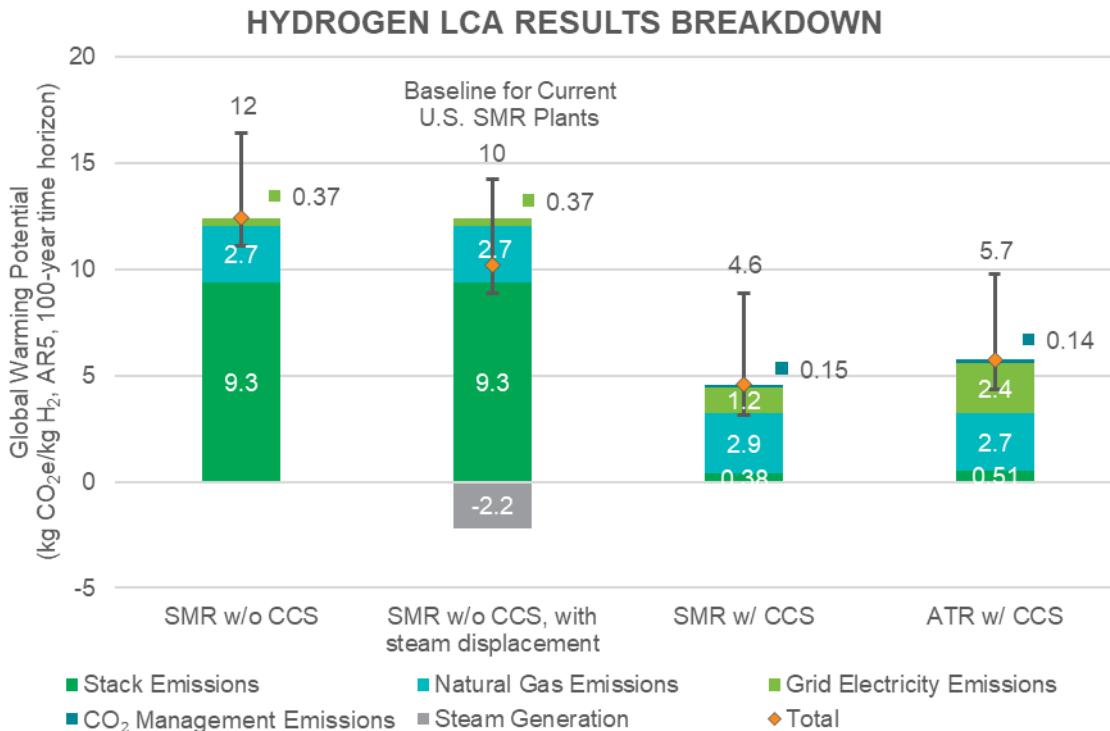
The baseline GWP results for SMR without CCS are 12 kg CO_2e/kg H_2 produced. Of that value, about 75 percent of the GWP results are estimated to be the exhaust stack emissions at the SMR facility, and about 22 percent are from the upstream emissions of extracting, processing, and delivering the NG to the facility. There are small contributions from the upstream production of electricity, about 3 percent. If the displaced steam is considered, then the total GWP results are reduced to 10 kg CO_2e/kg H_2 produced.

SMR with CCS decreases the GWP results to 4.6 (a roughly 60 percent reduction), and ATR with CCS decreases to 5.7, a roughly 50 percent reduction. These life cycle results may be higher than expected given the addition of CCS. However, the added NG and electricity needed to run the CCS facility on a per kg of H_2 produced basis means that there remain significant upstream GWP impacts even with CCS. Current ATR technologies with CCS would have slightly higher upstream NG GWP impacts than SMR, and about double the upstream GWP impacts from grid electricity. The results in Exhibit 16 also show error bars associated with a Monte Carlo simulation on the created models.

DOE has developed an initial CHPS to meet requirements of Section 40315 of the BIL. The initial CHPS establishes a target of 4 kg CO_2e/kg H_2 for lifecycle (i.e., "well-to-gate") GHG emissions. A takeaway from Exhibit 16 is that the SMR and ATR baseline configurations considered meet this target but only if variability to the underlying life cycle data is considered.

Exhibit 17 shows the variability in the GWP results for key components of the LCA model's reforming cases via error bars. The error bars for the "Total" category represent a summation of the variability of the individual GWP contributors.

Exhibit 17. Variability analysis from key components of H_2 life cycle GWP impacts
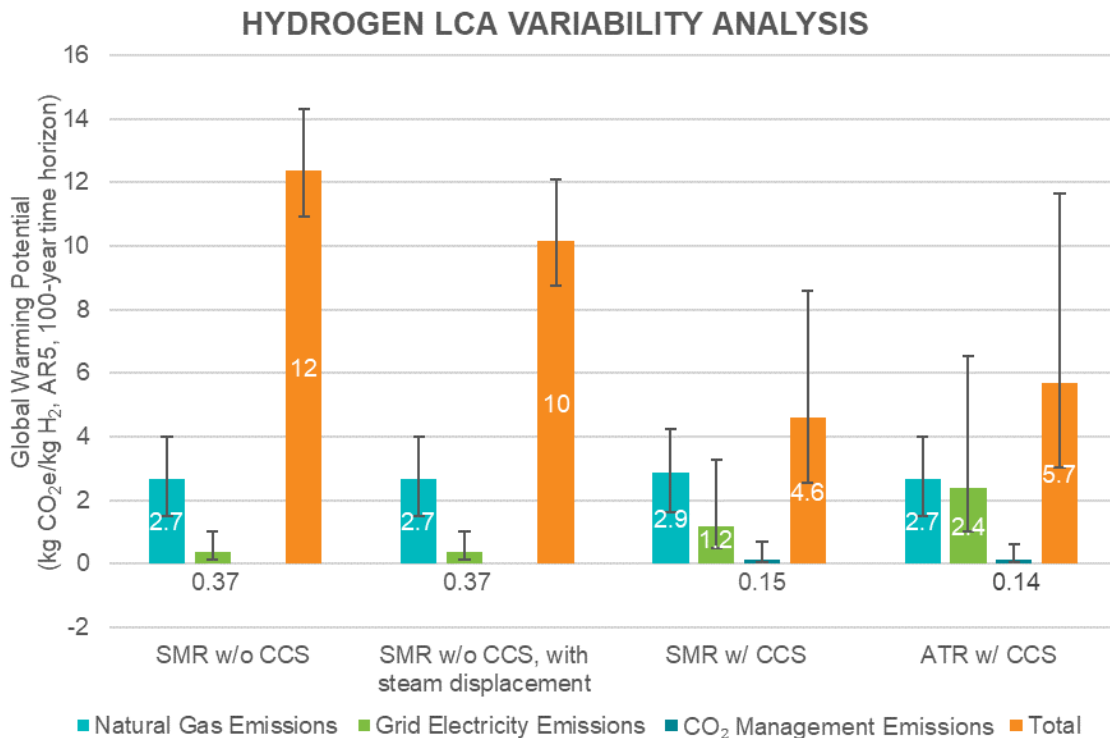
It should be noted that the error bars present in Exhibit 17 are not indicative of confidence intervals, but instead represent a maximum possible range of values for the given category. Within each category, the bar itself represents the value used in the baseline, whereas the error bars represent the minimum and maximum possible values for the given category. This is done to represent the current variability of the overall technology due to a scenario that varies from the baseline. Contribution categories were differentiated by grid balancing authority, NG basin and transportation, and CO_2 transport distance and storage.

For grid electricity contribution, the highest possible scenario was represented by the Homestead balancing authority with an emissions factor of 1.53 kg CO_2e/kilowatt hour (kWh), and the lowest being represented by Western Area Power Administration – Upper Great Plains West with an emissions factor of 0.1812 kg CO_2e/kWh [19]. For the NG basin variability, the highest and lowest scenarios were represented by the San Juan coalbed methane basin, 0.0198 kg CO_2e/megajoule (MJ) NG, and Alaskan Offshore basin, 0.007 kg CO_2e/MJ NG,

respectively [20] [21]. For T&S, upper and lower limits were found using the minimum expected piping distance of 200 miles when using Public Utility District No. 1 electricity, and 2,400 miles when using Homestead electricity, respectively. This, in combination with a fixed emissions factor of 0.042 kg CO_2e/kg CO_2 stored, was used to determine the upper and lower bounds for T&S.

The results show that generally, a main contributor to the variability in estimated GWP results for each case are the inputs of the primary fuel source. For SMR without CCS, the main variability comes from the upstream NG supply chain. For SMR and ATR with CCS, the CCS system adds significant grid electricity use, and the variability of the GWP of the grid electricity is comparable to, but slightly larger than, the upstream NG.

Given the relatively small overall magnitude, the T&S variability is never a significant contributor to the overall estimated variability in the GWP results.

From these results it can be inferred that strategies for NG reforming project developers to lower their GWP include procuring NG and power from regional supply chains where producers and suppliers effectively manage the emissions of the respective product. Various strategies exist which include managing fugitive emissions, electrification of NG compressor stations, renewable NG blending, and decarbonization of power generation through CO_2 capture and/or renewables. Efficiency gains made through NG reforming RD&D are another strategy to GWP improvements from lowering feedstock usage per unit of H_2 produced.

Cost Reduction Pathways

Although there is a limit to how much RD&D can drive down the LCOH from NG reforming, improvements achieved through process intensification, advanced reactor concepts, commercial technology optimizations, or a combination thereof are necessary. For example, companies have commercialized technologies that improve energy efficiency of the primary SMR reactor using optimized catalyst tubes incorporating recuperative heating or similar techniques within the reactor.

Furthermore, alternative CO_2 capture systems were explored for SMR, ATR, and POX systems. Technologies that incorporate a combination of cryogenic CO_2 separation and membrane H_2 separation were considered. In addition to improving the overall CO_2 capture rate, recycling of a H_2-rich stream recovered in the membrane step further improves H_2 yield. The Air Products vacuum swing adsorption (VSA) system for syngas CO_2 capture prior to the PSA unit is another technology development. This system eliminates the steam demand for pre-combustion capture system and the reoccurring cost of the amine solvent [22].

Advanced SMR concepts employ solid CO_2 sorbents that remove CO_2 formed during the reforming reaction within the reforming reactor itself. Such concepts are either based on fixed bed or fluidized bed reactor designs and provide H_2:NG yield improvements by driving the equilibrium-limited reforming reaction towards the products side to create more H_2, as well as additionally achieving capital cost reductions through elimination of traditional solvent- or cryogenic-based CO_2 removal processes [23]. A more-advanced concept for ATR is integrating a H_2-selective membrane within the ATR, which continuously extracts H_2 produced from the

reforming reactions and drives the chemical equilibrium towards the products side, creating more H_2. A CO_2-rich stream exits the top of the reformer that can be cleaned up and compressed into a captured CO_2 product. This concept allows for the elimination of the WGS reactors, syngas CO_2 capture unit, fired heater, and PSA unit while claiming to improve the H_2:NG mass yield by 30 percent [24].

Additionally, advanced catalysts have several potential applications in ATR, SMR and POX concepts that may provide improvements to process efficiency or enable process intensification by performing WGS within the reformer itself.

Non-technology factors considered during the planning stages of a project are also drivers towards the $1/kg H_2 goal for SMR, ATR, and POX technologies. One option is to increase the plant scale. SMR technologies can implement an additional train to increase the scale by 2 times and the ATR technologies can be scaled up to a maximum, which is 2.7 times the baseline, as demonstrated in industry. Site location is selected based on NG and electricity market prices. Next, the sale of by-products can provide additional plant revenue. Although there are no by-products available for sale in the SMR with CCS plants, the argon (Ar) produced from the ASU needed for the ATR with CCS can be sold as a by-product. The CO_2 T&S costs can be optimized by implementing shared trunkline and hub options and relocating the plant close to storage sites within the state. Captured CO_2 can be valued up to $50/metric ton (t) CO_2, to estimate the effect of a tax on carbon, to further lower costs toward the $1/kg H_2 goal.

Given all of the options, there are many possible cost reduction pathways to $1/kg H_2 for SMR and ATR technologies. Not all options are explored and included herein, but the example options for each technology improvement are shown in Exhibit 18.

Exhibit 18. Summary of parameters needed to achieve a pathway to $1/kg H_2 for SMR and ATR with CCS

Parameter	SMR with CCS			ATR with CCS	
Technology Improvement	Reformer Efficiency Improvements and Cryogenic CO_2 Capture System	VSA CO_2 Capture System	Reformer Efficiency Improvements	Cryogenic CO_2 Capture System	Advanced Membrane-Integrated ATR
Plant Scale	Additional SMR train			Scale to maximum ATR	No change from baseline
Site Location	Missouri				
EIA Price Scenario	Reference				
By-Products	n/a	n/a	n/a	Argon at $1.27/kg (7% above market price)	Argon at $1.00/kg (16% below market price)
Optimized CO_2 T&S	Relocation to East Central MO, high-capacity trunkline for CO_2 pipeline transport, storage hub for CO_2 storage operation				
CO_2 Valuation	$30/t	$50/t	$46/t	$0/t	$0/t
Final LCOH	$1.00/kg H_2				

To visualize cost reductions, waterfall charts have been developed for select pathways. The waterfall chart shows the baseline SMR or ATR LCOH, including the H_2 pressure credit, on the left side. Then relevant cost reduction parameters—technology RD&D improvement, plant scale, sale of by-products, site location, and CO_2 valuation—and how much they increase or decrease the cost are shown. The site location cost reduction parameter is influenced by multiple factors and has been broken up into three sub-parameters: state-specific NG and electricity prices based on the chosen Energy Information Administration (EIA) scenario, state-specific non-optimized CO_2 T&S costs which assume dedicated CO_2 T&S operations from the state's geographic centroid, and state-specific optimized CO_2 T&S costs as discussed previously. The final LCOH for each pathway is $1/kg H_2.

The waterfall chart for the membrane-integrated ATR technology, Exhibit 19, shows that the biggest contributor to the cost reduction is the technology improvement gained by integrating the membrane within the reformer. To achieve the $1/kg H_2 goal, the Ar needs to be sold at a price of $1.00/kg Ar, which is 16 percent below typical market prices. The net result on the LCOH of locating this plant in the state of Missouri is a reduction of about $0.068/kg H_2.

Exhibit 19. Waterfall chart showing a cost reduction pathway to $1 for the membrane-integrated ATR technology
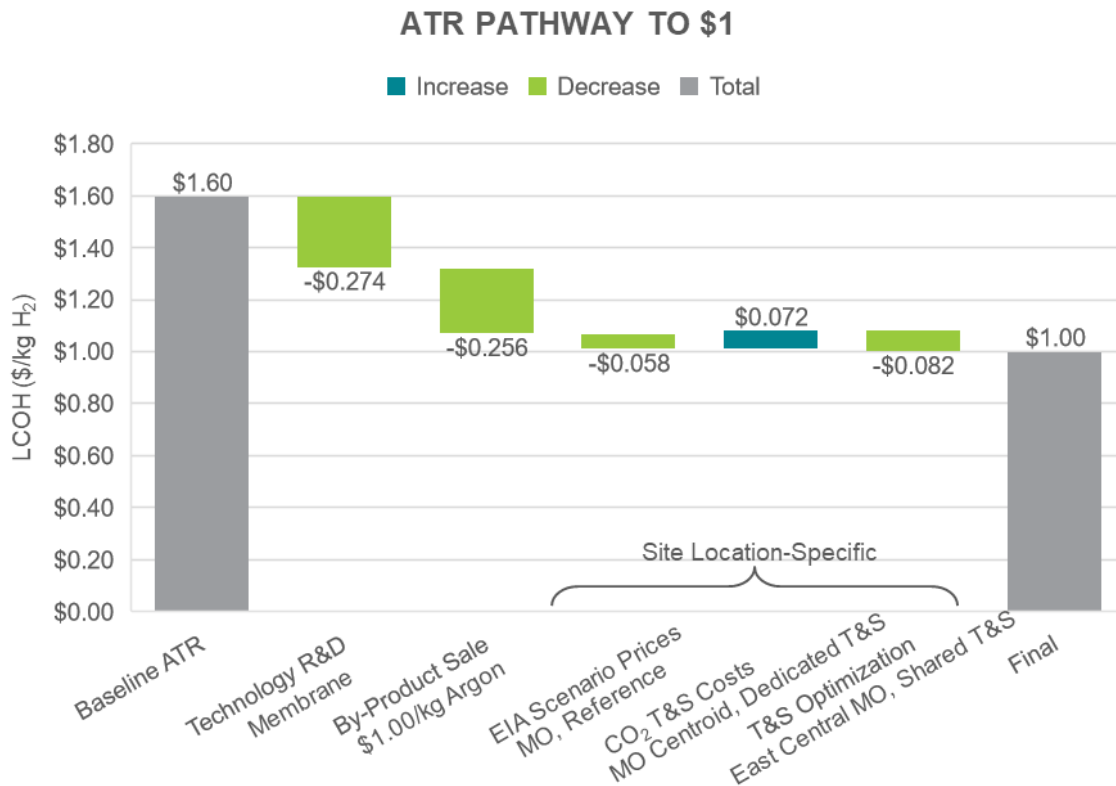
Exhibit 20 shows a waterfall chart for the pathway to $1/kg H_2 for reformer efficiency improvements with cryogenic CO_2 capture. In this pathway, CO_2 sales at $30/t CO_2 is the most significant cost reduction pathway. Next, the utilization of cryogenic CO_2 capture technology creates a $0.28/kg H_2 reduction in the LCOH. The relocation to Missouri creates a net reduction in the LCOH of about $0.067/kg H_2. In the SMR technologies, including a valuation of the CO_2 is

necessary to reach the $1/kg H_2 goal, due to the lack of a salable by-product and lack of economies of scale benefits through increasing plant size.

Exhibit 20. Waterfall chart showing a cost reduction pathway to $1 for the SMR reforming efficiency improvements with cryogenic CO_2 capture technology
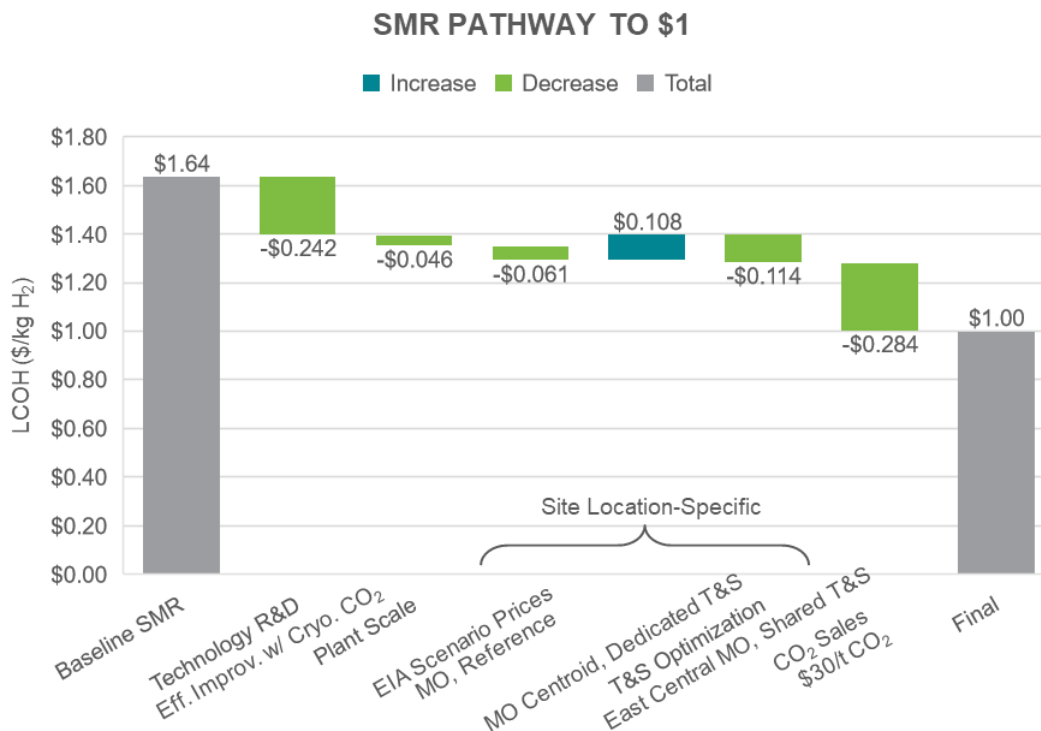
Although results are only available on a qualitative level, cost reduction pathways for POX systems can highly leverage the sale of Ar by-product. Comparing the chemistry for POX and ATR systems shows that the POX reaction uses twice as much O_2, allowing for the production of twice as much Ar by-product, which is sold as additional revenue to lower the LCOH. The sale of Ar as well as technology improvements like cryogenic CO_2 capture are pathways for reducing the cost of POX with CCS systems to $1/kg H_2.

Although not all pathways can be explored fully in this report, it is clear from what has been discussed that SMR, ATR, and POX technologies have multiple feasible options for achieving the $1/kg H_2 goal.

GASIFICATION OF SOLID FUELS WITH CARBON CAPTURE

Introduction

Solid fuel gasification for clean H_2 production involves reacting carbonaceous feedstocks with controlled amounts of O_2 and/or steam in a gasifier to produce syngas (a mixture rich in CO and H_2), often at high pressure. Gasification involves multiple reactions, including reactions of carbon with O_2, steam, and product gases—the product gases themselves can react in complex ways. Minor feedstock constituents will transform into possible pollutant species (such as sulfur

resulting in hydrogen sulfide), which must be controlled to meet emissions requirements. Major gasification reactions are depicted in Exhibit 21 along with a syngas composition range that depends on gasifier operating temperature, pressure, and choice of gasification agents and feedstocks (e.g., coal, coal and biomass, or biomass).

Exhibit 21. Gasification reactions and typical syngas composition range for O_2-blown gasification of carbonaceous feedstocks
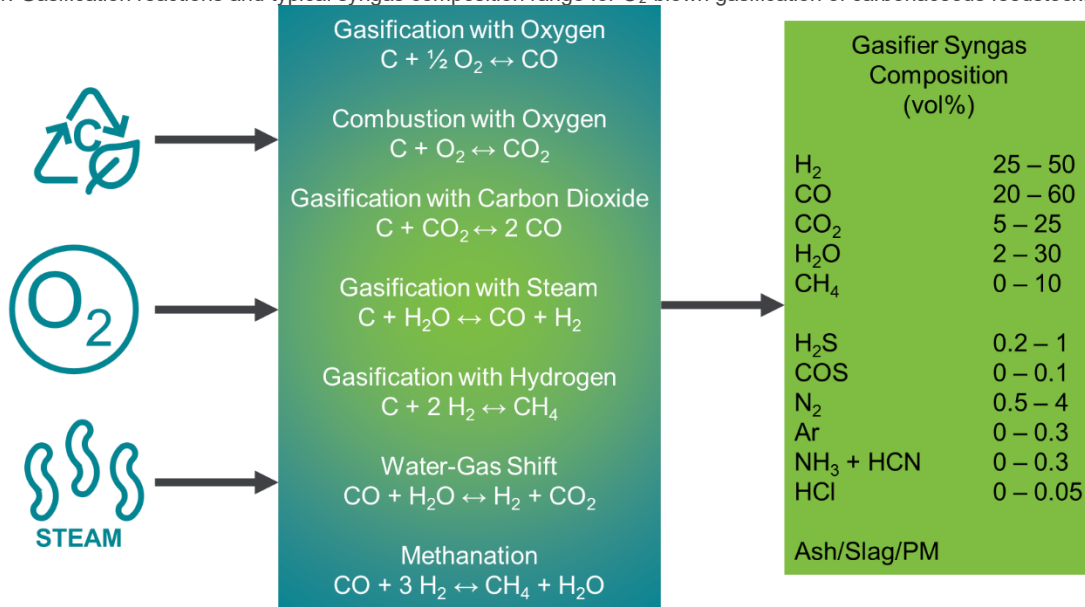
For decarbonized H_2 production, syngas is cleaned and converted to mostly H_2 and CO_2 using excess moisture through a WGS reaction. This is followed by separation of the H_2 from the CO_2, with the CO_2 compressed, transported, and stored, and the relatively pure H_2 available for use. Exhibit 22 depicts a typical process for coal and biomass gasification-based decarbonized H_2 production.

Exhibit 22. Hydrogen production from coal and biomass gasification with CO_2 removal
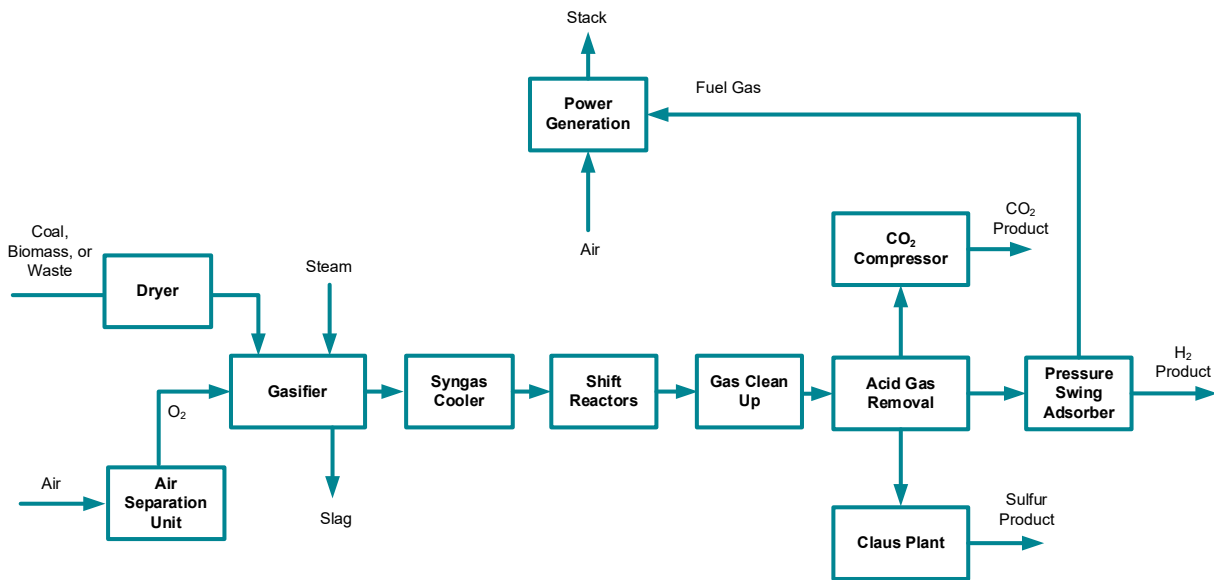
Conventionally, separation of H_2 from CO_2 in gasification systems utilizes solvent-based technologies associated with relatively high capital costs and system energy penalties. Innovative separation methods using membranes, sorbents, cryogenics, and hybrid approaches may offer higher efficiencies, but additional RD&D is needed to achieve sufficient cost reductions to be economically attractive for the next generation of clean H_2 production systems.

Gasification is versatile in being able to accept widely varied feedstocks and mixtures such as coal and waste coal, biomass, and various waste materials such as MSW and unrecyclable plastics. Gasification of coal has been used for decades as a basis for large-scale syngas generation plants for various end-products in the United States and around the world. In many of these plants, trials of biomass additions have been conducted to investigate mixed feedstock viability and possible environmental and cost benefits from utilization of low-cost and carbon-neutral biomass. Dedicated biomass gasifiers have been deployed for power and combined heat and power applications internationally. These processes normally use lower-pressure gasifier types at smaller scales, taking advantage of their relative flexibility in handling varying quality feed streams and suitability to the sizes needed for typical biomass feed opportunities.

Baseline Performance and Cost

A full TEA was conducted for a coal and biomass co-gasification case in which the amount of biomass was selected to attain a net-zero LCA emissions level [9]. Exhibit 23 provides an overall summary of the plant performance. The plant produces 5,531 kg/hr of H_2 at a CGE of 57.7 and an ETE of 57.9 percent (HHV basis). The CGE is defined as the ratio of the heat content (Btu/hr) of the H_2 product to the total fuel heat content (Btu/hr), expressed as a percent. The ETE is defined as the ratio of the H_2 product heat content plus the net power in equivalent units (Btu/pound [lb]) to the total fuel heat content (Btu/lb), expressed as a percent. Of the total auxiliary load, 37 megawatt electric (MWe), the ASU accounts for approximately 51 percent and the two-stage Selexol process and CO_2 compression account for an additional 29 percent. The steam turbine generates slightly more power than is consumed, resulting in a small net power export of 1 MWe to the grid.

Exhibit 23. Coal and biomass co-gasification baseline plant performance summary

Parameters	Coal/Biomass Co-gasification with CCS
H_2 Production Rate (kg/hr)	5,531
CO_2 Capture Rate (%)	92.7
Total Gross Power (MWe)	37
Total Auxiliaries (MWe)	37
Net Power Output (MWe)	1
As-Received Coal Flow Rate (kg/hr)	29,899
As-Received Biomass Flow Rate (kg/hr)	23,020
HHV Cold Gas Efficiency (%)	57.7
HHV Effective Thermal Efficiency (%)	57.9
Steam Turbine Cycle Efficiency (%)	42.9
Raw Water Consumption (L/kg H_2)	40.2
CO_2 Exhaust Stack Emissions (kg CO_2/kg H_2)	1.6

Exhibit 24 summarizes the contributions to the LCOH for the baseline co-gasification plant. The LCOH for the coal and biomass co-gasification case is more than double the LCOH for the reforming cases. Compared to the ATR case, the coal and biomass gasification case capital cost contribution is about five times larger, the fixed O&M cost is about six times larger, and the T&S cost is about double. The vast majority of the cost differences result from the much larger capital cost for the coal and biomass co-gasification plant.

Exhibit 24. Coal and biomass co-gasification baseline plant LCOH breakdown

Cost Component	Value (2020$/kg H$_2$)	Percentage
Capital	1.50	40%
Fixed O&M	0.77	21%
Variable O&M	0.45	12%
Fuel	0.82	22%
Total (excluding T&S)	**3.54**	**n/a**
CO$_2$ T&S	0.21	6%
Total (including CO$_2$ T&S)	**3.75**	**n/a**

The left chart in Exhibit 25 is a bar graph representation of the data in Exhibit 24 and the right chart is a donut chart that breaks down the capital costs by cost account for the coal/biomass co-gasification with CCS plant. The error bars on the left chart represent the potential LCOH range relative to the maximum and minimum capital cost uncertainty ranges. The largest contributor to capital costs is the gasifier, making up 40 percent of the total cost. The next-largest contributor is the BOP, accounting for 18 percent. The BOP includes cost accounts such as buildings and structures, feedwater systems, and instrumentation and control. The ASU accounts for 15 percent of the total capital costs.

Exhibit 25. Breakdown of coal/biomass co-gasification with CCS baseline LCOH by cost category (left) and capital costs (right)
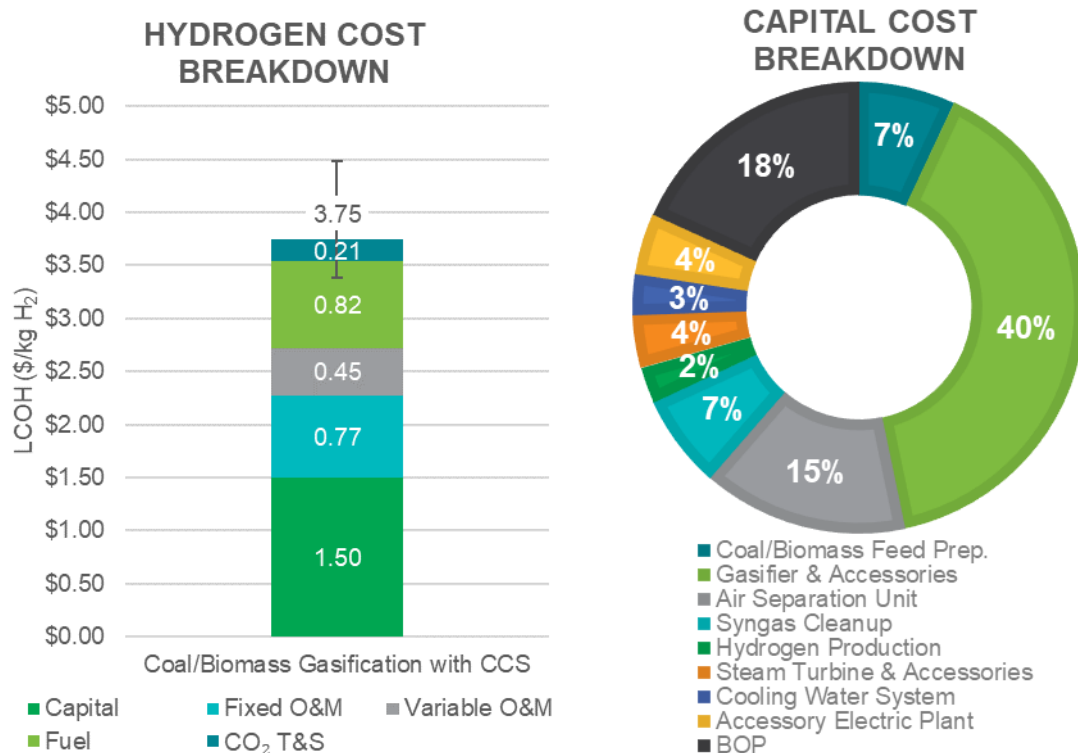
CO₂ Transport and Storage

The T&S tool, when comparing state-specific dedicated pipeline and storage project T&S costs against state-specific T&S costs assuming shared high-capacity trunkline and storage hub infrastructure, demonstrated that shared infrastructure can reduce T&S costs for the technology, depending on the state, from 34 percent to 66 percent (equivalent to $0.13/kg H_2 to $1.15/kg H_2). Exhibit 26 demonstrates coal/biomass co-gasification T&S cost reduction percentages by state. Exhibit 27 shows the optimized CO_2 T&S costs from shared high-capacity trunkline and storage hub infrastructure for coal/biomass co-gasification by state.

Exhibit 26. CO_2 T&S cost reduction percentage per state from T&S infrastructural optimization, from coal/biomass co-gasification
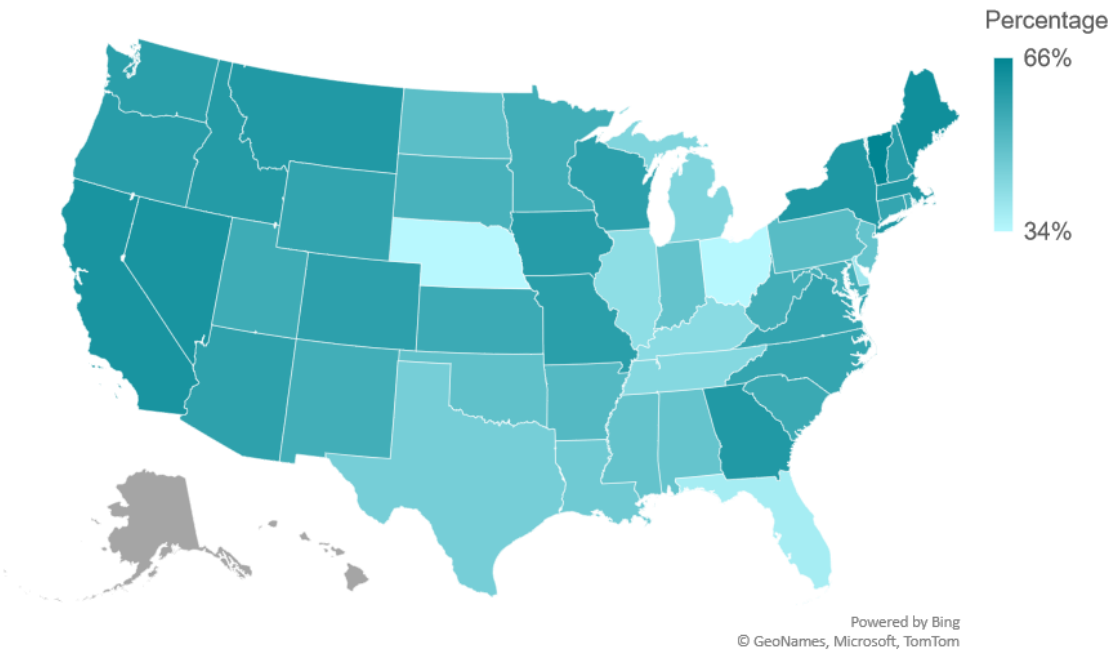
Exhibit 27. CO_2 T&S costs, optimized for shared infrastructure, for coal/biomass co-gasification, per state
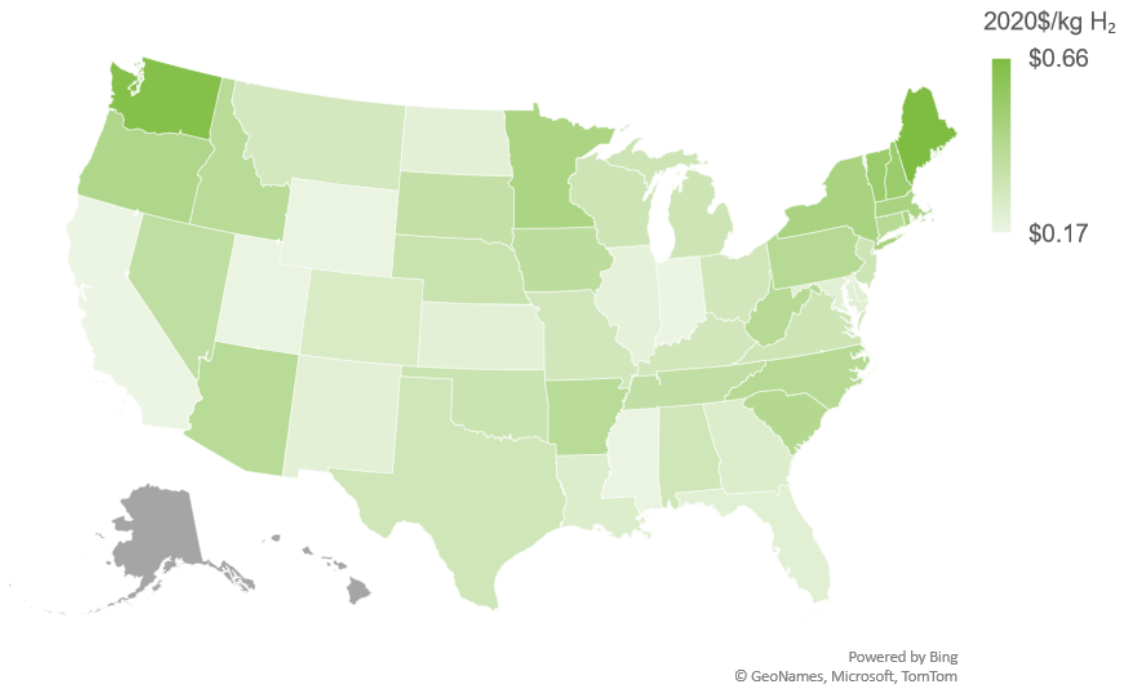
As discussed previously, additional T&S cost reductions can be generated by site selection optimizations; each case is geographically unique.

Emissions and LCA Discussion

LCA models were created for coal gasification (CG) without CCS, and coal and coal/biomass gasification with CCS, as shown in Exhibit 28.

Exhibit 28. LCA results for gasification technologies
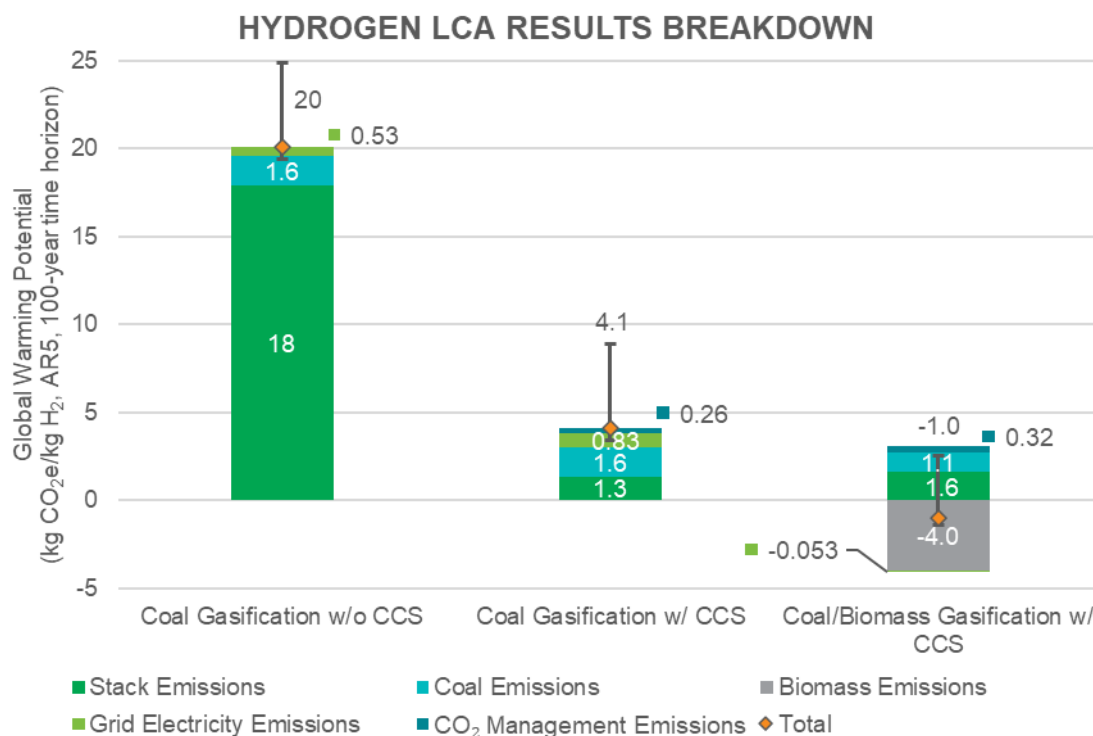
The baseline GWP results for CG without CCS are 20 kg CO_2e/kg H_2 produced. Of that value, about 90 percent of the GWP results are estimated to be the exhaust stack emissions at the facility, and about 8 percent are from the upstream emissions of mining, processing, and delivering the coal to the facility. There are small contributions from the upstream production of electricity, similar to those of the SMR facility without CCS.

CG with CCS decreases the GWP results to 4.1 (a roughly 80 percent reduction), and coal/biomass co-gasification with CCS decreases to -1.0. Like the SMR and ATR cases above, the addition of CCS does not eliminate GWP impacts. The biomass results are estimated to have net negative effects, given the estimated credit from the carbon that is stored in the biomass prior to its combustion. This is expected to be a key benefit from pursuing biomass gasification, with or without additional feedstocks.

As was observed of SMR and ATR w/ CCS, a takeaway from Exhibit 29 is that the CG w/ CCS baseline configuration considered meets this target but only if variability to the underlying life cycle data is considered. Net-zero life cycle GHG emissions are possible by co-feeding biomass and coal.

Similar to the reforming cases above, Exhibit 29 shows a variability analysis for the key model parameters for gasification.

Exhibit 29. Variability analysis for hydrogen gasification technologies
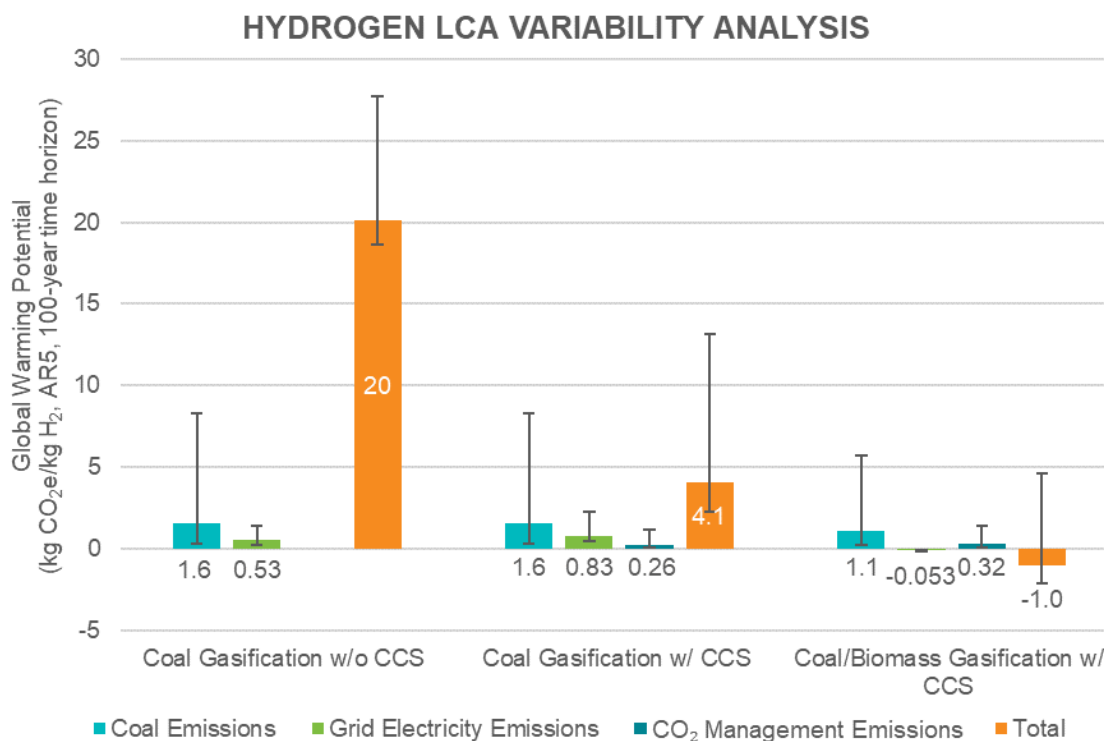
For the CG cases, the main variability is associated with the upstream coal supply chain. This is due to significant variability associated with the types of mines (surface or underground), the type of coal, and its delivery, etc. For the coal basin variability, bituminous coal in the Gulf Lignite and Southern Appalachia basins were used as the low and high cases with emissions factors of 0.037 kg CO_2e/kg coal delivered and 0.87 kg CO_2e/kg coal delivered, respectively. The CG process modeling done in this study specified Illinois No. 6 coal, and these results did not recheck thermodynamic requirements for all different types of coal in the gasifier, and so these variabilities shown may overstate or understate the actual variability that would be found if parallel analyses were done to derive the engineering parameters associated with all the different types of coal. The CG cases show only modest variability associated with the upstream grid electricity (albeit with higher magnitude for CG with CCS).

For coal and biomass gasification, the upstream coal and grid electricity are key contributors to variability. Note that the variability of the upstream biomass was not included in this analysis, due to lack of data on the GWP effects of biomass in different areas of the United States, but also would be expected to be variable. The GWP associated with managing CO_2 is only slightly variable, and a small overall contributor.

Cost Reduction Pathways

Although technologies exist for production of clean H_2 from solid fuel gasification-based systems, additional RD&D is needed to reduce the relatively high cost of gasification for clean H_2 production. Conventional gasification process technology has a large experience base for gasifiers for conventional coal or biomass gasifiers individually but there is a need to develop sufficient design information and operating experience gasifying mixtures of feedstocks that will aid in decarbonization and life cycle environmental performance. Introducing a complex feedstock blend of biomass mixed with legacy coal wastes, mixed plastics, MSW, and/or other wastes is likely to create issues with feed preparation/feeding to the gasifier vessel, new issues with syngas cleanup (given the slate of unusual contaminants that may be present in mixed wastes containing biomass and plastics), and corrosion issues, particularly in high-temperature zones of gasification vessels and certain other unit operations. Given the significant differences and lack of experience with mixed fuel (wastes from varied and inconsistent sources, and with biomass that may also exhibit variability), RD&D is needed to adapt or leverage known gasifier technology to a preponderance of mixed feedstock as demanded by decarbonization and life cycle performance goals.

The large capital and investment cost of gasification plants has been a hurdle to realization of a more widespread commercial gasification industry base; however, novel modular gasification systems could reduce costs to tractable levels that may attract market interest and investment. Modularity will be an important cost reduction pathway for both nearer-term gasification technology applications and advanced/developmental gasification systems that may emerge in the future.

In general, the concept of process intensification is a powerful path to reduce costs in gasification systems and units. Process intensification includes developing more efficient and compact systems through the optimization of critical parameters and/or combining multiple unit operations into a single subsystem that can accomplish multiple process steps simultaneously. Process intensification concepts to increase specific throughput (i.e., an increase in output per given equipment size) would have benefits for both energy efficiency and capital cost efficiency, thus reducing the cost per unit H_2 output of modular-scale systems.

Important auxiliary unit operations for gasification include O_2 production, syngas cleanup, and H_2 separation, all of which could benefit from advanced, efficient, and low-cost modular and process-intensified methods compared to conventional technologies. Some specific possibilities include 1) selective H_2 extraction from various gasification unit operations (e.g., the gasifier, or raw syngas quench, or WGS reactor) that might have combinatorial benefits for reducing equipment size, advantageously shifting reaction equilibrium and advantageously affecting gas phase space velocity via density change, etc.; or 2) CO_2 removal technologies integrated and combined with gasification system unit operations for capital cost efficiency; or 3) the combination of multiple unit operations (e.g., syngas cleanup systems, WGS) into a single unit operation to achieve an overall reduction in the system's unit operation count. Holistic approaches with gas separation/pollutant removal technologies would constitute the idea of process intensification to substantial cost and performance advantage.

Significantly overlapping opportunities are expected for cost reduction of CO_2 capture technologies that have applicability to both NG reforming and solid feedstock gasification. Capture technologies used on syngas in NG reforming cycles may apply to capture in gasification as well.

Pursuit of the above-suggested RD&D and advances in CO_2 removal are needed for significant cost reductions to achieve the DOE Hydrogen Shot goal targeting H_2 cost of $1 per 1 kg of clean H_2 by 2030.

PYROLYSIS OF NATURAL GAS

Introduction

The pyrolysis of CH_4 is a process that entails the breakdown of CH_4 into solid carbon and H_2 gas according to the following simplified chemical reaction: $CH_{4(g)} \rightarrow 2H_{2(g)} + C_{(s)}$. With plasma-based processes, the energy needed to drive the endothermic reaction comes from a plasma torch which typically operates at temperatures up to 2,000 °C, although "cold plasma" non-thermal processes have been proposed and are undergoing RD&D [25] [26]. The reaction has a standard state heat of reaction of 74.9 kJ/mol, which is within 10 percent of the heat of reaction for SMR on a per mole of H_2 basis. When the heat required for the steam generation for SMR is considered, the net heat of reaction for plasma pyrolysis is only about 60 percent of that for SMR [27].

The maximum theoretical yield of H_2 from plasma pyrolysis of CH_4 is two moles of H_2 per mole of CH_4. This is half the maximum theoretical yield as from SMR. However, the overall plasma pyrolysis yield is considerably lower than the maximum due to the presence of side reactions that can produce undesired hydrocarbon by-products requiring H_2 purification steps and by-product utilization or disposal. This issue is further exacerbated when the feedstock is NG, rather than CH_4, due to the presence of higher molecular weight hydrocarbons, e.g., C_2-C_{4+}.

An important factor to consider when comparing SMR with plasma pyrolysis is that SMR operates at elevated pressure whereas existing plasma pyrolysis units have operated at atmospheric pressure. This is likely to significantly impact capital costs but will definitely require additional auxiliary power to compress the H_2 product to the delivery pressure.

Exhibit 30 shows a simplified BFD for the pyrolysis process. In this process, the NG is desulfurized and then fed to the plasma reactor. The effluent is cooled prior to carbon product recovery and H_2 purification. The PSA off-gas is recycled back to the plasma reactor and a slip stream of the off-gas is used as fuel either in a combustion turbine for power generation or fired heater for heat recovery, depending on the needs of the pyrolysis system. This gaseous purge is also necessary to prevent build-up of inert products formed via side reactions.

Exhibit 30. BFD of plasma methane pyrolysis process
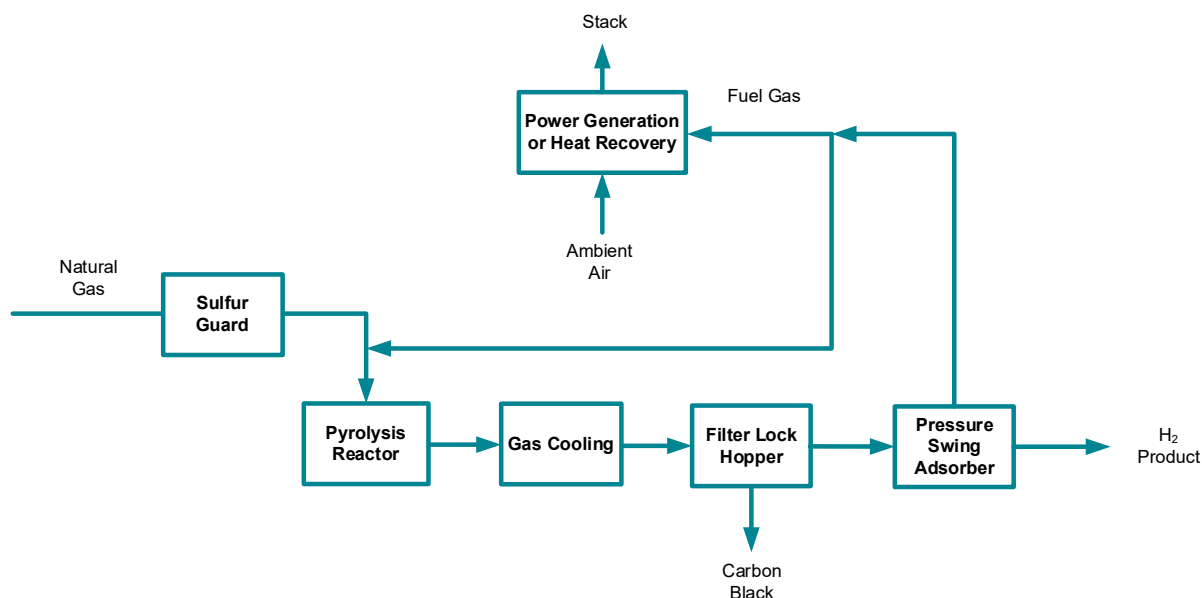
The initial efforts to develop a commercial plasma pyrolysis process focused on the carbon black product which is still by far the most valuable of the reaction products. More recently, commercialization efforts have been more focused on plasma pyrolysis as a process to produce H_2. A commercial example is the Monolith Olive Creek Plant, an operating plasma pyrolysis plant in Nebraska. This plant has a yearly carbon black capacity of 14,000 tons and produces 600 kg/hr (~6 MMSCFD) of H_2, which is used to create NH_3 for fertilizer use. Phase 2 of the Olive Creek project is planned for commissioning in 2023, which will utilize twelve 16,000-ton-capacity reactors, increasing production by about 13-fold [28].

Baseline Performance and Cost

Unlike the previously discussed technologies, a detailed TEA has not been performed for plasma pyrolysis process. Only highly approximate estimates for the cost and performance can be made through publicly available sources.

It is clear that considerable cost reduction can be achieved from the elimination of several unit operations that would be required for an SMR process. As a result, the LCOH for plasma pyrolysis will be even more dependent on the price of NG as for the SMR case. Publications state that the cradle-to-gate GHG emissions are 0.45 kg CO_2e/kg H_2 for the pyrolysis technology with NG and -2.08 kg CO_2e/kg H_2 when using RNG. No further details are provided but it is likely that these figures employ a plasma torch powered with renewable electricity.

Compared to the ATR and POX flowsheets, this scenario eliminates the need for a pre-reformer (ATR only), ASU, WGS reactors, pre-combustion CO_2 capture unit, fired heater, CO_2 compression, and CO_2 management. Compared to SMR, this scenario eliminates the need for a pre-reformer, WGS reactors, pre-combustion and post-combustion CO_2 capture units, fired heater, CO_2 compression, and CO_2 management. Due to the chemistry of pyrolysis, a 20

percent higher NG feed rate is required for the same H_2 production rate as used in the ATR case, resulting in a 0.24 H_2:NG mass yield. The power requirement for the plasma system is 8.2 kWh/kg NG. The carbon black produced is assumed to be a saleable by-product.

A screening assessment estimated that the LCOH would be approximately 3 percent higher than the baseline ATR case. According to this assessment, the savings in capital cost from the simpler pyrolysis systems is more than offset by an increase in operating cost for the assumed price of NG.

Emissions and LCA Discussion

With respect to the GWP impacts of pyrolysis, the current footprint of the technology is estimated to be comparable to, but slightly higher than, ATR with CCS, but lower than SMR without CCS. The relative contributions in the life cycle for pyrolysis are almost entirely from upstream NG and electricity. The upstream NG emissions have a significant amount of variability, including across production basins in the United States (where the emissions vary by a factor of 2), as well as via the different routing of gas through pipeline operators and networks that inconsistently manage equipment and leaks. Likewise, the upstream grid electricity emissions are highly variable (by a factor of 5) as a result of electricity grid mixes that are relatively low-carbon (e.g., in the Pacific Northwest) and higher carbon (e.g., in the mountain west region).

As has been mentioned for other H_2 production routes, strategies for pyrolysis project developers to lower their GWP include procuring NG and power from regional supply chains where producers and suppliers effectively manage the emissions of the respective product. Various strategies exist which include managing fugitive emissions, electrification of NG compressor stations, renewable NG blending, and decarbonization of power generation through CO_2 capture and/or renewables. Efficiency gains made through pyrolysis RD&D are another strategy to GWP improvements from lowering feedstock usage per unit of H_2 produced.

Overall, this means that considering across the variability of upstream NG and electricity, the GWP of pyrolysis could be as low as SMR with CCS or as high as SMR without CCS, in the near term. However, this qualitative analysis does not consider credits or avoided emissions associated with the by-production of conventionally produced carbon black, which is a GWP-intensive process, which could further decrease the footprint of this technology.

Cost Reduction Pathways

Although plasma pyrolysis processes appear to have a slightly higher LCOH than the reference ATR plant, the economics dramatically improve when the carbon black becomes a saleable product. The screening analysis used an assumed carbon black selling price half that used in a recent DOE Advanced Research Projects Agency – Energy (ARPA-E) presentation and still calculated a negative LCOH, meaning that the owners would have to pay vendors to take the H_2 to limit the plant profitability to the target parameters [29]. Therefore, the plasma pyrolysis process has the potential to achieve extremely low-cost H_2. Given that the carbon-to-H_2 mass yield for the process is ~3:1, the size of existing and new markets for carbon products is a critical aspect of the success of this technology.

Pathways to reduce the cost further will need to focus on some of the technical shortcomings of the process including solid carbon deposition on equipment and product gas stream contamination requiring an extensive and expensive gas cleanup unit.

Another promising pathway for plasma pyrolysis entails the use of catalysts to accelerate the pyrolysis reactions, rather than extremes in temperature. This will certainly reduce the energy cost for the process but there are potential disadvantages including increased rate of by-product formation and the potential for catalyst deactivation from some of the by-products.

ADVANCED THERMAL CONVERSION TECHNOLOGIES

Introduction

A number of advanced technologies that are in relatively early stages of development appear to offer benefits compared to the current commercial offerings. One of these technologies is in situ H_2 generation. A simplified BFD for an in-situ reforming concept is shown in Exhibit 31 [30].

Exhibit 31. BFD for in situ reforming
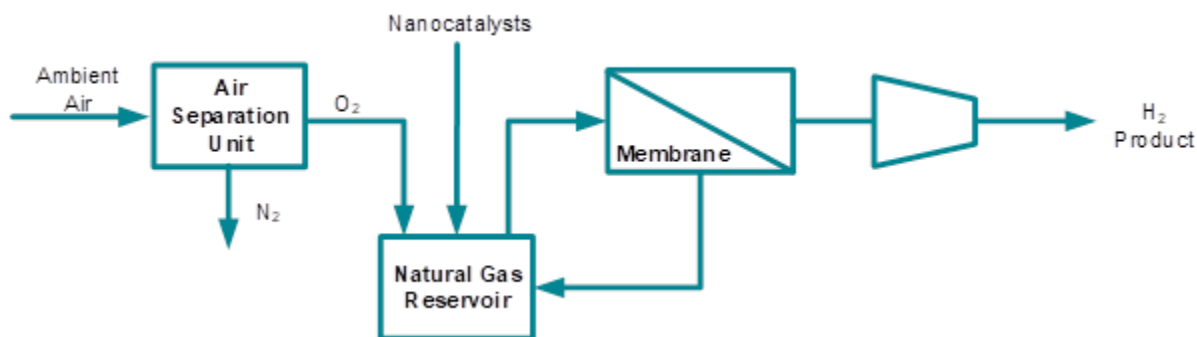
This unique concept proposes that combustion, gasification, and reforming processes all take place in subsurface locations where hydrocarbons are found. Nano catalysts would be used to achieve acceptable reforming rates at as low a temperature as possible and selective membranes would be employed to trap CO_2 behind while only extracting H_2.

Chemical looping is another technology with DOE-sponsored RD&D. Most chemical looping concepts utilize a metal oxide carrier that is circulated between two or three vessels at elevated temperature and pressure. In general, chemical looping achieves process benefits through intensification resulting from highly selective chemical reactions. Exhibit 32 shows a BFD for a chemical looping process that uses three reaction vessels.

Exhibit 32. BFD for 3-reactor reforming concept with O_2 carrier
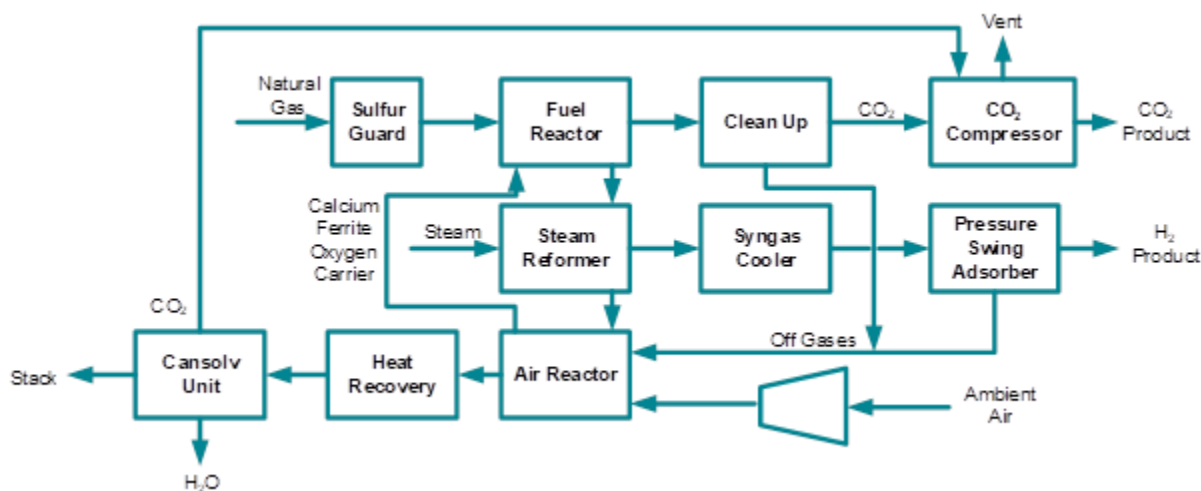
Exhibit 32 depicts a 3-reactor concept consisting of fuel, steam, and air reactors that circulate a calcium ferrite O_2 carrier. Reduction of the O_2 carrier occurs in the fuel reactor, producing CO_2 that is sent through a CO_2 purification unit (CPU). Steam reforming occurs in the second reactor through the addition of steam and the reduced O_2 carrier. Oxidation of the carrier occurs in the air reactor in which PSA and CPU off-gases are combined with air. This completes the 3-reactor cycle.

A third advanced technology for generating H_2 from NG via thermal conversion is known as DRM. This process is almost identical to the SMR technology except CO_2 replaces water (H_2O) as the oxidizing agent in the reformer. Exhibit 33 gives a BFD for a simplified and generic DRM process.

Exhibit 33. BFD for DRM concept
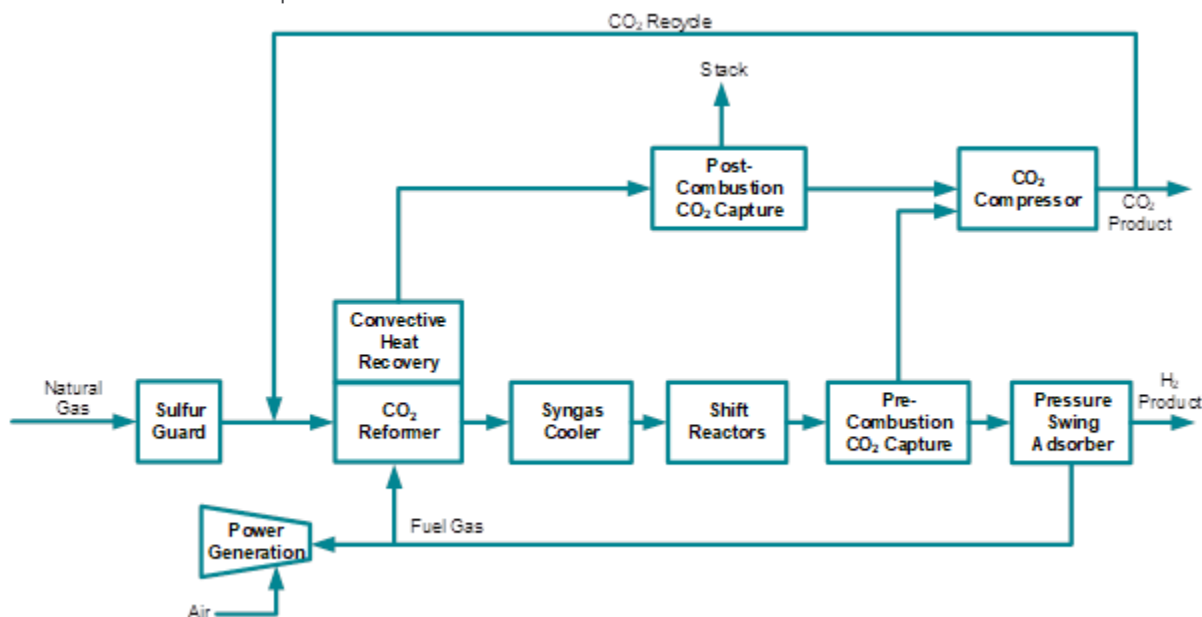
The overall chemistry for the DRM process is as follows: $CH_4 + CO_2 \rightarrow 2\,CO + 2\,H_2$. Unlike SMR, DRM produces a syngas with a H_2:CO ratio of 1. The overall H_2:CO ratio can be increased by performing one or more stages of WGS on a portion of the reformate stream. The process concept depicted in Exhibit 33 shows a combustion turbine for on-site power generation. This is an optional addition.

The primary application for DRM is to generate a syngas suitable for downstream hydrocarbon synthesis. However, it has received renewed attention recently as a process for the co-production of H_2 and electric power.

Baseline Performance and Cost

A detailed TEA was not performed for the in situ H_2 generation case. Rather, screening level analysis was performed to estimate the cost and performance in comparison to a reference ATR case.

Compared to the ATR flowsheet, this scenario eliminates the need for a sulfur guard, pre-reformer, ATR, WGS reactors, pre-combustion CO_2 capture unit, CO_2 compression, PSA unit, heat recovery/cooling systems, CO_2 transportation, and exhaust stack CO_2 emissions; however, this scenario needs a H_2 compressor. Due to the injection type of this scenario, it is assumed that there are no CO_2 T&S costs. It is assumed that the labor cost is 50 percent of the baseline labor costs. It is also assumed that the cost of the nano catalyst is equal to the cost of the ATR catalyst.

A screening analysis was performed on the 3-reactor reforming concept with O_2 carrier to develop estimates for the process performance and cost. Compared to the SMR flowsheet, this scenario eliminates the need for a pre-reformer, WGS reactors, and the pre-combustion CO_2 capture unit. An 18 percent lower NG flow rate is required for the same H_2 production rate, resulting in a 0.33 H_2:NG mass yield. The steam-to-carbon molar ratio is estimated to be 53 percent higher than the baseline SMR case. Furthermore, there is an 82 percent higher electricity consumption per unit of H_2 [31] [32]. An assumption is made that the cost of the O_2 carrier is equal to the cost of the SMR catalyst.

As with the other advanced technologies described in this section, a detailed TEA was not performed for the DRM process and the performance and cost can only be roughly estimated. Since the number and type of process units in the DRM process concept is the same as for the SMR process, the capital cost of DRM without on-site power generation would be expected to be similar to that for SMR. However, the DRM reaction is more endothermic than the SMR reaction and, hence, the effective thermal efficiency would be expected to be lower and the fuel and O&M costs higher. Unless a niche application can be identified, perhaps where CO_2 sources are available, it is unlikely that the DRM technology will be more economical than the SMR technology.

Emissions and LCA Discussion

With respect to the GHG emissions and GWP impacts of in situ H_2, the current footprint of the technology is estimated to be comparable to, but slightly less than, SMR with CCS, which makes it an attractive option. As mentioned previously, the upstream GWP effects of NG are

large and variable. However as applied to this technology, the NG upstream emissions are over-estimated as factors were used that include the life cycle of NG through transmission, while this technology would use gas straight from the ground that requires no transport effects. Reservoirs and basins have different upstream emissions, which leads to variability associated with this part of the life cycle. There are also potential differences in gas compositions and subsequent processing that were not considered for the in situ technology. On the other hand, the screening analysis done on this technology so far has not considered the potentially GWP-intensive production of nano catalysts and membranes required.

With respect to chemical looping, the estimated GWP from the technologies discussed is comparable to, but slightly less than, SMR with CCS. About 60 percent of the GWP is estimated to come from upstream NG emissions, and about 33 percent from upstream grid electricity. Modest emissions come from the exhaust stack and T&S. As noted above, to the extent that NG and electricity could be sourced from the least GWP-intensive options, significant further reductions are possible from the baseline discussed here.

No LCA modeling was attempted on DRM.

Cost Reduction Pathways

The in situ technology already achieves a very significant drop in capital cost compared to the reference ATR plant. The screening analysis estimates that the reduction in LCOH could be as much as 25 percent. However, this will still not achieve the goal of $1/kg H_2 but the goal can be achieved if Ar by-product sales are included.

While Exhibit 32 depicts an ASU with O_2 injection, concepts using air for the oxidation exist. This could result in a significant savings in capital costs, although the N_2 accompanying the air is an undesirable component that reduces the effective storage capacity of the reservoir.

In addition to in situ reforming, in situ pyrolysis concepts have also been considered. This is an even simpler process as molecular filtering of H_2 via membranes is not needed. This concept has not been developed to the point of identifying the type of catalyst that would be used, if any. Since the carbon left behind is solid, this concept may allay concerns about the long-term viability of storing CO_2.

As with other pyrolysis concepts, the fact that the highly enthalpic carbon remains unburned means that the process efficiency is relatively low. Further, designing a process where the valuable carbon black can be recovered will be a significant challenge.

For the 3-reactor reforming concept with O_2 carrier, considerable RD&D remains to be performed for the O_2 carrier material. It is a significant engineering challenge to transport very hot pressurized solids between the three reactor vessels. In addition, the usable lifetime of the O_2 carrier is unknown and if too low, it would render the process uneconomical.

One possible approach to circumvent these engineering challenges is to not circulate the O_2 carrier and instead, alternate the gas composition fed to the reactor between air, NG, and

steam. Exhibit 34 shows a simplified BFD for such a chemical looping with gas switching concept.

Exhibit 34. BFD for a chemical looping with gas switching concept
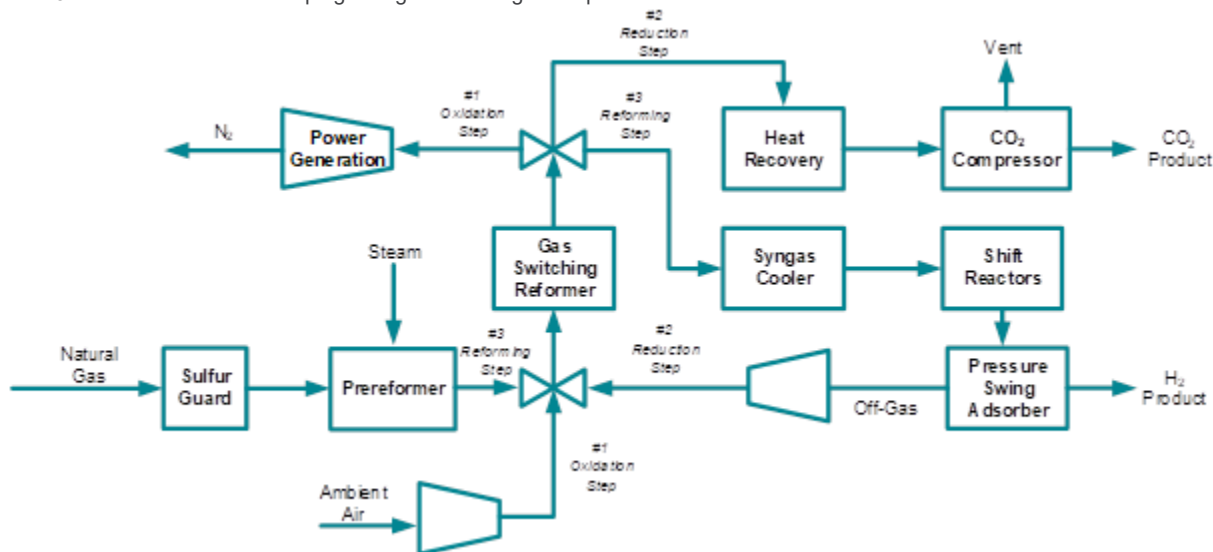
The O_2 carrier is oxidized via an air stream, resulting in a N_2 stream that is sent to a turbine to generate additional electricity. The O_2 carrier is reduced via the PSA off-gas, resulting in H_2O and CO_2, which is dried, compressed, and stored. The NG and steam mixture is reformed to produce syngas and is catalyzed by the nickel-based O_2 carrier [33].

Compared to the SMR flowsheet, this scenario eliminates the need for both pre- and post-combustion CO_2 capture units. A 9 percent lower NG feed rate is required for the same H_2 production, resulting in a 0.29 H_2:NG mass yield. A higher steam-to-carbon molar ratio of 2.66 is needed for this scenario. Finally, a 69 percent higher electricity consumption per unit H_2 is required due to additional compression requirements.

Because of its similarity to SMR, opportunities to reduce the cost of H_2 from a pathway based on the DRM technology are largely the same as those identified for SMR cost reduction. The largest cost components for DRM are expected to be the NG feedstock, CO_2 capture units, reformer, and heat recovery components. RD&D that improves the yield or effective thermal efficiency of the DRM reactor will reduce the NG requirement, which is the largest cost contributor. Improvements to the CO_2 capture unit and heat recovery components are expected to offer about the same degree of cost reduction as for SMR.

A recent literature search identified two advanced versions of the DRM concept and in both cases, the focus of the improvement is on the reforming catalyst. Linde has developed the DRYREF™ process, which relies on a version of the BASF developed SYNSPIRE™ G1-110 catalyst and is a hybrid of SMR and DRM [34]. The process can be configured in multiple manners to achieve target performance metrics. Case studies by BASF indicate that this technology can achieve a 3–5 percent reduction in capital cost and a 5 percent reduction in O&M costs. In some scenarios, CO_2 is imported to the plant and with H_2:CO ratios less than 1.5, it can achieve net negative emissions. Another such DRM process with an improved catalyst is

the process concept from the Gas Technology Institute (GTI) that employs a nano-engineered Ni catalyst on ceramic hollow fibers [35]. GTI claims that the GWP of their process is 40 percent lower than the state-of-the-art SMR process.

INTEGRATED ENERGY AND INDUSTRIAL SYSTEMS TO ENABLE DEEP DECARBONIZATION

Recent studies have highlighted opportunities for integrated energy systems (IES), which synergistically incorporate diverse energy sources, including renewable, nuclear, and fossil with carbon capture, to more effectively provide environmentally sustainable, cost effective, and reliable power, heat, mobility, and a variety of other consumer products and services [36]. An IES enables efficient utilization of multiple feedstocks to create multiple products and services through increased coordination and direct hybridization, allowing dynamic optimization of supply and demand. The development and deployment of such IES would enable deep decarbonization of the U.S. economy while providing significant opportunities for cost reductions to energy systems.

One such IES option for reforming technologies is to integrate an SMR with a gas turbine to create a system that uses the same feedstock to generate both H_2 and power while sharing the same carbon capture system. The power generated by the IES can provide low carbon electricity for on-site use, hence, avoiding the operating cost of grid electricity and its uncertainty due to price oscillations in the power market. IES power can alternatively serve as an additional revenue stream if sold to external consumers or to the grid. Furthermore, the thermal efficiency of an IES can be better optimized through process and heat integration compared to standalone systems for power and H_2 generation.

RD&D STRATEGIES FOR COST REDUCTIONS (DEPARTMENT OF ENERGY)

The following sections include a discussion of Department of Energy-sponsored research and development projects. Recent funding opportunity announcements (FOA) such as DE-FOA-0002400 provide funding to carry-out H_2 production RD&D in support of several FECM programs. This section also provides a brief analysis of how RD&D strategies can provide additional cost reduction opportunities for clean H_2 production technologies. The cost reduction opportunities considered here are at the site of H_2 production and apply to plant technologies capable of achieving or exceeding the BIL definition of clean H_2. If efforts are made to fully decarbonize thermal production routes, additional costs may be borne outside of the plant boundary.

Reforming of Natural Gas with Carbon Capture

Technology improvements to the baseline representations of current, state-of-the-art ATR and SMR with carbon technologies are needed for LCOH reduction. The technology improvements shown in Exhibit 18 are commercially available except the advanced membrane-integrated ATR

concept, which requires early-stage RD&D. However, large-scale demonstrations of these technologies in integrated process systems for clean H_2 production are limited.

An effective RD&D strategy for NG reforming technologies with carbon capture will advance large-scale demonstrations of commercially available technologies as well as the technical maturity of transformative reforming technologies. Early-stage RD&D is needed for transformational reforming concepts and will be discussed in the Advanced Thermal Conversion Technologies section. TEA and pre-front end engineering and design (FEED) studies to identify regions and markets most amenable to project economics and de-risking development of projects that incorporate commercial, and near-commercial, technology improvements have begun.

PRESENT RD&D

The DOE Office of Fossil Energy and Carbon Management (FECM) Carbon Capture Program has begun supporting RD&D of NG reforming technologies with carbon capture by providing funding through cooperative agreements with private industry, academia, and other government organizations resulting from two Funding Opportunity Announcements (FOAs) issued since 2020. In addition to the TEAs of the awarded projects, energy markets and LCA studies are needed to develop a rigorous understanding of the pathways highlighted in Exhibit 18. Furthermore, additional research is needed in the area of CH_4 emission quantification and management due to the high sensitivity of cradle-to-gate emissions to variations in NG emissions.

On January 15, 2021, DOE FECM released funding opportunity announcement DE-FOA-0002400 to fully utilize existing technology for net-zero carbon energy and commodity production through the production, transport, storage, and utilization of fossil-based H_2 with zero or negative carbon emissions [37]. Seven RD&D program areas are represented in the FOA, one of which provides funding opportunities for NG reforming technologies with carbon capture. The program area, objective, and associated Areas of Interest (AOIs) are as follows:

- Carbon Capture RD&D Program – The objective is to complete the initial design of a commercial-scale, carbon capture, storage, and utilization (CCUS) system that separates and stores more than 100,000 t/year net CO_2 of 95 percent purity, with 90+ percent carbon capture efficiency, from an SMR or ATR plant producing 99.97 percent H_2 from NG.
- AOI 7a: Advanced CCUS systems from SMR plants
- AOI 7b: Advanced CCUS systems from ATR plants

On April 23, 2020, DOE FECM released DE-FOA-0002187 under the Carbon Capture RD&D Program aimed at supporting initial engineering analyses on the design and implementation of carbon capture technologies specific to industrial CO_2 sources with CO_2 concentrations higher than coal-based flue gas at sites with emissions greater than 100,000 t/year of CO_2 [38]. The following AOI provides funding opportunities for NG reforming technologies with carbon capture under this FOA:

- AOI 1: CO_2 Capture and Compression from Industrial Sources

Collectively, five projects have been awarded under these two FOAs that represent current DOE FECM support for RD&D of NG reforming technologies with carbon capture. These projects largely focus on developing FEED studies for H_2 production with CCS, which helps to expand the knowledge base on large carbon capture projects.

Gasification of Solid Fuels with Carbon Capture
PAST RD&D

DOE FECM and its predecessors have been engaged in gasification systems RD&D from the founding of the department in the 1970s. At that time, NG shortages and the decreased access to petroleum products (in part due to the 1973 and 1979 oil embargos) strongly drove government-funded research on gasification technology for both power and liquid fuels production. An important focus of DOE research at that time was on large-scale, environmentally superior CG-based power generation through integrated gasification combined cycle (IGCC) systems. In the 1980s, the groundbreaking Cool Water IGCC project in California was the first successful demonstration of the basic IGCC concept at a commercial scale. Development continued in the 1990s with the commercial-scale Wabash River Coal Gasification Repowering Project (a Round IV Demonstration Project under DOE's Clean Coal Technology Program) in Indiana, and the greenfield IGCC unit at Tampa Electric's Polk Power Plant (a Round III demo under the Clean Coal Technology Program) in Florida. Both demos were highly successful, enabling gains in O&M experience, increasing gasifier and plant reliability, and increasing system uptime, and enabling experimentation with less expensive coal feedstocks. On completion of the demos, those IGCC units continued economical operation for years as the most efficient and cleanest coal-fired power units in the United States.

DOE's collaborations with industry to bring CG to commercial-scale operations shifted to focus on advancing specific key technologies within gasification systems and processes to reduce the cost and increase the efficiency of producing syngas and decreasing the carbon footprint of gasification. These included the following:

Syngas Cleanup – The conventional approach to syngas cleanup involves washing with water, but this means a severe temperature reduction of the syngas causing loss of thermodynamic efficiency. Methods to purify the syngas at elevated temperature (warm gas cleanup) were pursued as a high efficiency alternative. DOE/National Energy Technology Laboratory (NETL) partnered with the Research Triangle Institute on a near-commercial-scale demonstration of warm gas cleanup of syngas at the Polk Power Plant IGCC unit, on 20 percent of the syngas flow of the plant (50 MWe equivalent). This technology uses advanced regenerable sorbents to capture pollutant species from the syngas. The demonstration was successful, and the technology is ready for full-scale commercial implementation, allowing increased overall power generation efficiency at IGCC plants anywhere.

Integrated Water-Gas Shift/Pre-Combustion CO_2 Capture – Conventional WGS reactors require multiple stages at different operating temperatures and separate gas separation steps to reach adequate conversions of syngas to H_2. DOE/NETL has, therefore, been pursuing concepts to integrate CO_2 removal or H_2 separation directly into the WGS reactor (involving O_2 sorbents, selective gas separation membranes), thus reducing reaction stages and increasing efficiency.

Transport Gasification – DOE/NETL played a pivotal role in fostering the development of the Kellogg, Brown, & Root transport gasifier, an advanced circulating fluidized bed reactor for efficient conversion of low-rank, high-moisture, high-ash coals. This technology was tested and proved at the Power Systems Development Facility in Wilsonville, Alabama.

Gasifier Refractory – Refractory material lines a gasifier and gives it ability to withstand extremely high operating temperatures. The limited lifetime of refractories has been an ongoing problem in gasifier operation, demanding frequent replacement of this expensive material, and lowering system availability. DOE/NETL researchers addressed this problem with development of a series of innovative refractory materials. Aurex 95P is a patented and commercially deployed phosphate-modified chromium oxide refractory brick having decreased slag penetration, elimination of spalling, and high resistance to chemical corrosion. NETL's work in the area continued with the recent invention of the Chromia brick, which uses carbon treatment to fill void spaces and further increase durability and lifetime of the refractory in the extreme conditions of slagging gasifiers.

Feed Systems – Many commercial coal-based gasifiers use high-pressure, high-temperature entrained flow gasification, which limits feeding to slurried forms of coal that can be pumped at high pressure. The additional water compels use of higher ranks of coal (primarily bituminous) because slurrying water added to lower ranks of coal results in insufficient thermal value of the resultant slurry. Therefore, NETL has supported significant RD&D on cost-effective and reliable high-pressure solid feed systems to enable use of abundant and inexpensive low-rank coals in dry feeding of high-pressure gasifiers; to allow co-feeding of coal with other advantageous fuels (such as biomass, petcoke, or solid waste); and to encourage higher pressure (and therefore more efficient) operation of dry-feed gasifiers, reducing plant capital and O&M costs.

Oxygen Production – Many gasification technologies demand O_2 instead of air as an input, which is conventionally supplied by expensive and energy-intensive cryogenic ASUs. Innovative technologies such as high-temperature ceramic O_2 separation membranes/ion transport membranes have been investigated to reduce capital and operating costs of O_2 production and to enable fundamental increase of process cycle efficiency.

Catalytic Gasification – Catalytic gasification (as opposed to conventional high-temperature non-catalytic gasification) enables gasification at lower temperatures, reducing deterioration of gasifier vessels and refractory. Work included experiments, kinetic modeling, and computational fluid dynamics of advanced catalytic gasification of coal and coal-biomass mixtures to effectively gasify coal at lower temperatures and produce a cleaner syngas with elevated levels of H_2. Also, progress has been made in high-temperature steam reforming catalysts for use under the severe conditions of reforming tar, light hydrocarbons, NH_3, and CH_4 found in raw synthesis gas. The potential benefits of catalyst development include improving H_2 yield, reducing WGS requirements, and reducing downstream gas cleanup requirements.

PRESENT RD&D
DOE/NETL's work in the area of gasification of solid feedstocks currently focuses on early-stage RD&D for enhancement of environmental standards and increasing availability, efficiency, and

reliability of gasification systems. In so doing, the goals are to foster U.S. economic security through maintaining fuel diversity and energy resiliency, while helping to address the essential carbon reductions required to halve GHG emissions by 2030 and attain a carbon pollution-free electricity sector by 2035, leading to a zero-carbon U.S. economy by 2050. Gasification technology RD&D can help accelerate investment in coal, oil/gas, and power plant communities via clean energy that strengthens the economy and creates jobs, and foster environmental justice to address adverse human health, environmental, and climate-related impacts.

Gasification's inherent process advantages for implementing efficient CO_2 capture, and its ability to input carbon-neutral feedstocks (biomass) and waste materials, combine to enable net-zero or even net-negative carbon emissions performance, which will be invaluable to meet ambitious carbon reduction goals over the coming decades. Accordingly, current areas of RD&D feature the following technology:

Co-Gasification of Coal with Biomass and Plastic Wastes – This is an important area of research given its potential for net-negative CO_2 emissions. Waste plastics are desired as co-feedstocks due to their high volatile matter, low moisture, and low ash content, which would improve gasification performance, while also providing a means to disposition unrecyclable plastic waste and prevent it from becoming a waste disposal liability.

Novel Gasification/Process Intensification – As previously explained, successful implementation of process intensification would tend to strongly improve cost and efficiency of gasification systems. Current RD&D is targeting gasification integrated with selective gas separations, innovative gasifiers optimized for mixed feedstocks, and integrated syngas production and cleanup systems in gasification cycles tailored for H_2 production. Chemical looping gasification and microwave-assisted gasification are areas currently being explored that fall into the category of process intensified, novel gasification approaches. Microwave gasification is of particular current interest, as it leverages material interactions to enhance reaction rates, allows rapid start up and shut down allowing much easier integration with renewable energy than conventional gasification-based systems, and would easily allow modular design and integration.

Modular Gasification – DOE/NETL has focused research on smaller or modular gasification system scales (5–50 MWe equivalent). At this scale, the capital cost of the systems would be moderated, enabling better marketability especially in distributed generation scenarios. Also, modular systems could be better matched to local supplies of feedstocks, including limited biomass resources and localized waste materials, reducing or eliminating need for expensive transport of feedstock materials.

Gas Separations for H_2 Production from Coal/Waste Plastics/Biomass-Derived Syngas – Whether integrated with gasification itself or in downstream gas separators, innovative, highly efficient and energy-saving technologies for selective H_2 or CO_2 separation are being pursued. These may include advanced membranes, novel sorbents, or other innovative gas separation techniques. DOE has encouraged the use of accelerated technology development techniques including artificial intelligence/machine learning, computational modeling, and advanced

manufacturing-based approaches to lower the cost of advancing new technologies to commercialization.

Air Separation/Oxygen Production for Modular Gasification – Oxygen production/air separation technologies capable of meeting O_2 demand for modular gasification at lower cost and/or higher efficiency than state of the art air separation technologies. DOE/NETL's RD&D scope includes advanced membranes (e.g., those using mixed matrix materials and carbon molecular sieves), novel sorbents, O_2 carriers/chemical looping, novel cryogenics (including solid state cryogenics), and process integration approaches involving O_2 production.

21st Century Power Plant Initiative Design Studies – DOE/NETL has also funded notable design development efforts for DOE's 21st Century Power Plant Initiative, which seeks to advance power generation along with H_2 production beyond today's state-of-the-art, to make power plants more adaptive to the electrical grid with net zero carbon emission by 2035. Two projects are notable in the context of gasification systems:

- Wabash Valley Resources LLC and the GTI are developing the design, Environmental Information Volume, investment case, and a FEED study to redevelop the existing Wabash Valley Resources CG site (the former Wabash River IGCC plant) into a prototype gasification-based carbon-negative power and H_2 co-production plant.
- Electric Power Research Institute, Inc. is preparing a FEED study on an O_2-blown gasification system coupled with WGS, pre-combustion CO_2 capture, and PSA fueled by a coal/biomass mix (also waste plastic to be evaluated as co-feedstock) to yield high-purity H_2 (over 8,500 kg/hr) and a fuel off-gas that can generate power (50 MW net) from a flexible generator, all with net-negative CO_2 emissions. The plant will be hosted at one of two Nebraska Public Power District sites, where opportunities for enhanced oil recovery and storage have been investigated and the need for low-carbon power and H_2 is imminent. The GTI gasifier (a high-pressure, fluidized-bed type) and Hamilton Maurer International's gasifier (a lower pressure moving-bed type) has been selected.

In summary, current RD&D in gasification is focusing on deploying clean H_2 production to help address the nation's climate challenges through DOE's mission to minimize the environmental impacts of fossil fuels while working toward net-zero emissions. This work will help meet carbon reduction goals, develop cost-effective decarbonization for U.S. industry, and drive deployment and adoption of CCS. New projects to advance technologies for co-gasifying coal, biomass, and waste plastic at high efficiency, low cost, and with zero-carbon footprint are underway.

Pyrolysis of Natural Gas

In 2019, DOE's ARPA-E launched the Methane Pyrolysis Cohort consisting of funded partners focused on advancing H_2 production as well as generation, upgrading, and utilization of solid carbon products via CH_4 pyrolysis [39]. Participating cohort organizations span the product landscape as depicted in Exhibit 35. The primary RD&D focus areas for high volume H_2 generation is shown in Exhibit 36.

Exhibit 35. ARPA-E methane pyrolysis cohort approach
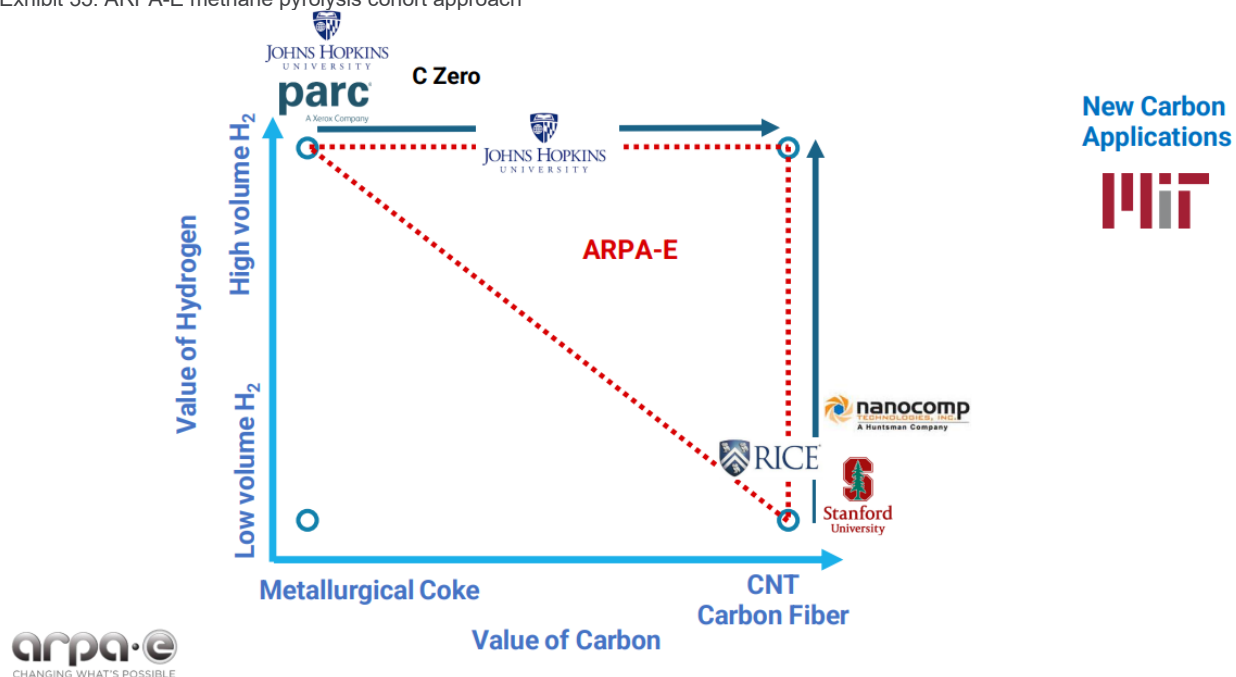
Source: ARPA-E [39]

Exhibit 36. ARPA-E methane pyrolysis cohort RD&D focus areas for H_2 generation from methane pyrolysis
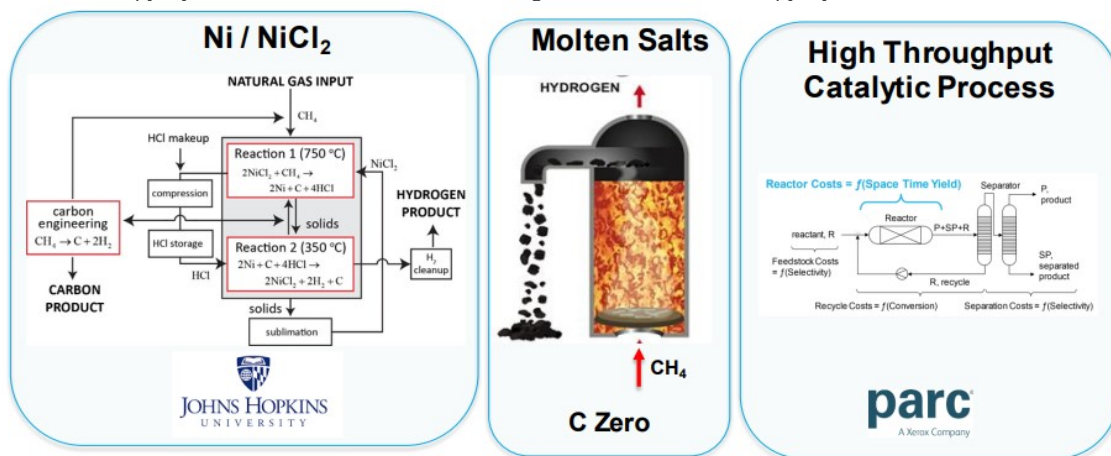
Source: ARPA-E [39]

In addition to the ARPA-E cohort, DOE FECM currently funds RD&D of catalytic pyrolysis technologies to convert associated gas from shale wells to H_2, carbon materials, and other value-added products [40]. The nature of this application focuses RD&D on low-volume,

distributed sources of NG for mitigation of fugitive emissions at the production site. Although no comprehensive FECM RD&D strategy currently exists for large-scale conversion of NG to H_2 as the primary product through advancements in pyrolysis technology, the current work forms the basis for the formation of such a strategy in coordination with the ARPA-E cohort.

Advanced Thermal Conversion Technologies

Along with the advanced membrane-integrated ATR concepts discussed previously, the advanced thermal conversion technologies discussed represent potentially transformational advancements in NG reforming and pyrolysis technology for clean H_2 production. Early-stage RD&D is needed for transformational reforming concepts in addition to TEA studies to develop performance and cost estimates for integrated systems at a greater level of rigor that initial screening analyses have provided to date. Generally, the RD&D focus areas are anticipated to enable process integration of CO_2/H_2 separation units and reforming/WGS chemistry in advanced reactor concepts. The following RD&D focus areas are needed to develop advanced thermal conversion technologies:

Solid CO_2 Sorbents – Solid sorbents enable CO_2 removal to be performed in the same process step as the reforming of NG. Such process-intensified reactors increase the H_2:NG yield by driving the equilibrium-limited reforming reaction towards H_2 production through in situ removal of CO_2.

Solid CO_2 Sorbent Handling & Regeneration Processes – Auxiliary process equipment for the efficient circulation and regeneration of solid CO_2 sorbents is needed to minimize sorbent degradation and energy requirements.

High-Temperature H_2/CO_2 Separation Membranes – Membranes may be applied to ATR reactors to enable separation of CO_2 at high pressure within the reforming reactor and increase H_2:NG yield. Such membranes avoid solid handling and regeneration challenges associated with solid CO_2 sorbents but must be able to withstand extreme reactor conditions.

Advanced Catalysts – Several potential applications exist for advanced thermal conversion. For NG reforming concepts, advanced catalysts may improve process efficiency or enable process intensification by performing WGS within the reformer. Controlling product selectivity and reducing carbon deactivation are primary challenges. Advanced catalysts may also be applied to pyrolysis concepts to reduce thermal demands and improve the overall process efficiency.

CONCLUSION

Thermal conversion pathways for H_2 production are critical to achieving DOE's Hydrogen Shot goal. This report explored the following thermal conversion technologies: SMR, ATR, POX, gasification, plasma pyrolysis, in situ H_2 generation, chemical looping, and dry reforming. Results of screening-level analyses show that technology advancement alone may not be enough to reduce H_2 production costs to the $1/kg H_2 goal. Therefore, beyond RD&D improvements, the report also explored the following factors for cost reduction: plant scale, market scenarios, plant site location, CO_2 T&S optimization, by-product sales, CO_2 valuation, and integration with other energy systems.

Performance and cost results were determined from baseline TEAs conducted for SMR, ATR, and gasification technologies as part of the NETL Hydrogen Baseline study. Furthermore, screening methodologies were developed for the estimation of performance and cost results for novel and advanced technologies. This work serves as the basis on which other analyses are built to create cost reduction pathways to the $1/kg H_2 goal.

Multiple EIA economic scenarios were considered, such as the High Oil & Gas Supply case which results in lower NG and electricity prices; however, only the most cost-advantaged locations under the Reference economic scenario prices were used in the cost reduction pathway analysis. For most technologies, the impact of site relocation to advantaged state candidates was minor but still net negative in terms of the LCOH.

The sale of by-products such as Ar and carbon black were also considered. Multiple cost reduction pathways showed that the sale of by-products was by far the most impactful in terms of achieving the H_2 cost goal. In lieu of considering a CO_2 tax credit, selling captured CO_2 up to a price of up to $50/t was another important method for cost reduction.

CO_2 T&S can be further optimized on a state-by-state basis. CO_2 T&S costs can be reduced by relocating the plant site within the state and utilizing shared CO_2 trunklines and hubs. These strategic choices allow CO_2 T&S costs to be reduced by up to 60 percent. For context, CO_2 T&S costs make up about 6 percent of the total LCOH for SMR, ATR, and gasification technologies.

The use of an IES for H_2 production has multiple benefits such as improved overall system efficiency and the ability to take advantage of fluctuations in electricity prices and other external factors.

Next, an important part of thermal conversion is the quantification of GHG emissions through LCA. Work done within the NETL Hydrogen Baseline Study supported this effort by providing a methodology for the analysis and qualitative results for cradle-to-gate emissions for ATR, SMR, and gasification baseline cases. Other novel and advanced technologies included a qualitative discussion of life cycle emissions. Although the BIL definition of clean H_2 is met with the inclusion of CO_2 capture and storage on today's H_2 production technologies, cradle-to-gate emissions are still estimated to be higher than non-fossil H_2 production routes and may be included in the initial CHPS established by DOE.

Finally, this report explored past and present DOE-sponsored RD&D projects and initiatives, many of which have been conducted either at DOE's national laboratories or through cooperative agreements with private industry, academic, and other government organizations through FOAs. RD&D seeks to reduce costs, improve efficiency and performance, reduce complexity, reduce emissions, increase scale, and more.

From improving and expanding analyses that can illuminate cost reduction pathways, to conducting RD&D on thermal conversion technologies, and finally, to funding and deploying technologies at larger scales, FECM's crosscutting blend of competencies are essential to bringing DOE's Hydrogen Shot goals to fruition. Looking forward, thermal conversion

technologies are well positioned to contribute to cost effective clean H_2 production in the years to come and to play an important role in achieving DOE's climate and energy goals.

ACRONYMS & ABBREVIATIONS

°C	Degrees Celsius
AACE	AACE International
AEO	Annual Energy Outlook
aMDEA	Activated methyldiethanolamine
AOI	Area of Interest
Ar	Argon
AR4	Fourth Assessment Report
AR5	Fifth Assessment Report
AR6	Sixth Assessment Report
ARPA-E	Advanced Research Projects Agency – Energy
ASU	Air separation unit
ATR	Autothermal reforming
b	Barrel
B&V	Black & Veatch
BFD	Block flow diagram
BIL	Bipartisan Infrastructure Law
BOP	Balance of plant
Btu	British thermal unit
C	Carbon
ccf	Carbon climate feedback
CCS	Carbon capture and storage
CCUS	Carbon capture, utilization, and storage
CF	Capacity factor
CG	Coal gasification
CGE	Cold gas efficiency
CH_4	Methane
CHPS	Clean Hydrogen Production Standard
CNT	Carbon nanotubes
CO	Carbon monoxide
CO_2	Carbon dioxide
CO_2e	CO_2 equivalent
COS	Carbonyl sulfide
CPU	CO_2 purification unit
DOE	Department of Energy
DRM	Dry reforming of methane
EIA	Energy Information Administration
EPA	Environmental Protection Agency
ETE	Effective thermal efficiency
FECM	Office of Fossil Energy and Carbon Management
FEED	Front end engineering and design

FLIGHT	Facility Level Information on GreenHouse gases Tool
FOA	Funding Opportunity Announcement
GHG	Greenhouse gas
GTI	Gas Technology Institute
GWP	Global warming potential
H_2	Hydrogen
H_2O	Water
H_2S	Hydrogen sulfide
HCl	Hydrogen chloride
HCN	Hydrogen cyanide
HHV	Higher heating value
hr	Hour
IGCC	Integrated gasification combined cycle
IES	Integrated energy systems
IL	Illinois
IPCC	Intergovernmental Panel for Climate Change
IRC	Internal Revenue Code
ISO	International Organization for Standardization
kg	Kilogram
kJ	Kilojoule per mole
kWh	Kilowatt hour
L	Liters
lb	Pound
LCA	Life cycle analysis
LCOH	Levelized cost of hydrogen
LHV	Lower heating value
mi	Miles
MJ	Megajoule
MMBtu	Million British thermal units
MMSCFD	Million standard cubic feet per day
MMt	Million metric tons
MO	Missouri
mol	Mole
MPa	Megapascal
MSW	Municipal solid waste
MWe	Megawatt electric
MWh	Megawatt hour
N_2	Nitrogen
N_2O	Nitrous oxide
NETL	National Energy Technology Laboratory
NG	Natural gas

NH_3	Ammonia	SCPC	Supercritical pulverized coal
Ni	Nickel	SMR	Steam methane reforming
$NiCl_2$	Nickel chloride	t	Metric ton
O&M	Operation and maintenance	T&S	Transport and storage
O_2	Oxygen	T&S Tool	T&S Screening Tool Module
PM	Particulate matter	TBD	To be decided
POX	Partial oxidation	TEA	Techno-economic analysis
PSA	Pressure swing adsorber	tpa	Metric tons per annum
psig	Pounds per square inch gauge	U.S.	United States
QGESS	Quality Guidelines for Energy System Studies	VSA	Vacuum swing adsorption
		WGS	Water-gas shift
R&D	Research and development		
RD&D	Research, development, and demonstration		

RECORD OF REVISIONS

Revision Number	Revision Date	Description of Change
1	February 2, 2024	Corrected in-text citation numbering

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[72] NETL, "Engineering Design of a Linde-BASF Advanced Post-Combustion CO2 Capture Technology at a Linde Steam Methane Reforming H2 Plant," NETL, 2020. [Online]. Available: https://www.netl.doe.gov/project-information?p=FE0031943.

APPENDIX: TEA PARAMETERS AND EXTERNAL FACTORS

A.1 Techno-economic Analysis Parameters

A full techno-economic analysis (TEA), as detailed in this section, was conducted for the steam methane reforming (SMR) with carbon capture and storage (CCS), autothermal reforming (ATR) with CCS, and coal/biomass co-gasification with CCS baseline cases. The other technology cases, including improvements to baseline technologies, pyrolysis technologies, and other advanced technologies, were not analyzed with the same rigor and will be discussed on a qualitative basis.

For the three cases with full-TEA results, an Aspen Plus® model was developed and used to generate material and energy balances as well as specifications for the major process equipment. The equipment list and material balances were used as the basis for generating the capital and operating cost estimates. Performance and process limits were based upon published reports, information obtained from vendors and users of the technology, performance data from design and build projects, and best engineering judgement. Capital and operating costs include scaled estimates from prior studies using the National Energy Technology Laboratory (NETL) Quality Guidelines for Energy System Studies (QGESS) methodology as well as estimates provided by Black & Veatch (B&V) using an in-house database and conceptual estimating models. Ultimately, a levelized cost of hydrogen (LCOH) was calculated for each of the cases.

A.1.1 PERFORMANCE DESIGN BASIS

Baseline cases are assumed to be located at a generic plant site in the midwestern United States, with the site characteristics and ambient conditions shown in Exhibit A-37. These properties are from the 2019 revision of the QGESS document "Process Modeling Design Parameters" [41].

Exhibit A-37. Site characteristics and ambient conditions

Category	Parameter	Value
Site Characteristics	Location	Greenfield, Midwestern U.S.
	Topography	Level
	Size (Gasification)	300 acres
	Size (Reforming)	100 acres
	Natural Gas Transportation	Pipeline
	Solid Fuels Transportation	Rail or Highway
	Slag Disposal	Off-Site
	Water	50% Municipal, 50% Ground Water
Ambient Conditions	Elevation	0 meter
	Barometric Pressure	0.101 MPa
	Average Ambient Dry Bulb Temperature	15 °C

Category	Parameter	Value
	Average Ambient Wet Bulb Temperature	10.8 °C
	Design Ambient Relative Humidity	60%
	Cooling Water Temperature	15.6 °C
Air Composition (mass %)	N_2	75.055
	O_2	22.998
	Ar	1.280
	H_2O	0.616
	CO_2	0.050

The natural gas (NG) feedstock utilized in reforming cases has the characteristics presented in Exhibit A-38, which are from the 2019 revision of the QGESS document "Specification for Selected Feedstocks" [42]. The NG primarily comprises methane (CH_4) and includes a small amount of methanethiol which is an odorant added as a safety measure.

Exhibit A-38. Composition and heating value of pipeline NG feedstock

Composition (vol %)	
Methane	93.1
Ethane	3.2
Propane	0.7
n-Butane	0.4
Carbon Dioxide	1.0
Nitrogen	1.6
Methanethiol	5.75×10^{-6}
Total	**100.0**
Heating Value (kJ/kg)	
HHV	52,295
LHV	47,201

The solid fuel feedstocks utilized in the gasification case, coal and biomass, have the characteristics presented in Exhibit A-39. The coal considered in the study is Illinois No. 6 coal and its properties are from the 2019 revision of the QGESS document "Detailed Coal Specifications" [43]. The biomass is assumed to be torrefied, non-pelletized, short rotation, and woody.

Exhibit A-39. Ultimate analysis and heating value of coal and biomass feedstocks

Ultimate Analysis (wt %)				
	Bituminous Illinois No. 6 Coal		Torrefied, Woody Biomass	
	As Received	Dry	As Received	Dry
Moisture	11.12	0.00	5.72	0.00
Carbon	63.75	71.72	59.89	63.52
Hydrogen	4.50	5.06	5.11	5.42
Nitrogen	1.25	1.41	0.41	0.44
Chlorine	0.15	0.17	0.00	0.00
Sulfur	2.51	2.82	0.00	0.00
Ash	9.70	10.91	0.51	0.54
Oxygen	7.02	7.91	28.36	30.08
Total	100.00	100.00	100.00	100.00
Heating Value (kJ/kg)				
HHV	27,113	30,506	22,676	24,051
LHV	26,151	29,544	21,406	22,853

The technologies were designed to produce a hydrogen (H_2) product with a minimum purity of 99.90 percent H_2, by volume. The maximum total concentration of all oxygen (O_2)-containing species, including carbon dioxide (CO_2), carbon monoxide (CO), H_2O, and O_2, is 10 ppm. The maximum allowed hydrogen sulfide (H_2S) concentration is 10 parts per billion. No particular end-use is considered; instead, the goal was to consider a H_2 product reflective of current, centralized fossil-based production facilities and suitable for a wide range of potential energy applications. The maximum impurity concentrations are suitable for ammonia (NH_3)-grade H_2 to avoid catalyst poisoning. The specification also results in a product suitable for the following applications per the International Organization for Standardization (ISO): [44]

- Type I, Grade A – Gaseous H_2; internal combustion engines for transportation; residential/commercial combustion appliances (e.g., boilers, cookers, and similar applications)
- Type I, Grade B – Gaseous H_2; industrial fuel for power generation and heat generation except proton-exchange membrane fuel cell applications

The H_2 product pressure specification was determined based on feedback from a commercial owner/operator of large-scale, centralized merchant H_2 facilities and a H_2 pipeline network. It was advised that pipeline operating pressures range from 800–900 psig, so a nominal H_2 product pressure at the plant fence is assumed to be 925 psig. This requires a H_2 compressor to be included in the flowsheet, which contributes additional power load and capital costs. Additional analyses conducted on the baseline results consider the removal of the H_2

compressor, which reduces the LCOH by a few cents and results in a product pressure ranging 316–394 psig.

The SMR with CCS and ATR with CCS plants are assumed to have a capacity factor (CF) of 90 percent, which is consistent with commercial plants that have a single reactor [9]. The coal/biomass co-gasification with CCS plant is assumed to have a CF of 80 percent, which is a minimum CF projected by technology suppliers and the Electric Power Research Institute for integrated gasification combined cycle plants without a spare gasifier [9]. A spare gasifier is required to match the 90 percent CF of the reforming plants. However, this additional cost was determined to not favor overall economics.

Additional details on biomass supply and cost considerations, environmental targets, and raw water withdrawal and consumption, etc., can be found in the NETL study "Comparison of Commercial, State-of-the-Art, Fossil-Based Hydrogen Production Technologies," hereafter referred to as the NETL Hydrogen Baseline study [9].

A.1.2 COST DESIGN BASIS

The figure of merit for the TEA is LCOH, which is defined as the amount of revenue required per kilogram (kg) of H_2 produced during the plant's operational life to meet all capital and operational costs. The real LCOH is a summation of the levelized capital cost, the levelized operation and maintenance (O&M) costs, the levelized fuel price, and CO_2 transport and storage (T&S) costs, in units of $/kg H_2.

The method used to determine capital recovery and levelization factors for O&M and fuel costs is found in the QGESS "Cost Estimation Methodology for NETL Assessments of Power Plant Performance," [45] but financial structure was adjusted slightly to reflect financing of H_2 production facilities, as shown in Exhibit A-40. The levelization assumes a 30-year plant operation period with an on-line year of 2023. All cost numbers are reported in the dollar year 2020.

Exhibit A-40. Nominal and real rates financial structure for hydrogen production

Type of Security	% of Total	Current Dollar Cost	Weighted Average Cost of Capital	After-Tax Weighted Average Cost of Capital
Nominal				
Debt	38%	7.25%	2.76%	2.05%
Equity	62%	5.16%	3.20%	3.20%
Total			**5.96%**	**5.25%**
Real (based on 2.01% average real gross domestic product deflator, 1990–2018)				
Debt	38%	5.15%	1.96%	1.45%
Equity	62%	3.10%	1.92%	1.92%
Total			**3.88%**	**3.37%**

The capital cost estimates reflect different uncertainty ranges depending on the technology considered. Gasification cases carry an uncertainty range of -25 percent/+50 percent,

consistent with AACE International (AACE) Class 5 cost estimates, based on the level of engineering design performed and limited recent development of coal gasification and coal/biomass co-gasification projects in the United States in recent years [9]. Reforming cases carry smaller uncertainty ranges of -15/+25 and fall within AACE Class 4 estimates, given recent experience with SMR and ATR plants.

The O&M pertains to those charges associated with operating and maintaining the H_2 plants over their expected life. These costs include the following: operating labor, material and labor for maintenance, administrative and support labor, consumables, fuel, waste disposal, and co-product or by-product credit. In the baseline TEA, no credit is considered for by-products other than power and of the six cases, only the coal/biomass co-gasification case has on-site power generation and only a small amount of power was available for export. Consequentially, this is the only case with a power credit. The cost and sale price of grid electricity was assumed to be $73.9/megawatt hour (MWh), which is the average price paid by an industrial consumer in the Midwest Independent System Operator region in 2019, inflated to 2020$ [46].

The cost of CO_2 T&S in a deep saline formation is estimated based on methodology available in the 2019 revision of the QGESS document "Carbon Dioxide Transport and Storage Costs in NETL Studies" [47]. Due to the variances in the geologic formations that make up saline formations across the United States, the cost to store CO_2 varies depending on maximum production rate, CF, and location. For the baseline TEA Midwest plant location, the CO_2 T&S cost value used is $10/metric ton (t) CO_2, in 2020$. In the baseline TEA, no tax credit for CO_2 capture or valuation for the CO_2 product is considered.

Feedstock costs for the coal and NG are specified according to the 2019 QGESS document "Fuel Prices for Selected Feedstocks in NETL Studies" [48]. The levelized, delivered prices, on a higher heating value (HHV) basis, are $4.56/million British thermal units (MMBtu) for NG and $2.30/MMBtu for Illinois No. 6 bituminous coal, inflated to 2020$. The cost for biomass was determined using a performance and economic model developed in a prior NETL study, which leveraged work completed by the Idaho National Laboratory [49]. The levelized, delivered price of as-received, torrefied biomass is $5.60/MMBtu on an HHV basis.

Technology cases including partial oxidation, pyrolysis, and advanced technologies, were not analyzed with the same rigor as the baseline cases and are discussed on a qualitative basis. The general methodology for the analysis of these other technologies included first conducting a general literature review of the technology and collecting performance and cost data. A block flow diagram (BFD) was created to describe the technology and understand the material flows on a high level. Each technology was assigned to a baseline case that best matched its characteristics and process equipment needs. The full-TEA results of the baseline were manipulated based on the individual technology's performance and cost claims to provide a high-level estimate of the cost of H_2 this technology may produce. Since these results are not based on technology-specific modeling data nor vendor-generated cost data, the results contain unknowns and must be viewed accordingly. Nevertheless, these high-level analyses can aid in the development of qualitative cost reduction pathways for each technology.

A.2 External Factors

The purpose of this section is to explore the assumptions and methodology behind the external factors that have a large influence on thermal conversion technologies and their cost reduction pathways. The following external factors are considered: plant scale, location of plant and location-specific feedstock price, by-product sales, and CO_2 T&S considerations. There is also a section on emissions and life cycle analysis (LCA) considerations, as that is an important consideration for thermal conversion technologies.

A.2.1 PLANT SCALE

Economies of scale usually provide favorable economics when increasing the capacity of a plant. Unless limited by the maximum practical size of a major process unit or the availability of feedstock, increasing plant scale will generally increase sales revenue faster than the increase in capital and O&M costs. This is because the capital costs typically follow a power law correlation with an exponent less than one. The scaling impact is particularly applicable for the ATR technology, which can accommodate a much larger scale than the SMR technology. Industry sources indicate that the maximum scale for an ATR plant is approximately 2.7 times that used in the baseline TEA. A sensitivity analysis was performed on the LCOH for an ATR plant as a function of plant scale using several possible power law exponents. The results are shown in Exhibit A-41 and indicate that for a power law exponent of 0.7, typical in the chemical process industry, the LCOH has the potential to be reduced by $0.113/kg H_2.

Exhibit A-41. LCOH sensitivity to increase in ATR scale
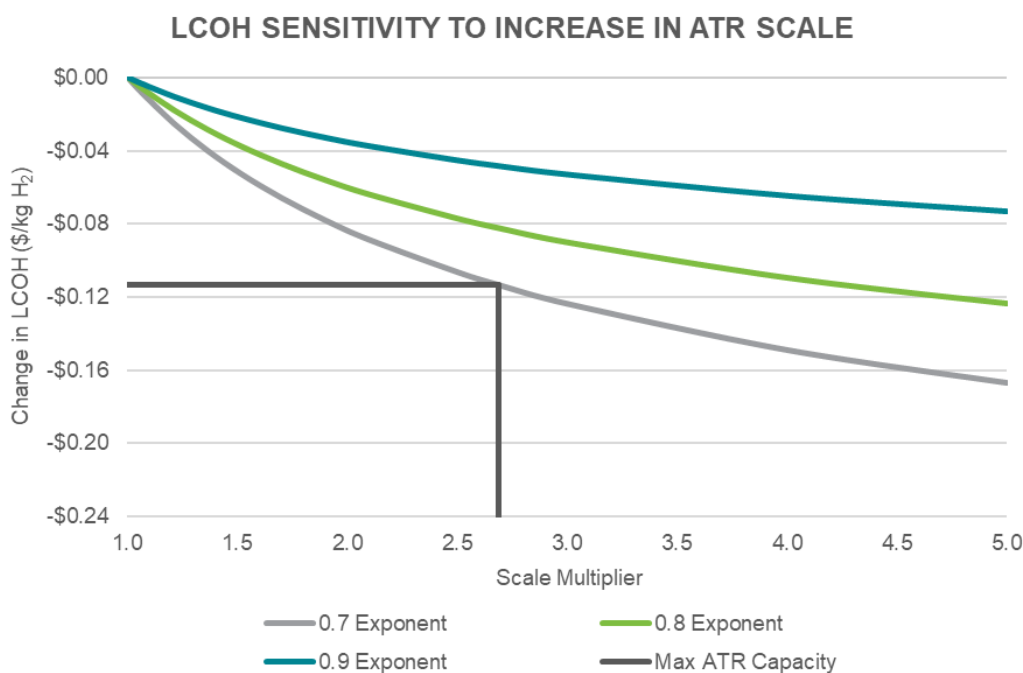

The plant design used in the NETL Hydrogen Baseline study for the SMR technology is based on the maximum single-train reformer capacity. While increasing the size of the SMR reactor is not practical, the plant could be designed to employ multiple SMR reactor trains. This would not significantly complicate the plant operation. The remaining balance of plant (BOP) components

in the baseline plant are of similar scale to that of the ATR plant and, thus, are amenable to the power law scaling. A sensitivity analysis was performed on the LCOH for a SMR plant at double the baseline plant scale using several possible power law exponents. The results are shown in Exhibit A-42 and indicate that for a power law exponent of 0.9, representing an additional reactor train and shared BOP components, the LCOH has the potential to be reduced by $0.046/kg H_2. Hypothetically, if the single-train capacity for the SMR could be increased a reduction in LCOH of about $0.11/kg H_2 would be realized.

Exhibit A-42. LCOH sensitivity to increase in SMR scale
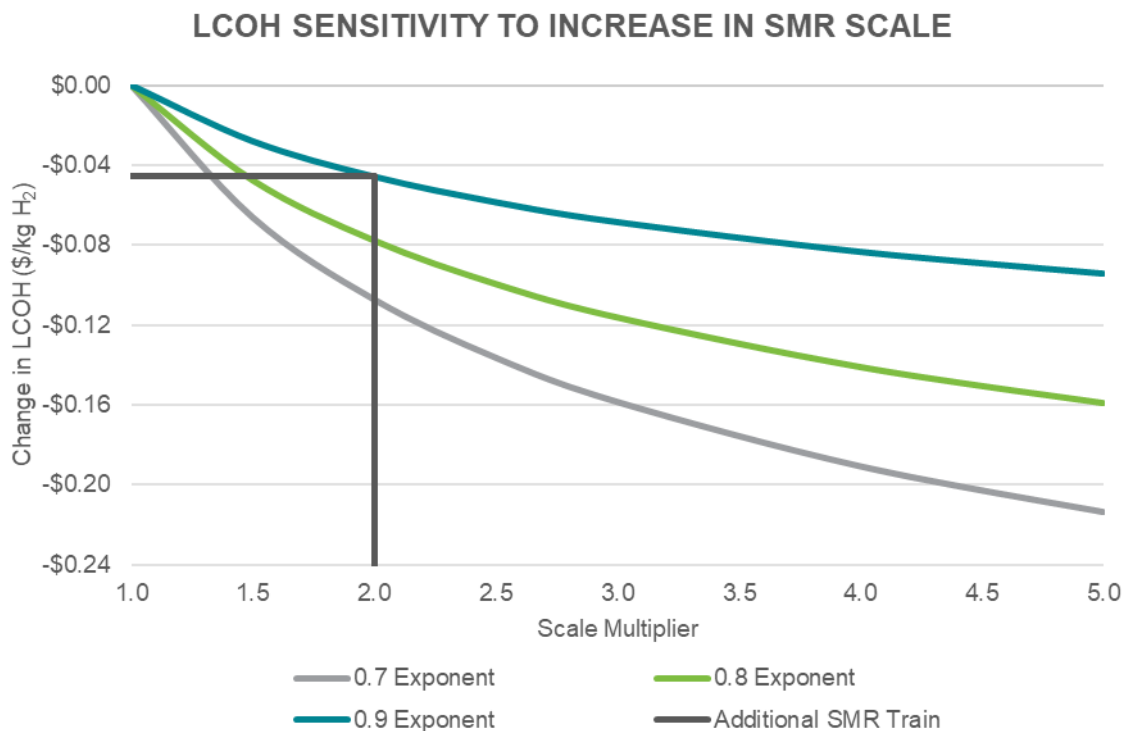
A.2.2 LOCATION AND FEEDSTOCK PRICE

Site location was chosen by comparing each of the contiguous 48 states' industrial NG and electricity prices. The prices for NG and electricity are based on the Energy Information Administration (EIA) Annual Energy Outlook (AEO) from 2021 [50]. Natural gas is both the raw material for H_2 conversion and a source of heat for the process. Natural gas prices were developed using the AEO2021 Reference case, the High Oil and Gas Supply case, and the Low Oil and Gas Supply case and expanded to state-by-state prices by comparing different NG hubs across the country to the Henry Hub NG price. In some cases, there were multiple NG hubs in a single state. When that was the case, the average was taken for the state. In other cases, a state did not have a NG hub and a neighboring state's hub was used. Industrial electricity prices were also determined on a state-by-state basis by comparing each state's average price to the U.S. average provided in AEO2021 for the year 2030. Although three EIA price scenarios were studied as part of this work, the cost reduction pathways presented only consider Reference case prices.

The AEO2021 Reference case represents EIA's best assessment of how U.S. and world energy markets will operate through 2050, based on key assumptions around existing energy policies in the United States and is intended to provide a baseline for exploring long-term trends. The Reference case serves as a reasonable baseline case that can be compared with the side cases that include alternative assumptions based on changes in current policy. EIA based the economic and demographic trends reflected in the Reference case on the current views of leading economic forecasters and demographers. For example, the Reference case project assumes improvement in known energy production, delivery, and consumption technologies. The Reference case generally assumes that current laws and regulations that affect the energy sector, including laws that have end dates, remain unchanged throughout the projection period. This assumption enables EIA to use the Reference case as a benchmark to compare with alternative policy-based cases [50].
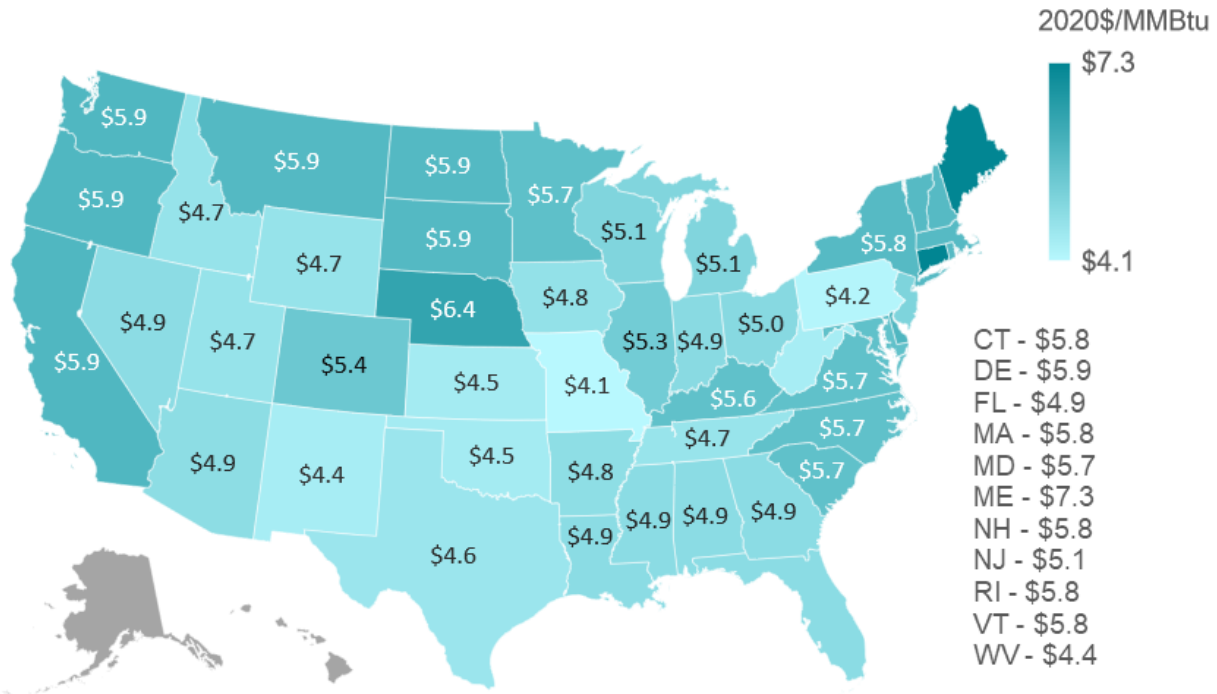
Global market balances, primarily influenced by factors that are not modeled in the National Energy Modeling System, will drive future oil prices. In the AEO2021 Low Oil & Gas Supply (high price) case, the price of Brent crude oil, in 2020 dollars, reaches $173 per barrel (b) by 2050, compared with $95/b in the Reference case and $48/b in the High Oil & Gas Supply (low price) case. Compared with the Reference case, the High Oil & Gas Supply case reflects lower costs and greater resource availability for oil and NG in the United States, which allows for more production at lower prices. On the other hand, the Low Oil & Gas Supply case assumes fewer resources and higher costs [50].

Both NG and electricity prices provided in AEO2021 are in 2020$. For both the NG and electricity prices, the EIA industrial prices were used for cases requiring power imports.

Natural gas prices were developed using AEO2021 cases described above and expanded to state-by-state prices by comparing different NG hubs across the country to the Henry Hub NG price. In some cases, there were multiple NG hubs in a single state. When that was the case, the average was taken for the state. In other cases, a state did not have an NG hub, and a neighboring state's hub was used. Exhibit A-43 shows 2030 NG prices for each state under the industrial Reference case.

Exhibit A-43. EIA AEO2021 NG prices per state for the reference case, in units of 2020$/MMBtu

Source: EIA [50]

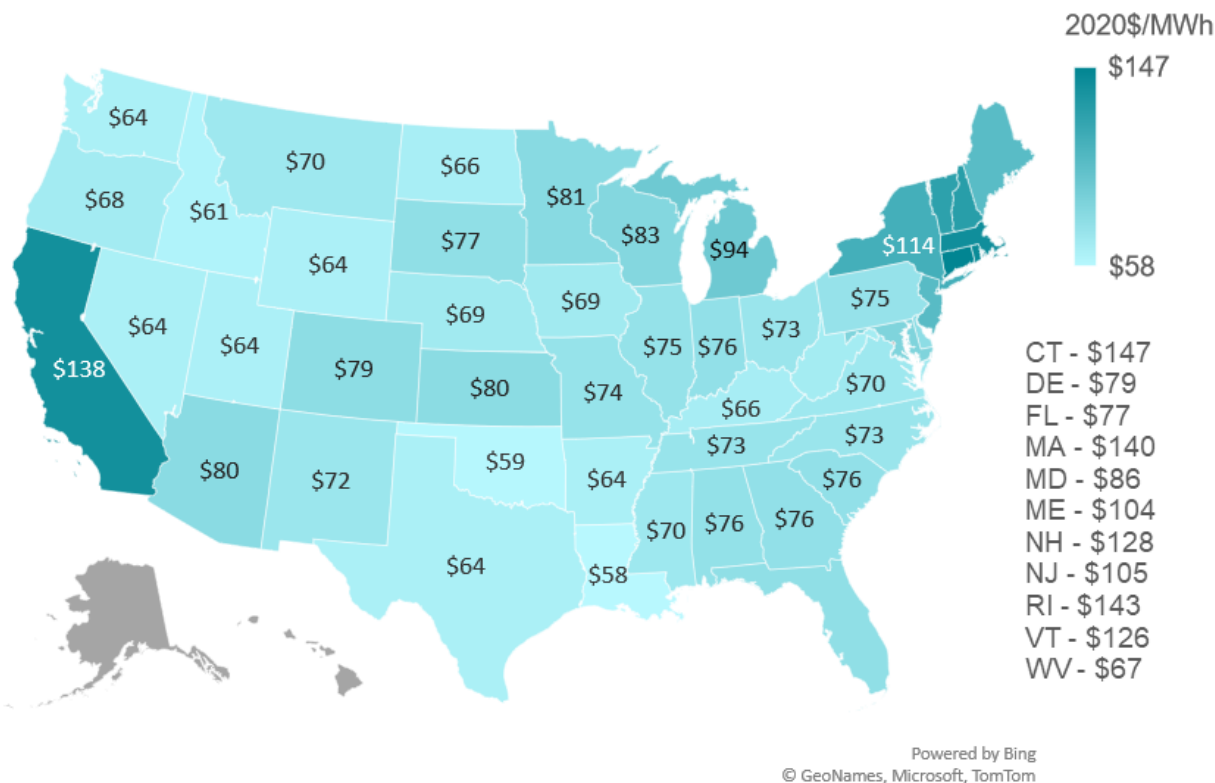To calculate state-by-state electricity prices, each state's average retail price was compared to the U.S. average provided in AEO2021 for the year 2030. Exhibit A-44 shows the 2030 electricity prices used in this analysis, in 2020 dollars.

Exhibit A-44. EIA AEO2021 industrial electricity prices per state for the reference case, in units of 2020$/MWh

EIA AEO2021 REFERENCE CASE ELECTRICITY PRICES

2020$/MWh

$147

$58

CT - $147
DE - $79
FL - $77
MA - $140
MD - $86
ME - $104
NH - $128
NJ - $105
RI - $143
VT - $126
WV - $67

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Source: EIA [50]

A.2.3 BY-PRODUCT SALES

The sale of valuable by-products can provide additional revenue, contributing to a reduction in the LCOH for certain technologies. Additional by-products beyond those considered in the baseline TEA include argon (Ar), carbon black, and pure CO_2.

Argon is a product of the air separation unit used in the ATR and partial oxidation (POX) technologies. While NETL currently does not have access to Ar market reports, research showed that 40-liter cylinders of argon cost $1.19/kg [51].

Carbon, as a product of the pyrolysis process, is considered to be a salable carbon black product. Exhibit A-45 shows that carbon black is a conservative representative with respect to potential market price of all valuable carbon products, and as more research into potential carbon markets and prices is published, additional revenue can be obtained from these carbon products [52].

Exhibit A-45. Summary of potential carbon ore use scenarios

	U.S. Production of Carbon Product (MMt)	Product Price ($2020/t)
Carbon Black	2.3	$951
Engineered Plastic Composites	108.1	$2,739
Activated Carbon	11.3	$2,060
Anodes for Aluminum	1.5	$3,719

The major by-product from the consumption of fossil fuels to make H_2 is CO_2. Pure CO_2 can be sold to the beverage industry or used for enhanced oil recovery; however, the current CO_2 market is already saturated by the ethanol and NH_3 industries. Therefore, in order to create a market incentive to store CO_2, leading to the implementation of capture technologies, the 45Q tax credit was passed by Congress. The tax credit for carbon oxide storage—often referred to using its Internal Revenue Code (IRC) section, 45Q—is computed per metric ton of qualified carbon oxide captured and stored. The amount of the credit, as well as various features of the credit, depend on when the qualifying capture equipment is placed in service. The Bipartisan Budget Act of 2018 (P.L. 115-123), which was signed into law on February 9, 2018, made numerous changes to the Section 45Q tax credit, as discussed below.

For the purposes of the tax credit, qualified carbon oxide is a carbon oxide that would have been released into the atmosphere if not for the qualifying equipment. To claim a tax credit, the emissions must be measured at the point of capture as well as at the point of disposal, injection, or other use. If the captured carbon oxide is intended to be stored, it must be disposed of in "secure geologic storage"; per IRC Section 45Q, "secure geologic storage" includes "storage at deep saline formations, oil and gas reservoirs, and un-mineable coal seams" [53]. The taxpayer has to repay the tax credit if the carbon oxide ceases to be captured, disposed of, or used in a qualifying manner (i.e., if it escapes into the atmosphere) [53].

The exact impact that the 45Q tax credit would have on the cost of H_2 produced by these plants is complex and cannot be fully explored. Therefore, no attempt was made to apply the 45Q tax credit. Instead, a set of values from $0 (no credit) to $50 at $10 increments, on a per metric ton CO_2 captured basis, was used to value the CO_2 product in this analysis.

A.2.4 CO_2 TRANSPORT AND STORAGE CONSIDERATIONS

CO_2 capture, transport, and storage are necessary to reduce the stack emissions of fossil energy-based H_2 production below 2 kg CO_2 emitted per kg H_2 produced. Fossil-based H_2 production pathways that incorporate CCS technologies are candidates to reach the Hydrogen Shot™ cost goal with moderately low carbon emission intensities. The cost of CO_2 T&S for fossil-based H_2 production projects must be accounted for when estimating the project's overall LCOH. The baseline TEAs assume a CO_2 T&S cost of $10/t; however, this value is not applicable throughout the contiguous United States due to variations in storage geology quality and availability across the country, as well as variations in distance between potential CO_2 capture and CO_2 storage sites. The $10/t CO_2 T&S cost is also not applicable for different H_2

production technologies due to variations in these technologies' CO_2 capture rates compared to the TEAs. Analyses were conducted to determine pathway-specific values for CO_2 T&S costs in place of the $10/t value assumed for the baseline TEAs as well as to provide additional opportunities for cost reduction.

CO_2 capture costs are H_2 production technology-dependent and are accounted for in baseline performance capital, fixed, variable, and fuel cost line items for each fossil-based H_2 production technology in this report (e.g., Exhibit 7). CO_2 T&S costs depend on additional factors like the relative locations of a H_2 production project and its CO_2 storage project, CO_2 transport pipeline capacity, CO_2 storage geology, and CO_2 storage project capacity, all of which can be optimized to lower LCOH. T&S cost assessment results, demonstrated previously, suggested shared T&S infrastructure (i.e., trunklines and storage hubs) are critical to reducing T&S contribution to a project's LCOH. Shared T&S infrastructure is a more plausible assumption for H_2 production projects sited near existing clusters of CO_2 emission point sources.

The Department of Energy (DOE) Office of Fossil Energy and Carbon Management (FECM) and NETL have developed the FECM/NETL CO_2 Transport Cost Model (hereafter referred to as CO2_T_COM) and the FECM/NETL CO_2 Saline Storage Cost Model (hereafter referred to as CO2_S_COM), which estimate the first-year break-even cost of CO_2 T&S, respectively, for various user-input parameters. A detailed description of CO2_T_COM and CO2_S_COM can be found in their associated user's manuals. Combined, the first-year break-even CO_2 T&S costs derived from CO2_T_COM and CO2_S_COM, reported in $/t CO_2, can be converted into a LCOH contribution if the production rates of H_2 and CO_2 are known.

CO_2 T&S cost optimization was performed for the three technology cases for which full-TEA results are available: SMR with CCS, ATR with CCS, and coal/biomass co-gasification with CCS. The average annual CO_2 mass flow rate and the ratio of the average to maximum CO_2 capture mass flow rate (hereafter referred to as CF) are reported for typical H_2 production projects, in million metric tons of CO_2 per annum (tpa), as shown in Exhibit A-46. CF is necessary for sizing different aspects of CCS infrastructure. Pipelines, for example, must be sized to accommodate the maximum CO_2 mass flow rate and the number of injection wells for a CO_2 storage project must be determined based on the maximum CO_2 mass flow rate. The storage project's storage capacity, on the other hand, must be sized to accommodate the average annual CO_2 mass flow rate over the project's lifetime.

Exhibit A-46. Fossil-based hydrogen technologies' CO_2 capture rates presented in NETL Hydrogen Baseline study

Fossil-Based Hydrogen Technology	Average CO_2 Capture Rate (tpa)	Maximum CO_2 Capture Rate (tpa)	CO_2 Capture Rate Capacity Factor (average/maximum)	CO_2 Storage Capacity Required per 30-year Project (t)
Coal/Biomass Gasification w/ CCS	0.78	0.98	80%	23.4
SMR w/ CCS	1.52	1.69	90%	45.6
ATR w/ CCS	1.91	2.12	90%	57.3

CO2_T_COM was used to generate a database of transport cost results for greenfield pipelines, sized to the CO_2 capture rates shown in Exhibit A-46, as well as for a larger "trunkline" capacity of 5.0 tpa (assuming a 90 percent CF). Transport costs were estimated for pipeline distances ranging 10–1,000 miles, in 10-mile increments for 10–50 miles, 50-mile increments for 100–500 miles, and 100-mile increments for 600–1,000 miles. Transport distance reflects the distance from the H_2 production project (i.e., the CO_2 source) to the CO_2 storage site. Trunkline costs were calculated to include the cost of the main pipeline, as well as a gathering pipeline from the CO_2 source to the trunkline, sized for the specific CO_2 source, and a distribution pipeline from the trunkline to the storage site, sized for the storage project type selected. Gathering pipeline length is assumed to be the greater of either 10 percent the calculated length of the trunkline, rounded to the nearest 10 miles, or 30 miles. Distribution pipeline length is assumed to be the greater of either 10 percent the calculated length of the trunkline, rounded to the nearest 10 miles, or 20 miles. Therefore, the minimum combined gathering and distribution pipeline length is 50 miles.

CO2_S_COM was used to generate a database of storage cost results for greenfield storage operations at each of its 314 unique saline aquifer geologic formations, for three different geologic structural regimes. Storage costs were generated for each of the H_2 production capture rates shown in Exhibit A-46, as well as a larger "storage hub" capacity of 5.0 tpa. CO2_S_COM calculates the total storage capacity for each of the 314 storage formations in the geologic database. This storage capacity is the maximum mass of CO_2 that could be stored in the formation.

When a storage project begins injecting CO_2, the injection starts to increase the pressure in the formation. Pressures will increase over time and eventually stabilize. CO_2 injection wells are regulated by the Class VI injection well regulations and must maintain pressures in the injection formation below 90 percent of the fracture pressure, which is a localized property of the formation. Pressure increases propagate faster and farther than the propagation of the CO_2 plume. If multiple CO_2 injection projects are implemented in the same storage formation at the same time, the pressure increases from the different projects will propagate and increase the pressure at nearby CO_2 storage projects. This effect of a CO_2 storage project affecting the pressure at a nearby CO_2 storage project is referred to as pressure interference in this report. If the projects are operating with pressures near the maximum allowed pressure, this presents an issue to the CO_2 storage projects. The projects could all reduce their injection rates to keep the pressures under the allowable pressure or basin-scale management could be imposed (presumably by the regulators managing the Class VI permit process) that limits the number of projects that can be implemented in the same storage formation at the same time. In this study, it was assumed the latter approach is implemented with each storage project injecting CO_2 at their design rate with minimal pressure influence from other projects operating in the same storage formation. A pressure interference correction factor was calculated based on the work of Teletzke et al. and used to reduce the maximum storage capacity in a storage formation to an effective pressure influenced storage capacity [54].

The two databases, derived from CO2_T_COM cost results, and from CO2_S_COM cost results and geologic data, were compiled into an Excel®-based T&S Screening Tool Module (T&S Tool). T&S Tool user input options are shown in Exhibit A-47.

Exhibit A-47. T&S Tool user input options

User Input Category	User Input Options	
	Option	**Note(s)**
Fossil-Based Hydrogen Production Technology	Coal/Biomass Co-gasification	Sets dedicated pipeline and dedicated storage options to 0.78 tpa at 80% CF
	SMR	Sets dedicated pipeline and dedicated storage options to 1.52 tpa at 90% CF
	ATR	Sets dedicated pipeline and dedicated storage options to 1.91 tpa at 90% CF
Hydrogen Production Site Location	U.S. State	User can select one of 48 contiguous U.S. states; sets H_2 production site at the selected states' centroid latitude and longitude coordinates
	User-Input	User can input specific latitude and longitude coordinates for the location of the H_2 production site
CO_2 Pipeline Transport	Dedicated	Sets pipeline size to meet the selected H_2 technology's CO_2 capture rate
	Trunkline	Sets pipeline size to meet 5.0 tpa at 90% CF; sets gathering pipeline size to meet the selected H_2 technology's CO_2 capture rate; sets distribution pipeline size to meet the selected storage operation's CO_2 injection rate
CO_2 Storage Operation	Dedicated	Sets storage operation's CO_2 injection rate to meet the selected H_2 technology's CO_2 capture rate
	Storage Hub	Sets storage operation's CO_2 injection rate to meet 5.0 tpa at 90% CF
CO_2 Storage Site Location	Formation Centroid	Sets the storage operation's coordinates to the centroid of the saline aquifer formation's areal extent
	1/3 Radius*	Subtracts 2/3 the saline aquifer formation's average radius from the calculated H_2 site location to the formation centroid distance; sets the storage operation's location nearer its saline aquifer formation's boundary (nearer the H_2 site location)
CO_2 Storage Site Geologic Structural Regime	Regional Dip	Sets the storage operation's structural regime to regional dip (relatively flat-lying formation)
	Anticline*	Sets the storage operation's structural regime to anticline (arch-like formation with closure on two of four sides)
	Dome*	Sets the storage operation's structural regime to dome (dome-like formation with closure on all sides)

The rightmost cell spanning Regional Dip, Anticline, and Dome rows: Impacts the total storage capacity of the formation and anticipated CO_2 plume size (and associated monitoring costs)

*It is recommended that geological data be used to justify these selections

Based on the user-provided inputs selected from Exhibit A-47, the T&S Tool 1) calculates the distance from the CO_2 source to each of the 314 CO_2 saline storage locations in CO2_S_COM, 2) records the transport cost associated with each storage location, 3) records the storage cost for each storage location that exceeds the calculated effective storage capacity, and 4) returns the storage site that represents the lowest combined T&S cost option.

A.2.5 EMISSIONS AND LCA CONSIDERATIONS

This report also discusses the emissions of greenhouse gases (GHGs) in the life cycle of producing H_2 from various technologies. Analysis was performed in accordance with ISO 14040/14044 Standards for Life Cycle Assessment [55] [56]. The goal of the LCA performed is to generate attributional life cycle GHG emissions estimates for each H_2 production case. The

final life cycle results are generated on a functional unit basis of 1 kg of H_2 (>99.90 %-vol, 20 bar) produced at plant gate.

A life cycle can include cradle-to-grave aspects of a product (i.e., all phases in the life of the product); however, in this analysis, as shown in Exhibit A-48, only the cradle-to-gate effects are included (i.e., up to the point of creating the H_2 at the facility gate). Thus, emissions will be discussed from two perspectives: from the exhaust stack at the production facility, and cradle-to-gate emissions, which include the exhaust stack emissions as well as major upstream sources of emissions. For example, emissions coming from an SMR process in a facility are exhaust stack emissions, and the emissions associated with extracting, producing, and delivering the NG to the SMR facility would be part of the cradle-to-gate emissions.

Exhibit A-48. Cradle-to-gate boundary representation
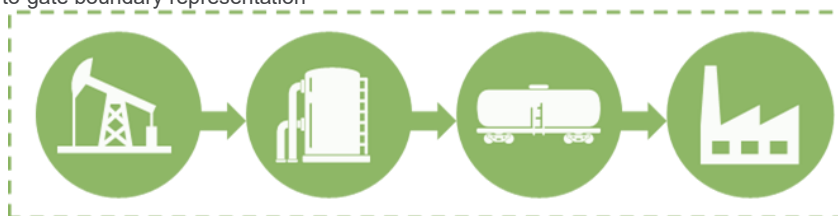
While LCA can include the inventory of many types of flows, such as criteria air pollutants, the focus in this LCA is on GHGs. Results were calculated using the Intergovernmental Panel for Climate Change (IPCC) Fifth Assessment Report (AR5) characterization model at a 100-year time horizon [57]. IPCC's global warming potential (GWP) characterization factors provide ways of converting emissions of individual GHGs into equivalent emissions of CO_2. GWP values are based on the most recent literature that considers the differences in radiative forcing in the atmosphere of different GHGs as compared to CO_2. In this report, GWP values from IPCC AR5 are estimated over a 100-year time horizon with atmospheric carbon feedback, as summarized in Exhibit A-49 [57].

Exhibit A-49. GWP values for select GHGs

GHG	Formula	GWP Factor
Carbon Dioxide	CO_2	1
Methane (biogenic)	CH_4	34
Methane (fossil)	CH_4	36
Nitrous Oxide	N_2O	298

With respect to existing DOE discussions about facility and life cycle emissions for H_2, the Bipartisan Infrastructure Law (BIL) defines clean H_2 as "hydrogen produced with a carbon intensity equal to or less than 2 kg CO_2 equivalent (CO_2e) produced at site of production per kg of hydrogen produced" [7]. There is no text in the BIL that otherwise suggests a carbon intensity target for the total cradle-to-gate emissions, and it notably does not specify definitions for H_2 production methods. However, "well-to-gate" lifecycle GHG emissions are included in the initial Clean Hydrogen Production Standard (CHPS) DOE published in 2023.

Generally speaking, two methods were used to generate facility and cradle-to-gate emissions in this study. For the main baseline pathways, LCA models were built using the openLCA software (employing methodologies compatible with DOE's GREET model). Life cycle modeling of the systems defined above uses openLCA software and various existing NETL LCA models. Notably, this effort builds upon past NETL work that developed life cycle models for producing the various feedstocks for the H_2 production plants:

- Upstream production of NG was modeled using the NETL NG model, which is documented in the NETL 2019 NG baseline report [20]. Regional basin-level data was updated to the year 2017 [58]. The boundaries for the NG are from NG extraction through transmission.
- Upstream production of biomass, specifically the torrefied Southern Yellow Pine used in this study, followed work previously done for the Connecticut Center for Advanced Technology [59]. Within models used for the current study, default parameters were used, except as follows. The biomass loss rate during harvesting was assumed to be 5 percent. Upstream potash fertilizer production was updated based on a 2018 Chen et al. journal article [60].
- The upstream production of coal leverages modeling and default assumptions from NETL's Supercritical Pulverized Coal (SCPC) Power Plant study [61]. The SCPC study considers upstream production of coal from the Illinois basin (Illinois underground bituminous coal was assumed to represent Illinois No. 6 coal). This study builds upon the upstream coal model in the SCPC study by modifying coal mine CH_4 emissions to 0.0086 kg CH_4/kg coal [62]. Transportation of coal from mine to plant assumes U.S. average distances of 3.8 miles by truck, 35.1 miles by barge, 42.1 miles by ocean/lake vessel, and 577 miles by train [63].
- Process information for storage of CO_2 in a saline aquifer followed modeling and assumptions used in the SCPC study.
- Electricity impacts are modeled using the NETL electricity baseline, represented by the U.S. average consumption mix by user [64] [19]. Electricity data considers all power generated and imported to the United States in the year 2016. Variability in these results is associated with the differing GHG intensities for the balancing authorities in the United States.

For the advanced pathways, rolled-up emissions values from other previous NETL work were applied to physical units of inputs estimated in the TEA methods discussed above. There is a high level of confidence related to the estimated GWP impacts for the upstream effects, although as noted above they would be expected to vary regionally by basin or grid region. The rolled-up values used for the advanced pathways are summarized in Exhibit A-50.

Exhibit A-50. Rolled-up U.S. average values used in advanced pathways

Upstream Process	Emissions Factor	Data Year
Grid Electricity (kg CO_2e/kWh)	0.586	2016
Natural Gas (kg CO_2e/MJ)	0.0133	2017
Coal (kg CO_2e/kg transported)	0.212	2016

Results were calculated with units kg CO_2e/kg H_2 using IPCC AR5 characterization factors with a 100-year time horizon and atmospheric carbon climate feedback (ccf). IPCC AR5 also provides factors with a 20-year time horizon, with and without ccf. IPCC has also published their Fourth Assessment Report (AR4) and Sixth Assessment Report (AR6) in recent years, both of which have published characterization factors at a 100-year and a 20-year time horizon [65] [66]. With so many impact assessment variations, it is helpful to compare results between methods. This comparison is shown in Exhibit A-51.

Exhibit A-51. GWP results for all cases by IPCC scenario (kg CO_2e/kg H_2)

Technology	AR6 -100	AR6 -20	AR5- 100 w/ ccf	AR5- 100 w/o ccf	AR5- 20 w/ ccf	AR5- 20 w/o ccf	AR4- 100	AR4 -20	CO₂ Capture Rate
SMR w/o CCS	13	15	12	12	16	15	13	15	-
SMR w/o CCS, w/ steam displacement	11	13	10	10	14	13	11	13	-
SMR w/ CCS	5.3	7.7	5.6	5.3	7.9	7.8	5.1	7.3	96.2
ATR w/ CCS	6.4	8.8	6.6	6.4	9.0	8.9	6.1	8.3	94.5
Coal Gasification w/o CCS	21	23	20	20	21	21	20	21	-
Coal Gasification w/ CCS	4.7	7.2	4.1	4.0	5.3	5.2	3.8	5.0	92.5
Coal/Biomass Gasification w/ CCS	-0.6	1.2	-1.0	-1.2	-0.23	-0.26	-1.3	-0.46	92.6