Assessment of usage of hydrogen as alternative fuel into NETPLAN

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CHAPTER 1. INTRODUCTION

1.1 Motivation

The electric power and the transportation sectors, two interdependent infrastructures, are the largest energy consuming sectors and the greatest contributors to carbon emissions in the U.S.

In 2010, the U.S energy consumed was 98 (Quadrillion Btu) Quads [1]. More than 67% of this energy was consumed for electric and transportation purposes, as shown in Figure 1.

Most of this energy came from non-renewable sources, (i.e., petroleum, natural gas, and coal) representing more than 80% of the total supply sources. In addition, approximately 74% of all greenhouse gas (GHG) emissions came from electric and transportation sectors in the U.S in 2010 [2].

Figure 1: Primary Energy Consumption by Source and Sector (Source [1])
As seen in Figure 1, the transportation sector relies almost entirely on refined petroleum products, accounting for over two-thirds of the oil used in the US. The U.S. light-duty transportation fleet (with over 225 million vehicles) requires over eight million barrels of oil each day [3]. Unfortunately, most of the petroleum consumed in the U.S. is imported and is expected to rise gradually for the near future.

The issues mentioned above motivates interest to replace current energy-related technologies with cleaner ones that support sustainable global economic growth including reduction of the impacts on air quality and potential effects of greenhouse gas emissions for the near, mid and long term future [4].

One of the solutions proposed is the use of hydrogen (H\textsubscript{2}) as an energy carrier. Hydrogen is being considered for its use as an energy carrier for stationary power and transportation markets. It can be used with a very high efficiency and near-zero emissions at the point of use [5].

Currently, the potential application of hydrogen as energy carrier is focused on the transportation sector through the use of hydrogen powered fuel cell vehicles (FCV). The advantage of using FCVs instead of internal combustion engines (ICEs) powered with gasoline is that when hydrogen is combusted only water vapor is emitted, unlike ICE that emits CO\textsubscript{2}.

The term hydrogen economy received a dramatic boost when U.S. president George W. Bush proposed a major initiative in his State of the Union address in January 2003. The amount of $1.2 billion was proposed by President Bush to invest in the hydrogen initiative in order to reverse America dependence on foreign oil and reduce greenhouse gas emissions [3].

President Bush stated in [3]:
“With a new national commitment, our scientists and engineers will overcome obstacles…so that the first car driven by a child born today could be powered by hydrogen, and pollution-free. Join me in this important innovation to make our air significantly cleaner, and our country much less dependent on foreign sources of energy”

Hydrogen, similar to electricity, is a secondary energy carrier that can be derived from a variety of primary sources, including fossil fuels, renewable, and nuclear power.

Currently, hydrogen is used mainly for producing ammonia (used in fertilizer) and to lower the sulfur content for the petrochemical sectors. Unfortunately, most of the hydrogen that is produced comes from non-renewable energy.

The widespread use of hydrogen as a major energy carrier will require considerable breakthroughs in several aspects of the U.S. energy system from production through end-use. The design and implementation of new hydrogen infrastructure is needed since there is no hydrogen infrastructure system today, unlike systems such as electricity, natural gas or gasoline, for example. In addition, the consumer is reluctant to purchase a vehicle if the infrastructure is not already in place. The famous “chicken and egg” (demand/supply) problem needs to be overcome in order that hydrogen can become an attractive alternative fuel for the future.

Extensive researches are being conducting for the implementation of hydrogen as an alternative fuel, as represented by [4], [6], [7] and [8]. The implementation of hydrogen as a fuel will not happen overnight; one way in which this transition might occur is presented in Figure 2, which illustrates that is will likely take decades in order to be integrated into the energy mix.
According to [6] there are considerable aspects that need to be considered when assessing future commercial hydrogen as a viable long-term alternative solution. For example: cost, operability, environmental impacts, safety and social implications are some attributes that need to be assessed. Also, there are important questions regarding when, where and how these technological options, some of which exist and some of which are still in development, will be implemented. Use of hydrogen cannot be analyzed in isolation. Operation of hydrogen infrastructure is done only in interaction with the overall energy system, as a shown in Figure 3.

**Figure 2: Transition to the Hydrogen Economy (Source [4])**
Figure 3: Hydrogen Markets as Part of the Overall Energy System (Source [9])

Following this line of thought, the *21st Century National Energy and Transportation Infrastructures–Balancing Sustainability, Costs, and Resiliency* project (NETSCORE 21 for short), funded by the National Science Foundation, was developed in order to respond to the lack of tools, knowledge, and perspective in designing a national system that integrates energy and transportation, considering the interdependencies between them as well as new energy supply technologies, sustainability and resiliency for a long term investment [10].

The goal of the NETSCORE 21 project is to identify optimal infrastructure designs in terms of future power generation technologies, energy transport and storage, and hybrid-electric transportation systems to achieve desirable balance between sustainability, costs, and resiliency. As a result, the project has been able to develop a tool called NETPLAN that is able to model and analyze long-term investment strategies for the transportation and energy systems [11] that account for interdependencies between them.
This thesis reports on work done to assess the use of hydrogen as an alternative fuel. The program NETPLAN is used to make this assessment.

1.2 Objectives

The objectives of this work are summarized as follow:

1. Identify the production, delivery, storage and application technologies for hydrogen as alternatives fuel;
2. Identify the potential resources available for hydrogen production in the U.S;
3. Develop a long term investment for assessing hydrogen fuel;
4. Evaluate different scenarios for the implementation of fuel cell vehicles.

1.3 Thesis Organization

The following thesis is organized in 7 chapters. The first chapter describes the motivation for this work as well as the goal of the NETSCORE 21 project, and the objectives. The second chapter presents information concerning the current use and potential resource of hydrogen in the U.S. The third chapter introduces hydrogen as a transportation fuel, and described its production processes. The fourth chapter presents the infrastructure required for the hydrogen economy. The fifth chapter explains the end-use technologies for the applications of the hydrogen as a fuel. The sixth chapter describes the NETPLAN tools, how they are used, and results for the long-term investment assessment for the hydrogen systems. Finally, the seventh chapter concludes and provides recommendations for future work.
CHAPTER 2. CURRENT USE AND HYDROGEN POTENTIAL RESOURCE IN USA

2.1 Overview

Hydrogen is being considered as an alternative clean fuel for a sustainable future. Similar to electricity, hydrogen is a secondary energy carrier that can be produced from any primary energy source such as coal, natural gas, oil, biomass, solar, wind, hydro, and nuclear power. Its introduction in the energy mix will result in profound environmental benefits, such as reduction on air pollution, greenhouse emissions, and energy supply security; especially in the transportation sector.

Hydrogen is a large and emergent industry. Based on [12] worldwide, 50 million tons of hydrogen, equivalent to about 170 million tons of petroleum, was produced in 2004, and the production is increasing by about 10% every year. Worldwide hydrogen production is mainly used in the following areas: approximately 60% to produce ammonia for use in fertilizer manufacturing and 40% in chemical, refinery and petrochemical sectors [12]. According to [13] around 11 million metric tons of hydrogen is produced in the U.S each year. This is sufficient to power 20-30 million cars or about 5-8 million homes.

This chapter describes the current hydrogen market and the hydrogen potential in the U.S based on primary energy resource available.
2.2 Hydrogen Current and Future Markets

Worldwide, hydrogen is consumed in the following sectors: 61% for ammonia production, 23% oil refining and 9% to methanol. The U.S consumes about 20% of the total global hydrogen production [12].

Approximately 9 million metric tons per year of hydrogen were produced in 2007 in the U.S and came from non-renewable energy sources. This corresponds to about 60 million metric tons of CO$_2$ emissions generated, as summarized in Table 1 [14].

**Table 1: Estimate Hydrogen Production by Business Sector (Source [14])**

<table>
<thead>
<tr>
<th>Sectors</th>
<th>Annual Hydrogen Production (million metric tons per year)</th>
<th>Estimated CO2 Emissions (million metric tons per year)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Merchant hydrogen</td>
<td>2.0</td>
<td>17</td>
</tr>
<tr>
<td>Oil refineries</td>
<td>2.6</td>
<td>~25</td>
</tr>
<tr>
<td>Ammonia plants</td>
<td>2.1</td>
<td>18</td>
</tr>
<tr>
<td>Methanol plants</td>
<td>1.5</td>
<td>None</td>
</tr>
<tr>
<td>Chlorine plants</td>
<td>0.4</td>
<td>None</td>
</tr>
<tr>
<td>Other</td>
<td>0.3</td>
<td>&lt; 1</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>8.9</strong></td>
<td><strong>~60</strong></td>
</tr>
</tbody>
</table>

Today, hydrogen is principally used to produce ammonia that is in turn used as fertilizer for agricultural purposes. A map of U.S. industrial hydrogen production facilities is shown in Figure 4. Also, hydrogen is used to help the transportation fuel to meet the environmental regulations (e.g., lower sulfur emissions) [9].
According to [15], the hydrogen production in the U.S is used in two ways: on-purpose and byproduct. The estimated U.S hydrogen production capacity of these two groups is showed in Table 2. The on-purpose hydrogen is produced at the site of consumption or nearby. It can be classified as captive or merchant hydrogen. The main difference is the producer of the hydrogen. For example, the hydrogen that is produced by the owner of the plant is denoted captive hydrogen [16]. Ammonia, hydrogen from oil refineries, and methanol are in this category. U.S locations of these three markets are shown in Figure 5.
On the other hand, merchant hydrogen is produced in order to be sold on the market when hydrogen is required in large volume as an input or to be traded as smaller specified volumes [16].

Unlike on-purpose hydrogen, by-products hydrogen is produced as a result of the overall production process. This hydrogen is not needed for additional steps, and so it is generally sold.
Table 2: Estimated U.S. Hydrogen Production Capacity (2003 and 2006) (Source [15])

<table>
<thead>
<tr>
<th>Capacity Type</th>
<th>Production Capacity (Thousand Metric Tons per Year)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2003</td>
</tr>
<tr>
<td><strong>On-Purpose Captive</strong></td>
<td></td>
</tr>
<tr>
<td>Oil Refinery</td>
<td>2,870</td>
</tr>
<tr>
<td>Ammonia</td>
<td>2,592</td>
</tr>
<tr>
<td>Methanol</td>
<td>393</td>
</tr>
<tr>
<td>Other</td>
<td>18</td>
</tr>
<tr>
<td><strong>On-Purpose Merchant</strong></td>
<td>976</td>
</tr>
<tr>
<td>Off-Site Refinery</td>
<td>2</td>
</tr>
<tr>
<td>Non-Refinery Compressed Gas (Cylinder and Bulk)</td>
<td>201</td>
</tr>
<tr>
<td>Compressed Gas (Pipeline)</td>
<td>43</td>
</tr>
<tr>
<td>Liquid Hydrogen</td>
<td>&lt;1</td>
</tr>
<tr>
<td>Small Reformers and Electrolyzers</td>
<td>&lt;1</td>
</tr>
<tr>
<td><strong>Total On-Purpose</strong></td>
<td>7,905</td>
</tr>
<tr>
<td><strong>Byproduct</strong></td>
<td></td>
</tr>
<tr>
<td>Catalytic Reforming at Oil Refineries</td>
<td>2,977</td>
</tr>
<tr>
<td>Other Off-Gas Recovery</td>
<td>462</td>
</tr>
<tr>
<td>Chlor-Alkali Processes</td>
<td>NA</td>
</tr>
<tr>
<td><strong>Total Byproduct</strong></td>
<td>3,439</td>
</tr>
<tr>
<td><strong>Total Hydrogen Production Capacity</strong></td>
<td>10,534</td>
</tr>
</tbody>
</table>

Having explained the current markets for hydrogen use, we now turn to future market possibilities. Currently, future markets such as liquid-fuel refining industrial applications, oil
and tar sand processing, mobile fuel cells applications, and others are being considered for a medium to long-term hydrogen production.

For instance, the coal liquefaction and shale oil (medium-to-long term) market will require 37.7 Mt of hydrogen in order to replace the entire current U.S crude oil from coal liquefaction. Hydrogen can also be used for electricity market (medium-to-long term) to replace natural gas for peak electricity production. Finally, hydrogen can be used within the transportation market via fuel cell vehicles. This last application is perhaps the most promising and is expected to be the main application for hydrogen [9]. Yet, it would require several decades for its implementation as can be seen in Table 3.

Table 3: Hydrogen Demand Scenarios for Transportation (Source [9])

<table>
<thead>
<tr>
<th></th>
<th>2020</th>
<th>2025</th>
<th>2030</th>
<th>2035</th>
<th>2040</th>
<th>2045</th>
<th>2050</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂ demand for transport (million tons)</td>
<td>1.8</td>
<td>5.4</td>
<td>16.2</td>
<td>35.6</td>
<td>67.1</td>
<td>89.8</td>
<td>100</td>
</tr>
</tbody>
</table>

2.3 Hydrogen Potential in USA

Hydrogen is a secondary energy carrier that can be produced from coal, natural gas, oil, biomass, solar, wind, hydro, and nuclear energy. Its future market will depend on which energy resources are available and where those energy resources are located.

The U.S. Department of Energy’s (DOE) National Renewable Energy Laboratory (NREL) has performed two important analyses to assess the potential for using hydrogen in the U.S. In both analyses, 30% of the current annual production capacity of each of the energy resources, mention above, is assumed for hydrogen production. All of the maps that
are presented in the following sections correspond to the resource assessment from the NREL.

The first resource assessment is described in a technical report titled *Hydrogen Potential from Coal, Natural Gas, Nuclear, and Hydro Power*; here, it is estimated that the quantity of hydrogen that could be produced from coal, natural gas, nuclear, and hydro power by county in the US is approximately 72.5 million metric tons per year [17]. This would displace 80% of the 396 million tons of gasoline used in the US in 2007.

The second resource assessment, titled *Potential for Hydrogen Production from Key Renewable Resources in the United States*, estimated the potential for hydrogen production from key renewable resources (onshore wind, solar photovoltaic, and biomass) by county for the United States [18]. Figure 6 shows the hydrogen potential from renewable energy resources as presented in this report. The study found that about 1 billion tons per year, or more than 10 times the potential from the other resource group (coal, natural gas, hydroelectric, and nuclear) is available for producing hydrogen from renewable energy.
Figure 6: Hydrogen Potential from Renewable Energy Resource (Source [18])

The U.S. has high potential for hydrogen production as presented in Table 4. Yet, there are several economic and technical challenges which must be overcome before this potential can be fully tapped.
Table 4: Hydrogen Potential in the U.S. (Source [17] and [18])

<table>
<thead>
<tr>
<th>Hydrogen from</th>
<th>Potential Hydrogen Production in U.S.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Natural Gas (tons/year)</td>
<td>26,805,697</td>
</tr>
<tr>
<td>Coal (tons/year)</td>
<td>40,485,759</td>
</tr>
<tr>
<td>Nuclear Energy (tons/year)</td>
<td>3,930,351</td>
</tr>
<tr>
<td>Hydro-Power (tons/year)</td>
<td>1,234,945</td>
</tr>
<tr>
<td>Wind Energy (tons)</td>
<td>301,328,935.5519</td>
</tr>
<tr>
<td>Solar Energy (tons)</td>
<td>790,631,720.3101</td>
</tr>
<tr>
<td>Biomass (tons)</td>
<td>33,299,723.8599</td>
</tr>
</tbody>
</table>

The following subsections overview the resource potential for hydrogen production in the U.S.

2.3.1 Natural Gas Potential

Natural gas is the most commonly used resource for hydrogen production. Worldwide, 48% of the hydrogen production is made through natural gas. In the U.S., 95% of hydrogen production is made by central plant natural gas reforming. Figure 7 shows the hydrogen potential from natural gas in the U.S. Currently, this technology is the least expensive for hydrogen production.

According to [19] natural gas is a cost-effective feedstock for produce hydrogen. The reasons that support the use of natural gas for hydrogen production are: natural gas reforming
is a well-known technology; the necessary natural gas infrastructure is largely in place; natural gas is easy to handle; and natural gas has a high hydrogen-to-carbon ratio which minimizes the by-product carbon dioxide formation. Also, this feedstock can reduce by up to 60% the greenhouse gas emissions of light-duty vehicle transportation via fuel cell vehicles compared to internal combustion engine vehicles that used gasoline [20].

Hydrogen can be produced from natural gas by three processes: Steam Reforming Process, Partial Oxidation Process and Auto thermal Reforming Process. Each of these processes is explained in the Chapter 3. At the present time, the Steam Reforming Process is the most commonly used process for H₂ production. Because of the vast commercial experience with this technology, it has advanced in terms of cost reduction and in terms of efficiency increase.
Currently, the Department of Energy (DOE) is focused on natural gas reforming for hydrogen production for near term use of hydrogen and not for long term solution. The reasons are [19]:

- Natural gas is a non-renewable energy and is therefore a limited resource with 15% imported into U.S.;
- The price of natural gas is volatile and very sensitive to seasonal demand;
- It requires less capital investment for distributed plant and it does not require transportation and delivery infrastructure compared to central plants;
• It releases some carbon dioxide during the H₂ production process and therefore requires carbon capture and storage to reach low carbon dioxide emissions, which increases by 11 to 21% the capital cost of hydrogen plant. For distributed system this is prohibitive.

This production technology is therefore considered to be a provisional option for initiating use of hydrogen in the U.S.

2.3.2 Coal Potential

According to [12] coal is a source of energy that may play a major role for the next several hundred years due to abundant reserves worldwide. The U.S. possesses the world largest proven reserves of coal with 272 billion short tons, followed by Russia with 173 and China with 126. It is estimated that the U.S. has coal reserves which will satisfy current production levels for nearly 250 years [21]. Figure 8 shows the hydrogen potential from coal in the U.S.

Coal is an attractive candidate for initiating use of hydrogen, because it is plentiful domestically and can contribute to reducing the U.S dependence on imported petroleum.
Currently, most coal usage is for electricity production in a coal-fired power station, which operates by burning coal to boil water that produces steam which drives a steam turbine for electricity generation. However, this technology is not appropriate for producing hydrogen from coal. Hydrogen production from coal does not occur via a combustion process but rather via a conversion process called integrated gasification combine cycle (IGCC). The IGCC process for hydrogen production is described in Chapter 3.

The IGCC, when combined with carbon capture and sequestration, is called a clean coal technology because it is offers low emissions power production from coal as opposed to
conventional coal fires power plants. Also, it is considered to be a polygeneration technology since it can produce multiple energy products: electricity and hydrogen.

Nevertheless, one challenge is the high cost associate with the carbon capture and sequestration technologies. The current cost of sequestering carbon dioxide is about $100-300 per ton of carbon sequestered [21].

The emissions from coal are larger compare to any other fossil fuel for hydrogen production. It is estimated that 19 kg of CO$_2$ per kg of hydrogen is produced in the hydrogen production process from coal, compared with natural gas where about 10 kg of CO$_2$ per kg of hydrogen is produced [19]. In addition IGCC is in an early stage of development compared with other hydrogen production technologies.

According to [19] coal is most effectively used in producing hydrogen through very large central plants when the demand of hydrogen is high and the distribution systems are available.

In the future, coal usage for electricity production will play a declining role, and so coal usage for hydrogen will become more favorable.

### 2.3.3 Nuclear Potential

The United States is the world largest supplier of nuclear power in the world. It has the 4th largest uranium reserves. It operates 104 generating units in 65 nuclear power plants. In 2008, these units produced a total of 806.2 TWh of electric energy that corresponded to ~20% of the of the 2008 total electric energy generation [22]. Figure 9 shows the hydrogen potential from nuclear power in the U.S.

The Japan nuclear crisis as a result of the devastating 9.0 magnitude earthquake and massive tsunami on March 11 2011 has stimulated much discussion about the risks and
benefits of nuclear power in the U.S. However, the U.S. Nuclear Regulatory Commission, at the request of President Obama, has announced a comprehensive safety review of the 104 nuclear power reactors in the U.S. The Obama administration "continues to support the expansion of nuclear power in the United States, despite the crisis in Japan" [22].

The nuclear energy is an attractive candidate for large scale of hydrogen production. One reason for this is that use of nuclear power for hydrogen production does not result in the emission of any of the pollutant gases such as carbon dioxide, sulfur dioxide or nitrogen dioxide; moreover, in contrast to use of fossil fuel feedstock for hydrogen production, very pure hydrogen for fuel cell vehicles can be obtained from nuclear technologies. For near-term use of hydrogen, hydrogen from nuclear energy can be obtained from nuclear generation during time intervals corresponding to off-peak electric demand.
Figure 9: Hydrogen Potential from Nuclear Power (Source [17])

Hydrogen can be produced from nuclear energy by water electrolysis process, thermochemical process and hybrid process. The water electrolysis process is the most used and commercialized technology. However, it presents low energy efficiency. Many advances have occurred in the past few years for this technology. The so-called advanced light-water-reactor (ALWR) has been designed in order to increase the energy efficiency of this technology.

Both the Thermochemical Process and the High Temperature Steam Electrolysis (HTSE) Process have the potential to increase production efficiency of hydrogen to 50% or
higher. Both processes require high-temperature operation in order to achieve high efficiencies [23].

The Idaho National Laboratory (INL) is a leading institution for the development of HTSE. It has been demonstrated at INL that both technologies are attractive candidates for large scale production of hydrogen in an operationally cost effective way. However, the higher efficiency and operational cost improvement comes with higher complexity and capital cost [19].

Table 5 describes some advantages and disadvantages for the use of nuclear energy for hydrogen production [19].

**Table 5: Advantages and Disadvantages of Nuclear Energy (Source [19])**

<table>
<thead>
<tr>
<th><strong>Nuclear Energy Use for Hydrogen Production</strong></th>
<th><strong>Advantages</strong></th>
<th><strong>Disadvantages</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>1. <em>Long-term domestic source</em>: H$_2$ from nuclear energy will be an excellent candidate in the long-term time frame. Its price is not subject to foreign pressures.</td>
<td>1. <em>Efficiency of conventional electrolysis process</em>: Even though is a well know technology, it presents low energy efficiency.</td>
<td></td>
</tr>
<tr>
<td>3. <em>Efficiency of overall process</em>: Higher efficiency can be obtained by the future technologies, such as HTSE.</td>
<td>3. <em>Nuclear Waste</em>: The nuclear waste disposal scheme remains to be finalized</td>
<td></td>
</tr>
<tr>
<td>4. <em>Public Concerns</em>: The fear of widespread devastation in case of accident. For example, the Japan earthquake.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### 2.3.4 Wind Potential

The United States has abundant wind resources. The U.S. wind potential is estimated to be 10,777 TW h/ year [24]. Figure 10 shows the hydrogen potential from wind energy in the U.S.
The cumulative installed capacity of wind power in the United States was 41,400 megawatts (MW) in the first quarter of 2011. Comparing to other countries of the world, the U.S is second with more cumulative capacity installed behind China [25].

Hydrogen can be produced from wind energy through electrolysis of water, where the electrical power is produced from the conversion of the wind energy. This process has been used for decades, and pure hydrogen is produced through this process.

Figure 10: Hydrogen Potential from Wind (Source [18])

At the present time, this process is very expensive and consumes more energy per unit of hydrogen produced compared to fossil fuel. Chapter 3 describes use of electrolysis for hydrogen production.
Hydrogen from wind energy via electrolysis has advantages of improving energy security and environmental quality. This is because, first, wind energy is a domestic energy resource. Second, it can result in zero or near-zero greenhouse gas emissions if all the wind energy that it would use to electrolyze the water to produce hydrogen is independent from the grid. This system is ideal for a clean hydrogen production.

The disadvantage of this system, based on [24], is that due to the low capacity factor and the variable output of the wind turbine the hydrogen production would be highly variable, and the capacity factor of the electrolyzer would be low. Another design system for hydrogen production from wind is via a grid connection. The advantage is the constant supply of electricity that is needed for the electrolyzer. It will operate at a high capacity factor due to the accessibility of energy from the grid. However, the system is unattractive when the electricity from the grid is generated from non-renewable energy.

Based on [19], hydrogen production from wind energy needs to overcome the following issues for successful development and deployment in the future:

- Cost reduction for electricity generated by wind power. The electricity cost is the most significant contributor for H₂ cost produced via electrolysis process.

- Cost reduction on the capital cost of the electrolyzer

In addition, the wind resource site must be located near existing distribution networks, it must have a sufficiently rich wind resource, and it must be economically competitive with respect to other alternative energy resources to be useful for hydrogen production [24].
Hydrogen can be produced in small-scale distributed systems that can reduce the need for hydrogen distribution that it is appropriate to meet the early stages for the fuel cell vehicles market. [19].

2.3.5 Solar Potential

Solar energy is a clean, abundant and available renewable energy source over the globe. At the end of 2009, the U.S. ranked fourth with the highest amount of solar powered installed with 1,650 MW behind Germany with 9,875 MW, Spain with 3,386 MW and Japan with 2,633MW [26]. Even though the solar energy offers a great potential for supply energy, it only provides less than 1% of U.S. energy needs [27]. Figure 11 shows the hydrogen potential from solar energy in the U.S.

At the present time, photovoltaic (PV) and concentrated solar power systems (CSP) are used for the conversion of sunlight into electricity. Both technologies have been demonstrated in large scale systems. However, the PV and CSP have been hindered by their economics [28]. The electricity generated by solar energy is more than twice as expensive as electricity from fossil fuels. The reasons for this are the high cost of the solar panel for PV technology and the high cost of the heliostats for the CSP [19].

In addition, the capacity factor of the systems is around 20% for PV. This low capacity factor is due to that the sunlight that arrives at the earth surface is variable depending on location, time of day, time of year, and weather conditions [29]. In addition, solar energy does not always match demand, although its daytime availability enables it to match demand better than wind energy. This issue can be addressed with the use of backup systems when the sun is not available. The principal advantage is that solar energy is that it does not produce air pollutants or carbon-dioxide.
Solar energy may be used to produce hydrogen. The use of solar energy for hydrogen production is attractive in that, when coupled with a fuel cell for electricity generation, the fuel cell storage capability can be used to effectively meet varying electric demand [28]. Nevertheless, the most attractive way to use hydrogen from solar energy remains in the transportation sector.

Figure 11: Hydrogen Potential from Solar (Source [18])

Hydrogen can be obtained from solar energy by the following technologies: Photovoltaic Systems (PV), Concentrated Solar Thermal Energy (CSP), and Photolytic Process [30]. Each of these technologies are described in what follows.
2.3.5.1 Photovoltaic Systems

Hydrogen can be produced by electrolysis of water using the current generated by PV. Hydrogen production by PV is not cost-effective due to the high cost of PV panels. Moreover, the production of hydrogen through electrolysis from solar is not cost-competitive because of high electricity cost and because the electrolyzers require further development [19]. However, additional improvement in this technology is necessary for long-term hydrogen production from PV systems. The main benefit is that it does not produce greenhouse emissions when hydrogen is produced.

2.3.5.2 Concentrated Solar Thermal Energy

In the CSP technology, the solar radiation is concentrated into the solar receiver mounted on the top of a central tower. High temperature heat is provided by the receiver. This heat is used to operate a conventional power cycle through a steam turbine to generate electricity. This electricity can be used for the dissociation of water into H₂ and O₂ through the electrolysis process. Thermochemical routes of hydrogen production using CSP technology are presented in Figure 12. The CSP system is a relatively new technology that it has shown promise and is moving towards sustainable large-scale fuel production [28] and [31].

Based on [28], [30] and [32], the CSP technology is considered as the benchmark for other routes such as solar-driven water splitting thermochemical cycles for hydrogen production. These processes involve endothermic reactions. They require higher reaction temperature that yields higher energy conversion efficiencies. On the other hand, these higher
temperatures lead to greater losses by re-radiation from the solar cavity receiver [28]. These methods are further described in [30] and [32].

![Diagram of thermochemical routes for the production of solar fuels (H₂, syngas)](image)

**Figure 12: Thermochemical Routes of Hydrogen Production using CSP (Source [28])**

**2.3.5.2.1 H₂ from water by solar thermolysis**

The thermal decomposition of water in hydrogen and oxygen is made through the application of concentrated solar energy in a single step called water thermolysis. This process requires higher temperature in the order of 2200 °C for effective degree of dissociation. In order to avoid explosive mixtures, an effective technique for hydrogen and oxygen is required [28].

**2.3.5.2.2 H₂ from water by solar thermochemical cycles**

The water is dissociate at moderately high temperatures (927 °C) compared with the H₂ from water by solar thermolysis cycle. This cycle has the advantage of avoiding the
separation problem; but this method tends to cause corrosion. The leading candidates for this approach are Sulfur-Iodine Cycle and Calcium –Bromine-Iron cycle (UT-3). Both methods are further explained in Chapter 3.

2.3.5.2.3 H₂ by decarbonization of fossil fuels

Solar cracking, solar reforming and solar steam gasification are the three solar thermochemical processes for hydrogen production using fossil fuel. Each one is described in what follows.

**Solar cracking:** This cycle uses concentrated solar energy as heat for the thermal decomposition of the natural gas, oil and other hydrocarbons into hydrogen. The main reaction is the following: \( \text{CH}_4 \rightarrow 2\text{H}_2 + \text{C} \) (solid). Based on [31] it is an unconventional process for hydrogen production even though it is a cost-effective cycle. The reason is that carbon solid is generated as byproduct; however, this carbon solid can be sequestered or marketed. This process has the advantage of removal and separates the carbon in a single step as shown in Figure 13.

![Figure 13: Solar Cracking Schematic Diagram (Source [28])](image)
**Solar Steam Reforming / Gasification**: These processes consist in the use of concentrating solar energy for the necessary heat for achieving the reforming/gasification reaction between the fossil fuel (natural gas, oil, and coal) and steam or CO₂ for the production of hydrogen and carbon dioxide. It is an endothermic reaction and requires temperatures around 1000 °C. The principal reaction is as follows: \( \text{CH}_4 + \text{H}_2\text{O} (\text{g}) \leftrightarrow 3\text{H}_2 + \text{CO} \). This process requires additional steps for shifting CO and separating CO₂ compared with the solar cracking, as shown in Figure 14. Furthermore, these methods cause additional energy loss associated with sequestration of carbon.

The solar reforming process is advantageous because CO₂ emissions can be reduced and 40% of the fuel can be saved compared with the conventional steam methane reforming process (SMR) (the same advantage can be obtained through the use of nuclear energy for the heat required for the reforming reaction [19]). Also, solar gasification has the ability to also convert solid fuel such as coal into cleaner hydrogen fuel. However, based on [28], the solar reforming process is 20% more expensive compared to the conventional SMR. Nonetheless, it remains an attractive candidate for near-term implementation of hydrogen.
According to [28] and [32] the advantages of using solar energy as a source of heat for the hydrogen production by descarbonization of fossil fuel are:

- The calorific value of the feedstock is upgraded;
- The gaseous products are not contaminated by the byproducts of combustion; and
- The discharge of pollutants to the environment is avoided.

2.3.5.2.4 H₂ from H₂S (hydrogen sulfide) by solar thermolysis:

Hydrogen sulfide (H₂S) is a toxic industrial product derived from natural gas, petroleum and coal processing. This product can be used for hydrogen production, using the hydrogen wasted in the Claus process [33] when sulfur is recovered. It requires high temperature for decompose H₂ and sulfur.

2.3.5.3 Photolytic Process

This process is in early stage of research and offers the potential of producing sustainable hydrogen with low environmental impact. The photolytic process produces
hydrogen and oxygen through the use of energy from sunlight to separate water. According to [34], the photolytic process presents two possible routes for hydrogen production: photoelectrochemical water splitting and photo-biological water splitting, as described in what follows.

### 2.3.5.3.1 Photo Electrochemical Water Splitting

The use of sunlight and a special class of semiconductor materials are used for the production of hydrogen from water. Based on [35] this specialized semiconductor absorbs sunlight and uses the light energy to separate the water molecules. However, this technology needs highly durable and efficient materials for the hydrogen production.

### 2.3.4.3.2 Photo Biological Water Splitting

Some microorganisms such as unicellular green algae, cyanobacteria, photosynthetic bacteria and some forms of dark fermentative bacteria and sunlight are used for hydrogen production from water. These microorganisms consume water and produce hydrogen as a byproduct of their natural metabolic process. According to [35] the enzymatic pathways through which hydrogen is formed at the molecular level need to optimize it.

This process presents some disadvantages: the microorganism splits water too slow in order to be used for commercial hydrogen, and cost-effective productions need to overcome and lower the cost production [35].

In conclusion solar hydrogen production technologies are a long term candidate for hydrogen. Table 6 summarizes the solar hydrogen production processes mentioned above. The advantage is that solar energy is available all over the globe and is renewable. However, it is not competitive with fossil fuel in terms of cost, reliability and performance for hydrogen production [36].
Table 6: Solar Hydrogen Production Technologies (Source [32])

<table>
<thead>
<tr>
<th>Solar H₂ Production Systems</th>
<th>Type</th>
<th>Processes</th>
<th>Processes Description</th>
<th>End Products</th>
</tr>
</thead>
<tbody>
<tr>
<td>PV</td>
<td>Low Temperature</td>
<td>Electrolysis</td>
<td>Water Electrolysis</td>
<td>H₂, O₂</td>
</tr>
<tr>
<td>Photo electrochemical</td>
<td>Low Temperature</td>
<td>Photo electrolysis</td>
<td>Photo electrolysis of water</td>
<td>H₂, O₂</td>
</tr>
<tr>
<td>Photo biological</td>
<td>Low Temperature</td>
<td>Photo biolysis</td>
<td>Plant and algal photo-synthesis</td>
<td>H₂</td>
</tr>
<tr>
<td>Concentrated solar thermal</td>
<td>High Temperature</td>
<td>Thermolysis</td>
<td>Thermal dissociation of water</td>
<td>H₂, O₂</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Thermochemical Cycles</td>
<td>Thermochemical cycles using metal oxides</td>
<td>H₂, O₂</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Gasification</td>
<td>Steam-gasification of coal and others solid carbonaceous materials</td>
<td>H₂, CO₂</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Cracking</td>
<td>Thermal decomposition of natural gas, oil, and other hydrocarbons</td>
<td>H₂, C</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Steam-reforming</td>
<td>Steam-reforming of natural gas, oil, and other hydrocarbons</td>
<td>H₂, CO₂</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Electrolysis</td>
<td>High temperature water electrolysis and water electrolysis via solar thermal electricity generation</td>
<td>H₂, O₂</td>
</tr>
</tbody>
</table>

2.3.6 Biomass Potential

Biomass is organic materials such as plant and animals (microorganisms) that have stored energy through the process of photosynthesis. Its use as a renewable energy dates to when humans learned to use fire [37]. Biomass is one of the most plentiful and well-utilized forms of renewable energy in the world.

In the U.S, biomass contributes to approximately 3.9 quadrillion British thermal units (Btu) (Quads) and in 2009, for the first time, this renewable energy supplied over 4% of total
U.S. primary energy consumption as is indicated in Figure 15. This supply increased in the early 2000 due to ethanol production [38].

Figure 15: Total Primary Energy Consumption in 2009 in the U.S. (Source [38])

Biomass is an abundant, clean and renewable resource that will play an important role in initiating use of hydrogen. Figure 16 shows the hydrogen potential from biomass resource in the U.S.

One of the principal attributes of biomass is that compared to fossil fuel, biomass, during its growth, removes approximately the same amount of CO₂ as it releases when it is used for energy production. Therefore, CO₂ emissions generated for biomass-driven hydrogen production are approximately neutral. In addition, hydrogen from biomass has facilitates independence from oil imports [39].
Figure 16: Hydrogen Potential from Biomass (Source [18])

Hydrogen can be produced from biomass through two types of processes: thermochemical and biological. Further description of these processes is provided in Chapter 3.

Unfortunately, no commercial technology of biomass for hydrogen production is available at the present time. Moreover, one of the major drawbacks is the low efficiency of utilizing biomass for hydrogen production. High capital cost and feedstock costs are the main challenges for hydrogen production via biomass energy. However, hydrogen from biomass has the potential to accelerate the realization of hydrogen as a major fuel of the future.
CHAPTER 3. HYDROGEN ECONOMY

3.1 Overview

Hydrogen provides high-quality energy and is capable of becoming a diversified secondary energy source. It can be used with a very high efficiency and near-zero emissions at the point of use [5].

This chapter provides a review of the properties of H\textsubscript{2} and its production processes.

3.2 Hydrogen as a transportation fuel

Hydrogen is the most abundant element in the universe. At standard temperature and pressure, H\textsubscript{2} is colorless, tasteless, odorless, and nontoxic. It is virtually never found in its pure form; it occurs, rather, in the form of chemical compounds. For example, hydrogen is present in water, fossil hydrocarbons, and biomass components such as carbohydrates, protein, and cellulose [12].

Hydrogen is the lightest of all elements. It presents a very low density per unit volume, 0.08987 kg/m\textsuperscript{3}. Hydrogen transforms from a gas to a liquid at a temperature of -253°C (-422.99°F), and from a liquid to a solid at a temperature of -259°C (-434.6°F). Table 7 summarizes the physical properties of hydrogen and Table 8 presents the energy-related properties of hydrogen as compared with other fuels.
Table 7: Physical Properties of Hydrogen (Source [12])

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>2.01594</td>
</tr>
<tr>
<td>Density of gas at 0°C and 1 atm.</td>
<td>0.08987 kg/m³</td>
</tr>
<tr>
<td>Density of solid at −259°C</td>
<td>858 kg/m³</td>
</tr>
<tr>
<td>Density of liquid at −253°C</td>
<td>708 kg/m³</td>
</tr>
<tr>
<td>Melting temperature</td>
<td>−259°C</td>
</tr>
<tr>
<td>Boiling temperature at 1 atm.</td>
<td>−253°C</td>
</tr>
<tr>
<td>Critical temperature</td>
<td>−240°C</td>
</tr>
<tr>
<td>Critical pressure</td>
<td>12.8 atm.</td>
</tr>
<tr>
<td>Critical density</td>
<td>31.2 kg/m³</td>
</tr>
<tr>
<td>Heat of fusion at −259°C</td>
<td>58 kJ/kg</td>
</tr>
<tr>
<td>Heat of vaporization at −253°C</td>
<td>447 kJ/kg</td>
</tr>
<tr>
<td>Thermal conductivity at 25°C</td>
<td>0.019 kJ/(ms°C)</td>
</tr>
<tr>
<td>Viscosity at 25°C</td>
<td>0.00892 centipoise</td>
</tr>
<tr>
<td>Heat capacity (Cp) of gas at 25°C</td>
<td>14.3 kJ/(kg°C)</td>
</tr>
<tr>
<td>Heat capacity (Cp) of liquid at −256°C</td>
<td>8.1 kJ/(kg°C)</td>
</tr>
<tr>
<td>Heat capacity (Cp) of solid at −259.8°C</td>
<td>2.63 kJ/(kg°C)</td>
</tr>
</tbody>
</table>

Among the properties [12] that suggest its use as a combustible fuel are:

- **Energy Content** \( \text{H}_2 \) has the highest energy content per unit mass of any fuel. On a weight basis, it has three times the capacity of gasoline (48.6 MJ/Kg vs. 140.4 MJ/ Kg). On a volume basis, however, the relative energy capacities of liquid \( \text{H}_2 \) and gasoline are reversed (8,491 MJ/m³ vs. 31,150 MJ/m³).
• **Limits of flammability** define the ease with which something will burn or ignite, causing fire or combustion [40]. H₂ presents a broader range of flammability; for example, H₂ is flammable in 4-75% concentrations, while the range for gasoline is from 1-7.6%.

• **Ignition energy** is the minimum energy required to ignite a combustible vapor, gas, or dust cloud [41]. H₂ has a very low ignition energy (0.02 MJ) compared to gasoline (0.24MJ). This characteristic enables rapid ignition for a hydrogen engine, even for a lean mixture.

• **Detonation limits.** H₂, when confined, can be detonated over a very wide range of concentrations. However, like many other fuels, it is very difficult to detonate if released into the atmosphere.

• **Auto ignition temperature.** Compared to other fuels, hydrogen has a higher auto ignition temperature (585 °C).

• **Flame speed.** H₂ presents a higher flame velocity (1.85 m/s) than gasoline vapor (0.42 m/s).

• **Diffusion.** H₂ has very high diffusivity. This ability to disperse in air represents an advantage because hydrogen leaks can be quickly dispersed in the environment and unsafe conditions avoided.

• **Density.** H₂ has very low density. This may present problems when it is used for transportation purpose; for example, a very large volume is necessary to store enough hydrogen to provide an adequate driving range [12]
### Table 8: Properties of Hydrogen and Other Fuels (Source[12])

<table>
<thead>
<tr>
<th>Fuel</th>
<th>LHV (MJ/kg)</th>
<th>HHV (MJ/kg)</th>
<th>Combustible Range (%)</th>
<th>Flame Temperature (°C)</th>
<th>Min. Ignition Energy (MJ)</th>
<th>Auto Ignition Temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>50</td>
<td>55.5</td>
<td>5–15</td>
<td>1914</td>
<td>0.3</td>
<td>540–630</td>
</tr>
<tr>
<td>Propane</td>
<td>45.6</td>
<td>50.3</td>
<td>2.1–9.5</td>
<td>1925</td>
<td>0.3</td>
<td>450</td>
</tr>
<tr>
<td>Octane</td>
<td>47.9</td>
<td>15.1</td>
<td>0.95–6.0</td>
<td>1980</td>
<td>0.26</td>
<td>415</td>
</tr>
<tr>
<td>Methanol</td>
<td>18</td>
<td>22.7</td>
<td>6.7–36.0</td>
<td>1870</td>
<td>0.14</td>
<td>460</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>119.9</td>
<td>141.6</td>
<td>4.0–75.0</td>
<td>2207</td>
<td>0.017</td>
<td>585</td>
</tr>
<tr>
<td>Gasoline</td>
<td>44.5</td>
<td>47.3</td>
<td>1.3–7.1</td>
<td>2307</td>
<td>0.29</td>
<td>260–460</td>
</tr>
<tr>
<td>Diesel</td>
<td>42.5</td>
<td>44.8</td>
<td>0.6–5.5</td>
<td>2327</td>
<td></td>
<td>180–320</td>
</tr>
</tbody>
</table>

### 3.3 Hydrogen Production

As indicated in Figure 17, hydrogen can be produced from a variety of sources. It can be produced from both non-renewable energy sources like natural gas, coal, petroleum, and nuclear as well as from renewable energy sources like wind, solar, hydro, geothermal, algae, and biomass alcohols.
The principal elements underlying hydrogen deployment include supply, production, distribution, dispensing, and end use. Supply is discussed in chapter 2 and the remaining pathways are explained in the following chapters.

The following subsections describe in more detail the various technologies that can be used to produce hydrogen.

### 3.3.1 Steam Reforming Process

The steam reforming process, the most common hydrogen production method, is also known as Steam Methane Reforming (SMR) because of its use of natural gas as a feedstock. About 40% of hydrogen worldwide is produced by this method.

This process, endothermic catalytic conversion of light hydrocarbon using steam, is used, for example, to supply large centralized quantities of hydrogen gas to oil refineries,
ammonia plants, and methanol plants [15]. Figure 18 shows the main components used by
the Steam Reforming Plan [42].

![Steam Reforming Plan Diagrams](Source [42])

The four important steps in the Steam Reforming Process [42] are:

- **Feedstock**: the process commonly uses a light hydrocarbon like natural gas or
  naphtha, but could also use biogas or methanol

- **Desulphurization unit**: removes the sulfur compounds in the feedstock to avoid a
  potential threat to the catalysts used in other steps of the process.

- **Primary and Secondary Steam reformer**: designed to break down feedstock,
  e.g., natural gas into H₂ and carbon monoxide (CO). At high temperatures (700 –
  1100 °C) and in the presence of a metal-based catalyst (nickel), steam reacts with
  methane to yield carbon monoxide and hydrogen. The first reaction is strongly
  endothermic (consumes heat). The reaction is summarized by:

  \[
  CH_4 + H_2O \rightarrow 3H_2 + CO \quad \Delta H^\circ = 206 \text{ kJ/mol}
  \]

- **Water Gas Shift Reactor**: subjects the products from the primary and secondary
  steam-reforming process to a temperature reduction of about 350°C to generate
  steam fed into the water gas shift reactor (WGS). The CO reacts with steam using
  a catalytic process to produce H₂ and CO₂. This second reaction is mildly
  exothermic (produces heat) and is summarized by:
• **PSA:** Hydrogen purification with pressure swing adsorption (PSA) to remove CO, CO₂ and CH₄ gases from hydrogen.

### 3.3.2 Partial Oxidation Process

Partial oxidation (POx) of hydrocarbons is another method for hydrogen production. Light hydrocarbons like natural gas can be used to produce H₂ through this process. However, the POx process usually produces H₂ at a faster rate than the SMR process, resulting in less H₂ produced from a given feedstock quantity. POx more commonly uses heavy residual oils (HROs) and coal as feedstock.

The POx process combines fuel and oxygen (or air) in proportion such that the fuel is converted into a mixture of H₂, CO, and CO₂ as it is showed in Figure 19. The overall reaction is exothermic due to a sufficient amount of oxygen added to a reagent stream [12].

![Figure 19: Partial Oxidation Process (Source [43])](image)

The four important steps in the POx process are [21]:

- **Gasification.** Coal is turned into synthetic gas (syngas) (composed of carbon monoxide, hydrogen, and carbon dioxide.) at a very high temperature (up to 1800°C), through a gasification process accomplished by mixing pulverized coal with an oxidant, usually steam, air, or oxygen.
• **Cooling and Cleaning.** The syngas is cooled and cleaned to remove extraneous gases and particles, leaving only carbon monoxide, carbon dioxide, and hydrogen. During syngas cleaning, mercury, sulfur, trace contaminants, and particulate substances are removed.

• **Shifting** Next, the syngas is sent to a "shift reactor." During the shift reaction, the carbon monoxide is converted into additional hydrogen and carbon dioxide by mixing it with steam. At this point the syngas consists mostly of hydrogen and carbon dioxide.

• **Purification** Once the syngas has been shifted, it is separated into separate streams of hydrogen and carbon dioxide. The hydrogen, once cleaned, is then ready for use, while the carbon dioxide is captured and sent off for sequestration.

### 3.3.3 Auto thermal Reforming Process (ATR)

The ATR process uses a combination of SMR and POx technologies. The ATR process combines catalytic partial oxidation and steam reforming to convert both lighter and heavier hydrocarbons; the exothermic oxidation supplies the necessary reaction heat for the subsequent endothermic steam-reforming process [44].

ATR has the advantage of high efficiency, since the heat required is generated as part of the process itself. This process has not up to now been widely applied.

### 3.3.4 Electrolysis Process

The hydrogen produced by this process constitutes around of 4% of worldwide production and it has been in use for about a decade.
It is used in smaller markets and specialty applications in which higher-purity hydrogen is required. For example, in food processing H\textsubscript{2} can be used to increase the degree of saturation in fats and oils [12].

Hydrogen production via electrolysis is produced by both renewable (wind, solar) and nuclear options. The nuclear option will be explained in the next section.

Hydrogen is produced via electrolysis by passing a direct current between two electrodes in water. The water molecule is split in an electrolyzer cell, producing oxygen at the anode (positive electrode) and hydrogen at the cathode (negative electrode).

The following reactions take place in the electrolyser cell [12]:

In the electrolyte \( \text{H}_2\text{O} \rightarrow 2\text{H}^+ + 2\text{OH}^- \)

At the cathode \( 2\text{H}^+ + 2\text{e}^- \rightarrow \text{H}_2 \)

At the anode \( 2\text{OH}^- \rightarrow \frac{1}{2}\text{O}_2 + \text{H}_2\text{O} + 2\text{e}^- \)

Overall reaction \( \text{H}_2\text{O} \rightarrow \frac{1}{2}\text{O}_2 + \text{H}_2 \quad \Delta H_r = 285.6 \text{ kJ/mol} \)

Depending on the type of electrolyte, electrolyzers can be classified into two basic categories: alkaline-water electrolyte (liquid electrolyte using potassium hydroxide KOH) and solid-polymer electrolyte membrane (PEM). Both types work at low temperature.

The operating voltage, rate of hydrogen production, and capital costs are factors that influence the performance of electrolyzers [45].

**3.3.4.1 Alkaline Electrolyte**

Alkaline electrolyzers use an electrolyte composed of an aqueous solution of potassium hydroxide (KOH), as shown in Figure 20. In this system, the oxygen ions migrate
through the electrolytic material, leaving hydrogen gas dissolved in the water stream. This hydrogen is readily extracted from the water stream directed into a separating chamber [19].

The electrolyzer unit can be either unipolar (tank) or bipolar (filter press).

3.3.4.1.1 Unipolar Electrolyzer Unit

This unit has its anodes and cathodes alternatively suspended in a tank containing a 20%-30 % electrolyte (KOH) solution. The cell electrodes are connected in parallel. This design has the advantage that it is simple to manufacture and repair. Its disadvantage is that it operates at lower current densities and lower temperatures.

Figure 21 shows the design of the unipolar electrolysis unit.
3.3.4.1.2 Bipolar Electrolyzer Unit

The bipolar unit is similar to a filter press. Its cells are connected in series. The advantages of this design are that it reduces the stack footprint, produces a higher current density, and has the ability to produce higher-pressure gas. Its disadvantage is that it cannot be repaired without servicing the entire stack [45].

Figure 22 shows the design used for bipolar electrolysis units.
3.3.4.2 Polymer Electrolyte Membrane (PEM) Electrolyzer

The PEM electrolyzer uses a solid ion-conducting membrane. Water is introduced into the PEM electrolyzer cell and hydrogen ions are drawn through the membrane where they recombine with electrons to form hydrogen atoms. Oxygen gas remains behind in the water. Hydrogen gas is separately channeled from the cell stack and captured [45].

3.3.5 Thermochemical and Other Advance Processes

Hydrogen can be produced through thermochemical, electrochemical, and/or hybrid processes using nuclear energy as the primary energy source, as shown in Figure 23.

The nuclear energy hydrogen production can be accomplished using the following process [46]

- A Water Electrolysis process using electricity generated by the nuclear plant
- High-temperature steam electrolysis or hybrid processes using high-temperature heat and electricity from the nuclear plant
- Thermochemical processes using heat from the nuclear plant
Figure 23: Hydrogen and Nuclear Technologies (Source [46])

- SMR: Steam Methane Reforming
- S-I: Sulfur iodine
- UT-3: University of Tokyo 3 (Ca-Br-Fe thermochemical cycle)
- WSP: Westinghouse sulfur process
- Water ES: Water electrolysis
- HTSE: High temperature water electrolysis
- MHR: Modular helium reactor
- AHTR: Advanced high temperature reactor
- STAR: Secure transportable autonomous reactor
- GT-MHR: Gas turbine modular helium reactor
- SCWR: Super critical water reactor
- ALWR: Advantage high temperature reactor
In the future, nuclear energy might be an option for replacing fossil fuel in the transportation sector. Table 9 describes the nuclear-derived energy carriers for transportation, their conversion processes, and their present-day status.

According to [47], possible future roles of nuclear energy as a key supplier of electrical energy will be:

- To produce electricity through the implementation of **Plug-in Hybrid Electric Vehicles**, PHEV, also called the “Electrified Economy”;
- To support synthetic fuel production from natural gas, coal, biomass and water, called the “**Synthetic Fuel Economy**”, and
- To produce hydrogen through the use of fuel-cell-based vehicles, FCV, called the “**Hydrogen Economy**”.

**Table 9: Nuclear-derived Energy Carriers for Transportation (Source [47])**

<table>
<thead>
<tr>
<th>Primary Energy</th>
<th>Path/Energy Carrier</th>
<th>Status</th>
<th>Prospect</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nuclear Energy</td>
<td>Electricity</td>
<td>Nuclear Conversion Process</td>
<td>Commercialized</td>
</tr>
</tbody>
</table>
|                | Liquid Fuels        | Proposals/ Research Started | Engine, almost ready | FCV a few decades more | Intermediate Environmen
tal Compatibility |
|                | Hydrogen            | R&D in progress | FCV a few decades more | Long term broader uses |
3.3.5.1 Thermo-chemical Process:

Hydrogen can be produced, from hydrocarbon and water through thermo-chemical cycles that combine heat sources (thermo) with chemical reactions.

Such process can be more efficient than water electrolysis, for example, due to the excellent thermodynamic reactions occurring at elevated temperature, requiring less electric energy to produce a given amount of hydrogen.

Despite the fact that they are relatively new technology, thermo-chemical cycles are considered excellent candidates for hydrogen production. These processes, however, tend to present corrosion problems and can also generate greenhouse emissions.

Thermo-chemical processes for hydrogen production are [46]

- Nuclear Steam Methane Reforming (N-SMR)
- Sulfur Iodine (SI) cycle
- Ca-Br-Fe (UT-3) cycle
- Cu–Cl cycle

The following sections describe the processes mentioned above. In all these processes water is used along with high-temperature chemical reactions, with hydrogen and oxygen obtained as byproducts. The other components can be recycled.

3.3.5.1.1 Nuclear Steam Methane Reforming (N-SMR)

As mentioned above, the SMR process requires high temperatures throughout the natural gas burning. One option for producing such high temperatures is nuclear energy. The SMR can be coupled to the high-temperature helium-cooled reactor, and use the heat from the modular helium reactor to replace the natural-gas burning.
Some advantages of this process are: reduction of the CO$_2$ emissions to the atmosphere, achieving up to 80% efficiency, and elimination of a natural-gas furnace in the process that may reduce the CH$_4$ consumption by as much as 40% [19]. However, along with the improvements mentioned, SMR continues to produce problematic CO$_2$ emissions.

### 3.3.5.1.2 Sulfur Iodine (SI) Thermo-chemical Water Splitting

The SI cycle takes in water and high-temperature heat, and releases hydrogen and oxygen. To release hydrogen as a byproduct, the following three chemical reactions are necessary [12]:

1. \[ \text{I}_2 + \text{SO}_2 + 2\text{H}_2\text{O} \rightarrow 2\text{HI} + \text{H}_2\text{SO}_4 \quad (120^\circ \text{C}) \]  
2. \[ \text{H}_2\text{SO}_4 \rightarrow \text{SO}_2 + \text{H}_2\text{O} + \frac{1}{2} \text{O}_2 \quad (830-900^\circ \text{C}) \]  
3. \[ 2\text{HI} \rightarrow \text{I}_2 + \text{H}_2 \quad (300-450^\circ \text{C}) \]

1. In this cycle, iodine and sulfur dioxide are added to water, forming hydrogen iodide and sulfuric acid in an exothermic reaction.

2. The sulfuric acid will decompose at about 850°C, releasing the oxygen and recycling the sulfur-dioxide.

3. The hydrogen iodide will decompose at about 400°C, releasing the hydrogen and recycling the iodine.

The net reaction is the decomposition of water into hydrogen and oxygen.
3.3.5.1.3 Calcium–Bromine-Iron Cycle (UT-3)

The acronyms of UT-3 refer to the University of Tokyo and Calcium–Bromine-Iron (Ca-Br-Fe). It was first developed in 1978 by this university and is still in development.

This process presents the following advantages: easy gas-solid separation, circulation of gases only, and favorable thermodynamic reactions [46]. Energy efficiency is limited to only 40%.

UT-3 cycle process description is as follow [paper]:

\[
\begin{align*}
\text{CaBr}_2 + \text{H}_2\text{O} & \rightarrow \text{CaO} + 2\text{HBr} \quad (730 \, ^\circ\text{C}), \\
\text{CaO} + \text{Br}_2 & \rightarrow \text{CaBr}_2 + 1/2\text{O}_2 \quad (550 \, ^\circ\text{C}), \\
\text{Fe}_3\text{O}_4 + 8\text{HBr} & \rightarrow 3\text{FeBr}_2 + 4\text{H}_2\text{O} + \text{Br}_2 \quad (220 \, ^\circ\text{C}), \\
3\text{FeBr}_2 + 4\text{H}_2\text{O} & \rightarrow \text{Fe}_3\text{O}_4 + 6\text{HBr} + \text{H}_2 \quad (650 \, ^\circ\text{C}).
\end{align*}
\]

3.3.5.1.4 Cu–Cl Cycle

This cycle is being developed by the Argonne National Laboratory (ANL) Chemical Engineering Division. It offers the following advantages: moderate temperature (around 500
°C), inexpensive chemicals, reduced complexity, high energy efficiency (40-45%) and, if proven, moderate corrosion issues at 500 °C compared to SI and UT-3 [46] and [19] processes.

There are three main reactions as described in [12]

\[ 2\text{CuCl}_2 \cdot \text{nH}_2\text{O} + 2\text{HCl} \cdot \text{mH}_2\text{O} \rightarrow 2\text{CuCl}_2 \cdot (\text{n + m})\text{H}_2\text{O} + \text{H}_2 \text{, electrolysis (25–80°C)} \]
\[ 2\text{CuCl}_2 + \text{H}_2\text{O} \rightarrow \text{CuCl}_2 \cdot \text{CuO} + 2\text{HCL} \text{, hydrolysis (310–375°C)} \]
\[ \text{CuCl}_2 \cdot \text{CuO} \rightarrow 2\text{CuCl} + \frac{1}{2} \text{O}_2 \text{, decomposition (450–530°C)} \]

3.3.5.2 Electromechanical Processes

This process can be used for hydrogen production through an electrolysis process using a nuclear reactor to provide electricity as input.

The electromechanical processes for hydrogen production using nuclear energy are:

- Water Electrolysis using a Light-Water Reactor (LWR)
- High-Temperature steam electrolysis (HTSE)

3.3.5.2.1. Water Electrolysis by Light-Water Reactor (LWR)

The Light-Water Reactor is the most commonly-used type of nuclear technology in the world, constituting about 80 percent worldwide of the nearly 440 operating plants [19].

The LWR is a type of thermal reactor that uses normal water as its coolant and neutron moderator [48]. This process is the least energy-efficient, around 33%, but it does not emit greenhouse emissions.

A new version of LWR has been in development during the past few years. The Advances Light-Water Reactor (ALWR) is one of these. Even though is still in the research and development stage, it has potential to offer higher efficiency and lower cost.
3.3.5.2.2 High-Temperature Steam Electrolysis (HTSE)

The high-temperature steam electrolysis process shown in Figure 25 is one of the most promising technologies for hydrogen production. HTSE uses steam electrolysis at high temperatures. The motivations that suggest use of this process is that it provides a clean pathway and can possibly increase the efficiency of hydrogen production from water to 50% or higher. It also doesn’t present the corrosion problem that it faced by the thermochemical process because the materials of the HTSE cell can be made of ceramic material to avoid this problem.

Figure 25: Nuclear Hydrogen Plant Using High Temperature Electrolysis (Source [49])

The thermal energy to provide power and the heat the steam for the electrolysis process is provided by the reactor, a High Temperature Gas-cooled Reactor, HTGR. The high-temperature heat exchanger supplies superheated steam to the cells [49] at about 850ºC, and at a pressure of 5 Mpa (725 psi)
The Idaho National Laboratory is leading a research effort in using nuclear energy for high-temperature electrolysis through use of solid-oxide cells for the production of hydrogen. These cells have been used for power production by combining hydrogen and oxygen to produce water while liberating heat and electricity. Conversely, such cells can achieve water-splitting to produce separate streams of hydrogen and oxygen while consuming electrical power and heat [46].

This process can be explained with the help of Figure 26:

- Here, the total energy required (ΔH), for water and steam decomposition, is the sum of required thermal energy, (Q_es), and electrical energy demand (ΔG).
- It can be seen that electrical energy demand decreases with increasing temperature, while the total energy increases slightly with temperature.
- Higher efficiency can be obtained through the decrease in electrical demand.

![Figure 26: Energy vs. Temperature in a High Temperature Electrolysis Process (Source [46])](image-url)
Thermodynamically, operation at high temperature reduces the electrical energy requirement for electrolysis and also increases the thermal efficiency of the power-generating cycle [46]. The electric energy consumption of the electrolysis process is a significant contributor to the price of hydrogen production. For example, hydrogen production from Central-Wind Electricity consumes 57.09 kWh/Kg H₂.

Table 10 summaries the options for nuclear hydrogen production mention above [46].
### Table 10: Nuclear Hydrogen Production Process (Source [46])

<table>
<thead>
<tr>
<th>Feature</th>
<th>Electrochemical</th>
<th>Thermochemical</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Water electrolys</td>
<td>High-temperature steam electrolysis</td>
</tr>
<tr>
<td>Required temperature, (°C)</td>
<td>&lt;100, at Patm</td>
<td>&gt;500, at Patm</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Efficiency of the process (%)</td>
<td>85–90 (at T &gt;800 °C)</td>
<td>90–95</td>
</tr>
<tr>
<td>Energy efficiency coupled to LWR, or ALWR%</td>
<td>~ 27</td>
<td>~ 30</td>
</tr>
<tr>
<td>Energy efficiency coupled to MHR, ALWR, ATHR, or S-AGR (%)</td>
<td>&gt;35</td>
<td>&gt;45, depending on power cycle and temperature</td>
</tr>
<tr>
<td>Advantage</td>
<td>Proven technology</td>
<td>• High efficiency • Can be coupled to reactors operating at intermediate temperatures • Eliminates CO2 emissions</td>
</tr>
<tr>
<td>Disadvantage</td>
<td>Low energy efficiency</td>
<td>• Requires development of durable, large-scale HTSE units</td>
</tr>
</tbody>
</table>
3.3.6 Biomass to Hydrogen

Biomass is the oldest form of energy used by humans. This renewable energy resource can be directly used by burning it or can be converted to other forms of energy like ethanol and biodiesel, for example.

Biomass has the potential to produce hydrogen in a sustainable and environmentally-friendly way. Hydrogen production from biomass is considered to be a sustainable option for the near- and mid-term future according to [44]. Among the reasons that support its implementation are abundance, cleanliness, and renewability.

Biomass resources can be divided into the following categories: Energy crops, Agricultural residues, Wood waste, Municipal Solid Waste (MSW), Landfill gas, and Livestock Manure [50].

Currently, the production of hydrogen from biomass can be divided into thermochemical and biological [51] categories, as shown in Figure 27 and Table 11.

![Figure 27: Pathways from Biomass to Hydrogen (Source [51])](image)
Table 11: Shows the advantages and disadvantages of the two main categories shows above (Source [51])

<table>
<thead>
<tr>
<th>Process</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermochemical</td>
<td>• Overall Efficiency (thermal to hydrogen) is higher (n~52%)</td>
<td>• The decomposition of biomass lead to char and tar formation</td>
</tr>
<tr>
<td></td>
<td>• Production Cost is lower</td>
<td></td>
</tr>
<tr>
<td>Biological</td>
<td>• More environmental friendly process</td>
<td>• H2 production using this process has limitations, one of which is the low hydrogen yields</td>
</tr>
<tr>
<td></td>
<td>• Less energy-intensive</td>
<td></td>
</tr>
</tbody>
</table>

3.3.6.1 Thermo-chemical Processes

The thermochemical conversion processes for hydrogen production can be classified as follows: Combustion, liquefaction, pyrolysis, and gasification [52].

The combustion process burns the biomass in air to convert it into heat, mechanical power, or electricity. This process produces low energy efficiency and pollutant emissions. However, it is the most-used process due to its low cost and high reliability [53].

In the liquefaction process, the biomass is converted into an oily liquid by combining the biomass with water at elevated temperatures (300-350°C) under a pressure of (12-20 MPa) in the absence of air, with a catalyst added in the process.

Based on [52] a low hydrogen production can be obtained by the liquefaction process. However, up to the present time, more attention has been given to the production of hydrogen through the gasification and pyrolysis processes.
3.3.6.1.1 Hydrogen from Biomass via Gasification

This process consists of applying heat under pressure to the biomass in the presence of steam and a controlled amount of oxygen, thereby converting it into a gaseous mixture of hydrogen, carbon monoxide, carbon dioxide, and other compounds [54]. The gasification process used for hydrogen production from biomass is similar to the partial-oxidation process explained in Section 3.2, with minor substitutions. Gasification is a combination of pyrolysis and combustion processes.

This conversion process can be expressed as:

\[ \text{Biomass} + \text{Heat} + \text{Steam} \rightarrow \text{H}_2 + \text{CO} + \text{CO}_2 + \text{CH}_4 + \text{light and heavy hydrocarbons} + \text{char}. \]

The principal disadvantages of the process are the char and tar formation. Figure 28 shows a diagram of a centralized hydrogen production from biomass gasification system.

**Centralized Hydrogen Production from Biomass Gasification**

![Diagram of centralized hydrogen production from biomass gasification](image)

*Figure 28: Centralized Hydrogen Production from Biomass Gasification (Source [55])*
This process has been selected as a near-term commercial application of hydrogen production from biomass due to its similarity to coal gasification [54].

### 3.3.6.1.2 Hydrogen from biomass via Pyrolysis

According to [54] this process consists of heating the biomass to 500 °C in the absence of air to convert it into liquid, solid, and gaseous fractions. This conversion process can be expressed as follows:

\[
\text{Biomass} + \text{Heat} \rightarrow \text{H}_2 + \text{CO} + \text{CH}_4 + \text{other products}
\]

Pyrolysis reaction is an endothermic reaction. It can be classified into two sub-processes: slow pyrolysis and fast pyrolysis. Slow pyrolysis is not commonly used for hydrogen production due to its charcoal production.

The fast pyrolysis process, on the other hand, uses a high temperature (around 800 to 900 °C) to which the biomass is heated rapidly in the absence of air to form vapor, followed by subsequent condensation to a dark brown bio-liquid [54].

The advantage of this process is that leaves a residual of as little as 10% of the solid char materials and converts up to 60% into gas-rich hydrogen and carbon monoxides. For that reason, this process is an excellent competitor compared to conventional gasification methods, even though it is in early stage of development [54].

### 3.3.6.2 Biological Hydrogen Production (BioH$_2$)

The biological process is another method for biomass-based hydrogen production. Hydrogen is produced through the use of natural biological processes used to convert and store energy produced by sunlight [35]. These processes are considered to be carbon-neutral and renewable energy resource for hydrogen production for the long-term future.
BioH₂ for hydrogen production can be classified into the following groups: Photosynthesis, Fermentation, and Microbial electrolysis cells. Table 12 describes the challenges and advantages associated with these processes [56]

**Table 12: Challenges and Advantages of Biological Hydrogen Production Processes**

(Source [56])

<table>
<thead>
<tr>
<th>Process</th>
<th>Characteristics</th>
<th>Challenges</th>
<th>Advantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Photosynthesis</td>
<td>This process use sunlight and specialized microorganisms such as green algae and cyanobacteria to split water and produce hydrogen. Due to its natural metabolic processes these microbes consume water and produce hydrogen as a byproduct.</td>
<td>The oxygen produced along with the hydrogen tends to accumulate and impede the work of the hydrogen-evolving enzymes, this being a key challenge for this process.</td>
<td>The net reaction of the process and the energy provided by sunlight are the two attractive properties for hydrogen production due to that does not involve any carbon byproducts.</td>
</tr>
<tr>
<td>Fermentation</td>
<td>This process uses bacteria that can act on organic material and decompose it into hydrogen and other byproducts without the aid of sunlight.</td>
<td>The greatest challenge for fermentative BioH₂ is that the H₂ yield is low.</td>
<td>The advantage of dark fermentation is that the H₂ production rate (H₂ volume/reactor volume-time) can be orders of magnitude larger.</td>
</tr>
<tr>
<td>Microbial electrolysis cells</td>
<td>The process combines bacterial metabolism with electrochemistry to achieve H₂ production. As the bacteria decompose the organic materials, they produce a low voltage at the anode. Hydrogen is produced at the fully submerged cathode with the input of just a tiny amount of additional energy.</td>
<td>The main challenge of this process is the requirement for an external energy supply to increase the energy of the generated electrons.</td>
<td>It can give high H₂ yields, as H₂ - capture efficiencies ranged from (67 to 91%) from diverse donor substrates (e.g. cellulose, glucose, butyrate, lactate, propionate, ethanol or acetate).</td>
</tr>
</tbody>
</table>
Even though the biomass is an excellent candidate for hydrogen production due to its sustainability and environmental-friendliness, at the present time no commercial plants exist to produce hydrogen from biomass.

**3.4 Hydrogen Production Technology Overview**

The sections above explained the details of the technologies for hydrogen production both in use and under development. Hydrogen production technologies must overcome present challenges in order to produce a sustainable energy solution for the future.

This section summarizes the principal technologies for hydrogen production, challenges, and benefits, and a time frame for their implementation as is indicated in Table 13.
<table>
<thead>
<tr>
<th>Technology</th>
<th>Challenges</th>
<th>Benefits</th>
<th>Time Frame</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distributed Natural Gas Reforming</td>
<td>• Improve reforming efficiency</td>
<td>• Lowest cost for hydrogen production</td>
<td>Near-to-mid-</td>
</tr>
<tr>
<td></td>
<td>• High capital and operation cost</td>
<td>• Natural gas infrastructure is in place</td>
<td>term</td>
</tr>
<tr>
<td></td>
<td>• Reduce carbon sequestration cost</td>
<td>• Key technology for begin hydrogen market</td>
<td></td>
</tr>
<tr>
<td>Coal and Biomass Gasification Plant</td>
<td>• Feedstock impurities</td>
<td>• Provides low-cost synthetic fuel in addition to hydrogen</td>
<td>Near-to-mid-</td>
</tr>
<tr>
<td></td>
<td>• System efficiency</td>
<td>• Uses abundant and affordable coal feedstock</td>
<td>long-term</td>
</tr>
<tr>
<td></td>
<td>• Reduce cost for carbon capture and storage</td>
<td>• Produce more H₂ from synthesis gas at a lower cost</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Produce more H₂ from synthesis gas at a lower</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Electrolysis Process</td>
<td>cost</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Low system efficiency and high capital costs</td>
<td>• Zero or near to zero GHG emissions is result from hydrogen production</td>
<td>Long-Term</td>
</tr>
<tr>
<td></td>
<td>• Integration with renewable energy sources</td>
<td>from hydrogen production from electrolysis process,</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Balance storage and production rate capacity</td>
<td>depending the electricity source used</td>
<td></td>
</tr>
<tr>
<td></td>
<td>for variable demand</td>
<td>• Use existing infrastructure</td>
<td></td>
</tr>
<tr>
<td>Thermochemical Process</td>
<td>• Cost-effective reactor</td>
<td>• Produces hydrogen using only water, energy from nuclear reactors,</td>
<td>Long-Term</td>
</tr>
<tr>
<td></td>
<td>• Develop efficient heat transfer for chemical</td>
<td>• Clean and sustainable</td>
<td></td>
</tr>
<tr>
<td></td>
<td>cycle</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Identify appropriate materials for construction for these high-temperature operations</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
According to [35] hydrogen cost, competitiveness, and time to market will be affected by both the location and the scale of the technology.

The scale of production of hydrogen can be classified into Distributed and Central types, as shown in Figure 29.

- **Distributed Production:** These types of technologies produce hydrogen on-site at the refueling station. They will be used in the early stages of hydrogen introduction with closely available feedstock. This technology could help to reduce the “chicken and egg” problem of the hydrogen. It could reduce the initial infrastructure costs and lead to lower infrastructure-transition costs.

- **Central Production:** These plants will be used to satisfy high demand for hydrogen. It will offer lower cost once the scale is realized, resulting in a transition from distributed to centralized production. These plants require an efficient and low-cost delivery infrastructure [35].
Figure 29: Timeframe to Market Distributed and Central Production Plants (Source [35])
CHAPTER 4. HYDROGEN DELIVERY, STORAGE AND FUELING INFRASTRUCTURE

4.1 Overview

To succeed as an alternative fuel of the future, hydrogen must overcome present-day technical and commercial challenges. There is, for example, no infrastructure system like those that exist for electricity, natural gas, or gasoline for delivering hydrogen to consumers.

The famous “chicken and egg” problem is one of the major challenges that it is facing the hydrogen pathways. Due to the lack of adequate fueling options, consumers will be unwilling to purchase hydrogen-fueled vehicles and, conversely, fueling infrastructure is unlikely to develop until a sufficient number of such vehicles are in use.

This chapter discusses the delivery and refueling infrastructure needed to transport hydrogen from the production plant (central or distributed) to the refueling station, and today’s available storage methods.

4.2 Hydrogen Delivery Systems

A delivery system is an essential component of the H₂ infrastructure, and is one of the principal contributors to the cost, emissions, and energy use related to the hydrogen pathway [57].

Hydrogen can be delivered via three main methods: compressed gaseous hydrogen by truck, liquid hydrogen by truck, and gaseous hydrogen by pipeline.

To deliver hydrogen two physical approaches, compression and liquefaction, can be used. Both methods are widely-used at the present time. Both have the objective of
increasing the volumetric energy density of hydrogen to achieve energy densities consistent with economic transport.

- **Liquefaction**: Liquefaction is accomplished by cooling H\(_2\) to below 20K (-253ºC) to form a liquid. It is a multi-stage process using a series of refrigerants and compression/expansion loops to produce the necessary extreme cold. It presents the advantage of high energy density but at a very high capital cost. It requires use of 1/3 of the energy in the hydrogen itself. This process is employed only in small plants by merchant hydrogen vendors [58] and [59].

- **Compression**: Compression of hydrogen is less energy intensive than liquefaction. It is a process that can be accomplished at small scales (on the order of a few kg/day) all the way up to very large scales (hundreds of tons per day). In this process, mechanical compressors are used to raise the pressure of a fixed quantity of gas, often delivering it into a high pressure storage device. Compressors require expensive materials to prevent hydrogen embrittlement and the associated risk of part failures during use [58].

According to [57] the selection of the lowest-cost of hydrogen delivery will depend on the attributes of geography and market characteristics, including population and radius, population density, size and number of refueling stations, and market penetration of fuel-cell vehicles. This study also analyzed two types of delivery models with an objective of identifying low-cost options for H\(_2\) delivery. The two types of delivery models considered were:

- **Hydrogen Transmission Model**: H\(_2\) is transported from one point to another under control of two parameters: flow rate (tons/day) and transport distance (km).
The model includes compressors or liquefiers at the hydrogen plant, and truck or pipeline methods for delivery.

- **Hydrogen Distribution Model**: This model includes the refueling-station network as along with compressors or liquefiers at the hydrogen plant and trucks and pipelines for delivery. The distribution distances, dependent in the population density of the city, the physical size (City Radius, km), and the size and the number of required refueling station were also considered.

**4.2.1 Delivery of Compressed Hydrogen**

The delivery of hydrogen in compressed gas tanks (tube trailer) is commonly used for industrial purposes. Figure 30 shows possible compressed hydrogen delivery pathways.

For transport $\text{H}_2$ gas by truck, a very high pressure is needed to maximize tank capacities. This method is used over short distances for relatively small volumes (~300 kg) of hydrogen. It is not feasible for large volumes and longer distance. Moreover, it requires a high-pressure interface for the vehicle fuelling application.

However, tube trailers can be used as storage systems at refueling stations, reducing the cost of storage. This also reduces the energy required to move hydrogen from one pressurized vessel to another [59].
As mentioned above, the hydrogen delivery method is a significant contributor to the cost, toxic emissions, and energy used in the entire cycle.

For delivery of compressed hydrogen by tube trailer, the principal factors that determine the delivery cost are the capital costs of the truck cabs and tube trailers, the driving distances, the driver labor, and diesel truck operation and maintenance, as presented in Table 14 [59].
Table 14: Compressed Gas Truck Delivery System Characteristics (Source [59])

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Truck Capacity</td>
<td>300 kg H₂</td>
</tr>
<tr>
<td>Truck P (max)</td>
<td>2350 psia</td>
</tr>
<tr>
<td>Truck P (min)</td>
<td>440 psia</td>
</tr>
<tr>
<td>Tube Trailer Cost</td>
<td>$150,000</td>
</tr>
<tr>
<td>Cab Cost</td>
<td>$90,000</td>
</tr>
<tr>
<td>Undercarriage Cost</td>
<td>$60,000</td>
</tr>
</tbody>
</table>

Also, this delivery method contributes to emission of a significant amount of CO₂ due to use of diesel fuel in the transport trucks.

4.2.2 Delivery of Liquid Hydrogen

The volume density of hydrogen is increased by truck delivery of liquid hydrogen. Figure 31 shows Liquid Hydrogen Delivery Pathways. This method of delivery is used for large volumes and medium to long distances. For example, it enables a single truck to carry up to 10 times the volume of an equivalent gaseous tube trailer (up to 4000 kg for liquid, compared with 300 kg for gaseous) [59].
Also, liquid hydrogen by truck is favored when gaseous pipeline cost is prohibitive. Using this method, a high-purity form of hydrogen can be used.

Nevertheless, according to [59], more energy is required to liquefy the hydrogen. This method consumes more than 30% of the energy content of the hydrogen and is therefore expensive. The study by [61] found that the value varies between 8-12.7 kWh/ kg H\textsubscript{2} for the electric energy needed for liquefy H\textsubscript{2}.

Many of the emissions associated with this method are due to source of electricity used to power the liquefaction process. Liquefaction can contribute up to 6.8 kg CO\textsubscript{2} / kg H\textsubscript{2},
i.e., approximately 50% of the CO$_2$ produced by an equivalent amount (on an energy basis) of gasoline, Table 15 shows the liquid H$_2$ truck capacity and cost.

### Table 15: Liquid Hydrogen Delivery System Characteristics (Source [59])

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Truck Capacity</strong></td>
<td>4000 kg H$_2$</td>
</tr>
<tr>
<td><strong>Liquid H$_2$ boil off</strong></td>
<td>0.3% / day</td>
</tr>
<tr>
<td><strong>Liquid H$_2$ tank cost</strong></td>
<td>$650,000</td>
</tr>
<tr>
<td><strong>Cab cost</strong></td>
<td>$90,000</td>
</tr>
<tr>
<td><strong>Undercarriage cost</strong></td>
<td>$60,000</td>
</tr>
</tbody>
</table>

#### 4.2.3 Gaseous Hydrogen by Pipeline

The merchant hydrogen producers are the owners of the 700 miles of hydrogen pipeline presently operating in the United State. These pipelines are needed where large amounts of hydrogen are required as, for example, in petroleum refineries and chemical plants [62].

This delivery method makes sense only if there is widespread use of hydrogen in fuel-cell vehicles. The principal reason for reluctance to commit is the high capital cost for new pipeline systems, even though is the lowest-cost option for delivering large volume of hydrogen once a pipeline is in place. Figure 32 shows the pipeline-delivery options proposed by [60].
Using existing natural gas infrastructure, an option currently being analyzed, can be an option for expanding the hydrogen delivery infrastructure.

The uncertainty related to the cost of a hydrogen pipeline is nevertheless significant compared to that for natural gas; Table 16 shows a list of pipeline cost equations for hydrogen delivery. The cost of special material (high quality hydrogen-certified steel) needed for the $\text{H}_2$ pipeline infrastructure is a main factor contributing to reluctance to commit. According to [59] costs are projected to be between 0-80% more than those of natural gas.
pipeline due to this expensive material and higher labor costs in joining the pipes is also anticipated.

Table 16: Pipelines Cost Equations for Hydrogen (Source [59])

<table>
<thead>
<tr>
<th>Source</th>
<th>Equation</th>
<th>Units</th>
<th>Notes</th>
<th>Life</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parker</td>
<td>([674D^2 + 11,754D +234,085]L + 405,000)</td>
<td>$</td>
<td>D[in], L[mi]</td>
<td>---</td>
</tr>
<tr>
<td>Yang and Ogden – rural</td>
<td>$1869(D)^2 + $300,000</td>
<td>$/km</td>
<td>D[in]</td>
<td>15 yrs</td>
</tr>
<tr>
<td>Yang and Ogden - urban</td>
<td>$1869(D)^2 + $600,000</td>
<td>$/km</td>
<td>D[in]</td>
<td>15 yrs</td>
</tr>
<tr>
<td>NAS transmission – current</td>
<td>$600,000</td>
<td>$/km</td>
<td>---</td>
<td>15.9%</td>
</tr>
<tr>
<td>NAS transmission – future</td>
<td>$450,000</td>
<td>$/km</td>
<td>---</td>
<td>15.9%</td>
</tr>
<tr>
<td>H2A transmission</td>
<td>$467,252</td>
<td>$/km</td>
<td>---</td>
<td>20 yrs</td>
</tr>
<tr>
<td>H2A distribution</td>
<td>$317,603</td>
<td>$/km</td>
<td>---</td>
<td>20 yrs</td>
</tr>
</tbody>
</table>

1Lifetime not specified, only equipment capital charge

4.2.4 Hydrogen Delivery by Rail

The delivery of hydrogen by rail is perhaps the most economical option for hydrogen production from renewable energy resources. This option is an excellent candidate for both long distance and high demand for hydrogen. This approach also offers higher load-carrying capacities and higher weight limits than those for over-the-road trailers [63].
According to [63], at present there is insufficient hydrogen transport by rail. The reasons given are a lack of timely scheduling and transport to avoid excessive hydrogen boil-off, and a lack of cryogenic rail cars capable of handling liquid hydrogen.

Figure 33 gives an analysis of Hydrogen rail-delivery pathways.

![Figure 33: Hydrogen Rail Delivery Pathways (Source [63])](image)

**4.3 Hydrogen Fueling Stations**

The fueling station is a vital component of the hydrogen economy, since it is the place where the end users and their vehicles will interface with the infrastructure. Hydrogen stations will usually be located along roads or highways, both in rural and urban areas.

The introduction of these stations will benefit from conventional gasoline stations already in place. For example, whether hydrogen stations will experience seasonal demands similar to those of gasoline station should be analyzed [60].
However, the fueling stations are components that must be carefully evaluated. For instance, due to the differing methods for hydrogen production, (onsite vs. centralized production) and delivery (compressed H$_2$ via truck delivery, liquid H$_2$ via truck delivery and compressed H$_2$ via pipeline delivery) the fueling station, unlike gasoline station, will need to adapt to a variety of new conditions [64].

Therefore, based on [5], evolution of several different types of fueling station, including a Compressed Hydrogen Station, a Liquid Hydrogen Station, a Pipeline Hydrogen Station, and a Mobile Hydrogen Station, is likely: Table 17 presents an overview of the station types.
Table 17: Hydrogen Fueling Stations Overview (Source [59])

<table>
<thead>
<tr>
<th>Station Type</th>
<th>Systems Diagram</th>
<th>Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compressed Hydrogen Station</td>
<td><img src="Image" alt="Compressed Hydrogen Station Diagram" /></td>
<td>• Takes advantages of the tube trailer in order to store the hydrogen. It can reduce the cost and energy use.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Two arrangements can be made: cascade and booster:</td>
</tr>
<tr>
<td></td>
<td></td>
<td>o <strong>Cascade</strong>: Divide the storage volume into multiple banks to sequentially fill the FCV.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Requires high compression energy</td>
</tr>
<tr>
<td></td>
<td></td>
<td>o <strong>Booster</strong>: Stores a larger volume of H$_2$ at an intermediate pressure. Less energy is required, but more compressors are needed.</td>
</tr>
<tr>
<td>Liquid Hydrogen Station</td>
<td><img src="Image" alt="Liquid Hydrogen Station Diagram" /></td>
<td>• The station has the possibility of dispensing either liquid or compressed hydrogen. Even though is not ideal from an energy-use perspective, it can reduce costs for delivery and storage.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Key components: storage tank, cryogenic hydrogen pump and vaporizer. The last unit can conserve energy by pumping the liquid up to pressure before vaporizing rather than compressing a gas.</td>
</tr>
<tr>
<td>Pipeline Hydrogen Station</td>
<td><img src="Image" alt="Pipeline Hydrogen Station Diagram" /></td>
<td>• The station consists of a gas meter, hydrogen compressor to increase pipeline pressures (typically below 1000 psi) to storage pressure (above 6000 psi), hydrogen storage tanks, and dispensers.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• The pipeline network improves the cost of H$_2$ for existing and additional station.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Stations built near an existing hydrogen pipeline have the advantage of a reliable low-cost source of hydrogen and eliminate the need for on-site production truck delivery.</td>
</tr>
<tr>
<td>Mobile Hydrogen Station</td>
<td><img src="Image" alt="Mobile Hydrogen Station Diagram" /></td>
<td>• This is the simplest type of station. It consists only of high-pressure gaseous hydrogen storage and dispenser.</td>
</tr>
</tbody>
</table>
The fueling station represents one of the major obstacles for the hydrogen economy. According to [65] the 'chicken and egg' problem will be difficult to overcome. “Who will invest in the manufacture of fuel cell vehicles if there is no widespread hydrogen supply?”

In order to address the “chicken and egg” problem facing the hydrogen economy, the National Renewable Energy Laboratory (NREL), in collaboration with the Department of Energy (DOE), has analyzed the minimum infrastructure that could support the introduction of hydrogen-fueling station in its paper titled “Analysis of Hydrogen Infrastructure needed to enable Commercial Introduction of Hydrogen Fueled Vehicles” [66].

The study was able to determine the location and number of possible hydrogen stations nationwide that would make hydrogen fueling feasible. Figure 34 shows Proposed Hydrogen Fueling Stations along Major Interstates. Population densities and traffic volumes (vehicles per day) were identified throughout the U.S. interstate system.
Figure 34: Proposed Hydrogen Fueling Stations in the U.S. (Source [66])

The study used a standard station configuration and cost for the analysis presented in [66]. Table 18 displays the Standard Station configurations and their construction costs.
Table 18: Standard Stations Configurations and Costs (Source [66])

<table>
<thead>
<tr>
<th>Station Type</th>
<th>Cost per Station</th>
<th>Abbreviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steam Methane Reformer, 100 kg/day</td>
<td>$1,052,921</td>
<td>SMR100</td>
</tr>
<tr>
<td>Steam Methane Reformer, 1,000 kg/day</td>
<td>$5,078,145</td>
<td>SMR1000</td>
</tr>
<tr>
<td>Electrolyzer, grid, 30 kg/day</td>
<td>$555,863</td>
<td>EL30G</td>
</tr>
<tr>
<td>Electrolyzer, grid, 100 kg/day</td>
<td>$945,703</td>
<td>EL100G</td>
</tr>
<tr>
<td>Electrolyzer, renewable, 30 kg/day</td>
<td>$667,402</td>
<td>ER30R</td>
</tr>
<tr>
<td>Mobile Refueler, 10 kg/day</td>
<td>$248,897</td>
<td>MR10</td>
</tr>
<tr>
<td>Delivered Liquid Hydrogen, 1,000 kg/day</td>
<td>$2,617,395</td>
<td>DLH21000</td>
</tr>
<tr>
<td>Pipeline Station, 100 kg/day</td>
<td>$578,678</td>
<td>PIPE</td>
</tr>
</tbody>
</table>

The study concluded that, based on aggressive penetration of 1% by fuel-cell vehicles in 2020, and the information above, approximately 284 stations, with a total cost of $837 million, were required to begin the transition to a national hydrogen-fueling infrastructure.

4.4 Hydrogen Storage

Hydrogen can be stored in different manners, each presenting specific advantages and disadvantages. Energy density, volume, efficiency, and safety are the main factors to be considered in contemplating hydrogen storage [61].

The methods via which hydrogen can be stored are: as a compressed gas, as a liquid, or chemically combined into a metal hydride. Underground storage is still another option for hydrogen storage, even though it is just a special case of compressed gas.

Hydrogen storage will be needed to meet the time-varying demand for fuel [60] similarly to today’s needs for natural gas and gasoline storage.
4.4.1 Compressed Hydrogen

High-pressure tanks are needed to store compressed gaseous hydrogen (CGH\(_2\)). Due to the low energy density of compressed hydrogen, the storage volume per unit of energy is high, resulting in higher capital and operating costs.

According to [61], 4-15% of the stored hydrogen energy content is needed to accomplish compression.

Cost, volume, and weight constraints are key factors that will determine the storage pressure and tank materials [59].

4.4.2 Liquid Hydrogen

Liquid hydrogen (LH\(_2\)) is stored in cryogenic vessels. To reach a full liquid state, LH\(_2\) must be cooled to below −252.87°C. Liquid-hydrogen storage presents losses due to liquid boil-off. At its boiling point any heat transfer to liquid causes some hydrogen evaporation, the major disadvantage of this method. This method results in a net loss of about 30% of the hydrogen energy content.

Liquid hydrogen storage is the most expensive storage method.

4.4.3 Metal Hydrides

Metal hydride systems can either be low temperature (-150 °C) or high temperature (300 °C). Either method is absent of safety concerns such as leakage that can be a problem with compressed hydrogen and LH\(_2\). This method is therefore one of the safest methods for storing hydrogen.
According to [67] the total hydrogen absorbed is around 1-2% of the total weight of the storage medium. The disadvantage of this method is that the considerable inert mass of metal must be installed or even moved around.
CHAPTER 5. END USE TECHNOLOGIES

5.1 Introduction

The need for use of more sustainable energy systems to reduce dependence on imported petroleum and replace high-carbon-emitting energy sources is one of the major efforts that the United State is conducting at the present time.

The U.S is facing paramount problems that relate to energy security and climate change. The transportation sector, for example, accounts for 28% of U.S. energy needs and is responsible for serious problems with respect to air pollution, global warming, and rapid depletion of the earth’s petroleum resources [68].

Due these problems, spokesmen for the transportation sector have called for the development of more cleaner, higher-efficiency, and safer systems to replace conventional vehicles in the near future.

Electric vehicles, hybrid electric, and fuel-cell vehicles are among candidates being proposed as alternatives for replacing conventional vehicles.

This chapter gives an introduction to fuel-cell technologies describes the various types of fuel cells, and presents discussion of various onboard storage systems.

5.2 Hydrogen Fuel Cell

Hydrogen is an energy carrier that can be used for power generation and industrial applications, commercial, residential, and transportation sector applications, Figure 35 shows the various hydrogen applications areas.

Presently, much attention is being addressed to the use of hydrogen in the transportation sector through deployment of fuel-cell vehicles.
It is important to note that hydrogen-based systems can be used for the production of electricity. For example, they could be used as backups for grid power in situations where the primary resource is remotely located or where the availability of the resource doesn’t coincide with the demand, (intermittent renewable energy resources).

Significantly efforts are presently dedicated to the production of electricity from hydrogen through the use of stationary fuel-cell systems. Hydrogen is, however, also potentially viewed as a transportation fuel for fuel-cell vehicles because of possible climate-change benefits.

**Figure 35: Hydrogen Energy Application Areas (Source [12])**

Hydrogen fuel-cell vehicles have the advantage of offering high energy efficiency and much lower emissions than conventional internal combustion engines (ICE).
According to [69], due to improvements in efficiency, resource requirements, and environmental attributes, hydrogen and fuel cells are being considered as an excellent alternative to gasoline. For these reasons, hydrogen can potentially reduce our national dependence on foreign oil, greenhouse gas emissions, and urban air pollution.

However, the widespread use of fuel cell vehicles does present various challenges that must be overcome to be cost-competitive with both conventional and advanced vehicle technologies. The main challenges for fuel cells are cost and durability.

Fuel-cell vehicles are estimated to cost fivefold more than those with internal combustion engine. Also, fuel-cell systems must be as durable and reliable as conventional vehicles. As an example of the challenge, note that today’s fuel cell operates for less than half the life span of a conventional internal combustion engine [19].

### 5.2.1 Fuel Cell Operation

Electricity can be generated by using a fuel-cell device employing a fuel (hydrogen) and oxygen through an electrochemical process. A fuel cell having two electrodes, a cathode and an anode, connected by an electrolyte, is depicted in Figure 36 [70].

Hydrogen and oxygen flow to the anode and cathode, respectively, giving the following electrochemical reaction:

$$\text{H}_2 + \frac{1}{2} \text{O}_2 \rightarrow \text{H}_2\text{O}$$

In general, hydrogen atoms enter a fuel cell at the anode where a chemical reaction strips them of their electrons. The hydrogen atoms are thus ionized and carry a positive electrical charge. The negatively-charged electrons provide the current that travels through wires to do work.
On the other hand, oxygen enters the fuel cell at the cathode and, in some cell types, combines with electrons returning from the electrical circuit and hydrogen ions that have traveled through the electrolyte from the anode. In other cell types the oxygen picks up electrons and then travels through the electrolyte to the anode, where it combines with hydrogen ions.

A single fuel cell produces about 0.7 volts; many separate fuel cells can be combined to form a fuel cell stack. They can also be connected in parallel to produce higher current and in series to produce higher voltage.

According to [44] to speed up the reaction of both hydrogen and oxygen, the electrodes are covered with a precious metal catalyst (e.g., platinum).

Figure 36: Fuel Cell Operation (Source [70])
The advantage of the fuel-cell system is that, if hydrogen fuel is used, the only by-product emitted is water. A fuel cell is a quiet, clean source of energy. Fuel cells are similar to batteries. Both are composed of positive and negative electrodes with an intervening electrolyte. The difference between fuel cells and batteries is that, unlike in batteries, energy is not stored through recharging. Fuel cells obtain their energy from the hydrogen or similar fuel supplied to them [7].

5.2.2 Types of Fuel Cells

There are six different types of fuel cells: (1) proton-exchange membrane fuel cell (PEM), (2) alkaline fuel cell (AFC), (3) phosphoric-acid fuel cell (PAFC), (4) molten-carbonate fuel cell (MCFC), (5) solid-oxide fuel cell (SOFC), and (6) direct-methanol fuel cell (DMFC). They differ generally in their applications, operating temperatures, costs, electrolytes used, and the chemical reactions involved, as indicated in Table 19.
Table 19: Main Characteristics of Fuel Cells (Source [44])

<table>
<thead>
<tr>
<th>Type</th>
<th>Name</th>
<th>Electrolyte</th>
<th>Temperature Range (°C)</th>
<th>Power Range</th>
<th>Electric Efficiency (systems)</th>
<th>Start-up Time</th>
<th>Field of Applications</th>
</tr>
</thead>
<tbody>
<tr>
<td>PEM</td>
<td>Proton-exchange membrane fuel cell</td>
<td>Proton-conducting polymer membrane</td>
<td>50-80</td>
<td>Up to 250 kW</td>
<td>25–45%</td>
<td>Immediate</td>
<td>Road vehicles, stationary electricity generation, heat and electricity co-generation, submarine space travel</td>
</tr>
<tr>
<td>AFC</td>
<td>Alkaline fuel cell</td>
<td>30-50% KOH</td>
<td>60-90</td>
<td>7 kW</td>
<td>37–42%</td>
<td>Immediate</td>
<td>Space travel, Road Vehicles, submarines</td>
</tr>
<tr>
<td>PAFC</td>
<td>Phosphoric-acid fuel cell</td>
<td>Concentrated phosphoric acid</td>
<td>160-220</td>
<td>&gt;50 kW</td>
<td>37–42%</td>
<td>30 mins from hot standby</td>
<td>Stationary electricity generation, heat and electricity co-generation, road vehicles</td>
</tr>
<tr>
<td>MCFC</td>
<td>Molten carbonate fuel cell</td>
<td>Molten carbonate (Li₂CO₃, K₂CO₃)</td>
<td>620-660</td>
<td>&gt;1 MW</td>
<td>40–60%</td>
<td>Several hours after cold start</td>
<td>Stationary electricity generation, heat and electricity co-generation</td>
</tr>
<tr>
<td>SOFC</td>
<td>Solid-oxide fuel cell</td>
<td>Ion-conducting ceramic</td>
<td>800-1000</td>
<td>&gt;200 kW</td>
<td>44–50%</td>
<td>Several hours after cold start</td>
<td>Stationary electricity generation, heat and electricity co-generation</td>
</tr>
<tr>
<td>DMFC</td>
<td>Direct Methanol fuel cell</td>
<td>Proton-conducting polymer membrane</td>
<td>80-100</td>
<td>&lt;10 kW</td>
<td>15–30%</td>
<td>Immediate</td>
<td>Portable, mobile</td>
</tr>
</tbody>
</table>
A fuel cell can use any source of energy containing hydrogen, e.g., natural gas, coal gas, biogas, methanol etc. However, pure hydrogen and oxygen are required to achieve highest fuel-cell efficiencies.

According to [44], fuel cells can be divided into low and high temperature categories. The PEM (50-80 °C) and AFC (60-90 °C) work at low operating temperature compared to MCFC (620-660 °C) and SOFC (800-1000 °C) that work at high operating temperature. The low-temperature fuel cell can tolerate only relatively small amounts of impurity in contrast with higher-temperature fuel cells that don’t make the same purity demands.

As mentioned above, fuel cells can be used in different applications, with the automobile market considered the most promising area for the use of hydrogen and fuel cells.

PEM fuel cell systems are presently considered the leading contenders for automotive fuel cell application; Table 20 shows their current status and future targets. Low operating temperature (about 80°C), high power density, rapid change in power on demand, and quick start-up is the major potential advantages for their implementation in vehicles [12].

**Table 20: PEM Fuel Cells Present and Future Target (Source [44])**

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Unit</th>
<th>Today</th>
<th>Target</th>
</tr>
</thead>
<tbody>
<tr>
<td>Investment</td>
<td>$/kW</td>
<td>2000-4000</td>
<td>50-60</td>
</tr>
<tr>
<td>Life Time</td>
<td>h</td>
<td>&lt; 2000</td>
<td>&gt; 5000</td>
</tr>
<tr>
<td>Efficiency (System)</td>
<td>%</td>
<td>38</td>
<td>&gt;45</td>
</tr>
</tbody>
</table>

Even though the PEM fuel cell offer many advantages like higher efficiency, lower emissions, greater fuel flexibility, etc., over internal combustion engines (ICE) for vehicle propulsion, they must still compete on the bases of cost and durability.
5.2.3 Fuel-Cell Vehicle Applications

At the present time, the gasoline-fueled (or diesel-fueled) vehicle powered by an internal combustion engine represents a well-known technology with a vast infrastructure already in place and performance that has improved significantly in the last few years.

However, the motivation of the U.S. to reduce dependence on imported petroleum, and to reduce atmospheric pollutants and CO$_2$ emissions by improving fuel economy and achieving zero tailpipe emissions for passenger vehicles, has focused the attention of automobile manufacturers on developing clean new alternatives like direct hydrogen fuel-cell vehicles [19].

A fuel-cell vehicle (FCV) is an electric automobile that runs on hydrogen gas rather than gasoline and emits zero emissions. The FCV stores its energy in a hydrogen tank unlike electric vehicles that store energy in batteries. The principal components of a FCV are presented in Figure 37 [71] and described as follows:

- Fuel Cell Stack: Converts hydrogen gas and oxygen into electricity to power the electric motor
- Hydrogen Storage Tank: Hydrogen gas is stored at high pressure to increase the driving range
- Electric Motor: Electric motors work more quietly, smoothly, and efficiently than ICEs.
- Power Control Unit: Governs the flow of electricity
- High-Output Battery: Storage energy generated from regenerative braking to provide supplemental power to the electric motors
Commercialization of hydrogen and fuel-cell technologies will compete with both conventional and advanced technologies. However, the FCV must overcome several unique challenges before its widespread implementation is likely.

At the present time, the FCV is facing two major challenges [72]:

- The fuel cell systems must be as durable and cost-effective as gasoline ICEs.
- A small, lightweight hydrogen storage system is needed to provide an acceptable driving range of 300 miles or more.

Additionally, the uncertainty and risk involved in the introduction of a new fuel and new vehicle technology to the market makes the task very difficult. On one hand, there is prevailing misconception that hydrogen is unsafe and unreliable, and the public has very little awareness of hydrogen and fuel cell systems [19]. The major demand parameters for a light-duty vehicle are shown in Table 21.
### Table 21: Light-duty Vehicle Parameters (Source [19])

<table>
<thead>
<tr>
<th>Demand Category</th>
<th>Parameter</th>
</tr>
</thead>
</table>
| **Customer**    | Initial cost  
|                 | Operational and maintenance costs 
|                 | Quality  
|                 | Range (between refueling) and refueling convenience 
|                 | Passenger/cargo space  
|                 | Performance (acceleration, speed, ride quality, acceptably low levels of noise, vibration, and harshness) 
|                 | Safety |
| **Regulatory**  | Emissions of pollutants (carbon monoxide [CO], oxides of nitrogen [NOx], hydrocarbons [HC], particulates)  
|                 | Fuel efficiency  
|                 | Greenhouse gas emissions  
|                 | Safety |

Nevertheless, fuel cell vehicles are attractive potential replacements for ICE-based vehicles. Over the past year significant progress has been made in fuel-cell technology. For example, the cost has decreased while performance and durability have increased considerably. Still, the production quality of the vehicles is at an early stage [72].

Currently, several well-to-wheel studies have evaluated the fuel economy of FCVs relative to their conventional gasoline ICE counterparts.

The U.S. Department of Energy’s (DOE), for example, is pursuing a portfolio of technologies that have the potential to significantly reduce greenhouse-gas (GHG) emissions and petroleum consumption, as shown in Figure 38 and Figure 39, respectively. The technical report titled *Well-to-Wheels Greenhouse Gas Emissions and Petroleum Use for*
Mid-Size Light-Duty Vehicles presents an updated well-to-wheels analysis of GHG performance for various vehicle/fuel combinations and petroleum energy use [73]. The report shows that fuel-cell vehicles operating on hydrogen are among the lowest emitters of GHGs per mile and petroleum energy use (see figure) even though the hydrogen is produced from non-renewable energy resources. Conventional gasoline vehicles generate roughly 2 to 10 times more GHGs per mile than FCVs.

![Well-to-Wheels Greenhouse Gas Emissions](source: [73])

Figure 38: Well to Wheels Greenhouse Gas Emissions (Source [73])
5.2.4 Onboard Storage Systems

Hydrogen can be stored on board vehicles as a gas, liquid, or solid. At the present time, high-pressure gaseous storage system seems to be the best solution with respect to short-term introduction.

The main challenge of fuel-cell vehicle commercialization is the onboard hydrogen storage system. On a weight basis, hydrogen has nearly three times the energy content of gasoline (120 MJ/kg for hydrogen versus 44 MJ/kg for gasoline). However, on a volume basis, the situation is reversed (8 MJ/liter for liquid hydrogen versus 32 MJ/liter for
gasoline). This challenge must be overcome in order to be able to compete with gasoline or diesel-fueled vehicles.

The Hydrogen Fuel Initiative, launched by President George H. W. Bush in 2003, has dedicated a significant effort to development of hydrogen storage systems [74]. Through this effort the Department of Energy (DOE) has focused on applied research and development (R&D) on onboard hydrogen-storage technologies supporting a driving range of greater than 300 miles (500 km) while meeting packaging, cost, safety, and performance requirements competitive with comparable vehicles in the marketplace [75].

The DOE has developed a system-level target taking into consideration six broad categories for hydrogen onboard storage performance: hydrogen capacity, cost, durability, hydrogen charging/discharging rates, fuel quality and environmental, and safety and health, as shown in Figure 40. These targets are based on equivalency to current gasoline storage systems in terms of weight, volume, cost, and other operating parameters.
Table 2 Technical Targets: Onboard Hydrogen Storage Systems

<table>
<thead>
<tr>
<th>Storage Parameter</th>
<th>Units</th>
<th>2010</th>
<th>2017</th>
<th>Ultimate</th>
</tr>
</thead>
<tbody>
<tr>
<td>System Gravimetric Capacity:</td>
<td>kWh/kg</td>
<td>1.5 (0.045)</td>
<td>1.8 (0.055)</td>
<td>2.5 (0.075)</td>
</tr>
<tr>
<td>Usable, specific-energy from H₂ (net useful energy/max system mass)</td>
<td>kg H₂/kg system</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>System Volumetric Capacity:</td>
<td>kWh/L</td>
<td>0.9 (0.028)</td>
<td>1.3 (0.040)</td>
<td>2.3 (0.070)</td>
</tr>
<tr>
<td>Usable energy density from H₂ (net useful energy/max system volume)</td>
<td>kg H₂/L system</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Storage System Cost b.</td>
<td>$/kWh net</td>
<td>TBD</td>
<td>TBD</td>
<td>TBD</td>
</tr>
<tr>
<td></td>
<td>($/kg H₂)</td>
<td>(TBD)</td>
<td>(TBD)</td>
<td>(TBD)</td>
</tr>
<tr>
<td></td>
<td>$/gge at pump</td>
<td>3-7</td>
<td>2-4</td>
<td>2-4</td>
</tr>
<tr>
<td>Durability/Operability:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Operating ambient temperature °C</td>
<td></td>
<td>-30/50 (sun)</td>
<td>-40/60 (sun)</td>
<td>-40/60 (sun)</td>
</tr>
<tr>
<td>Min/max delivery temperature °C</td>
<td></td>
<td>-40/65</td>
<td>-40/65</td>
<td>-40/65</td>
</tr>
<tr>
<td>Operational cycle life (1/4 tank to full)</td>
<td>CyClico</td>
<td>1000</td>
<td>1500</td>
<td>1500</td>
</tr>
<tr>
<td>Min delivery pressure from storage system, FC= fuel cell, ICE= internal combustion engine</td>
<td>bar (abs)</td>
<td>5 FC/35 ICE</td>
<td>5 FC/35 ICE</td>
<td>3 FC/35 ICE</td>
</tr>
<tr>
<td>Max delivery pressure from storage system</td>
<td>bar (abs)</td>
<td>12 FC/100 ICE</td>
<td>12 FC/100 ICE</td>
<td>12 FC/100 ICE</td>
</tr>
<tr>
<td>Gross Efficiency</td>
<td>%</td>
<td>90</td>
<td>90</td>
<td>90</td>
</tr>
<tr>
<td><strong>Net</strong> to Powerplant Efficiency</td>
<td>%</td>
<td>60</td>
<td>60</td>
<td>60</td>
</tr>
<tr>
<td>Charging / Discharging Rates:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>System fill time (5 kg)</td>
<td>min</td>
<td>4.2</td>
<td>3.3</td>
<td>2.5</td>
</tr>
<tr>
<td></td>
<td>(kg H₂/min)</td>
<td>(1.2)</td>
<td>(1.5)</td>
<td>(2.0)</td>
</tr>
<tr>
<td>Minimum full flow rate (g/s/kW)</td>
<td>g/s/kW</td>
<td>0.02</td>
<td>0.02</td>
<td>0.02</td>
</tr>
<tr>
<td>Start time to full flow (20°C)</td>
<td>s</td>
<td>5</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>Start time to full flow (-20°C)</td>
<td>s</td>
<td>15</td>
<td>15</td>
<td>15</td>
</tr>
<tr>
<td>Transient response 10%-90% and 90% - 0% b.</td>
<td>s</td>
<td>0.75</td>
<td>0.75</td>
<td>0.75</td>
</tr>
<tr>
<td>Fuel Purity (H₂ from storage)</td>
<td>% H₂</td>
<td>SAE J2719 and ISO/PDTS 14687-2 (99.97% dry basis)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Environmental Health &amp; Safety:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Permeation &amp; leakage</td>
<td>Scc/h</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Toxicity</td>
<td></td>
<td>Meets or exceeds applicable standards</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Safety</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Loss of usable H₂ a.</td>
<td>g/kWh H₂ stored</td>
<td>0.1</td>
<td>0.05</td>
<td>0.05</td>
</tr>
</tbody>
</table>

Useful constants: 0.2778 kWh/MJ; 33.3 kWh/kg H₂; 1 kg H₂ = 1 gal gasoline equivalent.

**Figure 40: Onboard Hydrogen Storage Systems for Light-duty Vehicles (Source [12])**

The targets are emphasized with respect to the driven systems and not based on hydrogen storage methods. Both attributes must be taken into consideration [12].

Figure 41 shows the current status of vehicular hydrogen-storage systems, including gravimetric, volumetric, and system cost targets.
It is evident that none of the existing vehicular hydrogen-storage systems meet the combined gravimetric, volumetric, and cost targets for either 2010 or 2015. Table 22 describes some challenges and corresponding characteristics that must be overcome for the onboard-storage hydrogen system [12].
### Table 22: Onboard Storage Hydrogen System Challenges (Source [12])

<table>
<thead>
<tr>
<th>Challenges</th>
<th>Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weight and Volume</td>
<td>The FCV must overcome the high weight and volume required to store H₂ on vehicles, resulting in inadequate vehicle range compared to petroleum vehicles.</td>
</tr>
<tr>
<td>Efficiency</td>
<td>The energy required to store H₂ in a liquid or gaseous stage is high, creating a challenge for energy efficiency systems of hydrogen storage.</td>
</tr>
<tr>
<td>Durability</td>
<td>The storage systems have short durability or lifetime. A lifetime of 1500 cycles is needed to overcome this challenge.</td>
</tr>
<tr>
<td>Cost</td>
<td>Compared to conventional vehicle, the cost of onboard hydrogen systems is extremely high. Improvements in low cost materials, storage components, and low cost-high volume methods are the keys for overcoming these challenges.</td>
</tr>
<tr>
<td>Codes and Standards</td>
<td>Actually, it has not code or standards have been established for hydrogen storage to facilitate its implementation and commercialization.</td>
</tr>
<tr>
<td>Life-Cycle and Efficiency Analyses</td>
<td>Hydrogen systems present a lack of full life cycles cost and efficiency.</td>
</tr>
</tbody>
</table>
CHAPTER 6. STUDY OF HYDROGEN FUEL INTO NETPLAN

6.1 Introduction

New alternative and renewable technologies are being developed in the U.S in order to produce, transport and convert clean energy for the electric and transportation systems. These two systems are the largest energy consuming and the greatest contributors to carbon emissions in the U.S.

In the transportation sector for example, new transportation fuels such as electricity, natural gas, biomethane, propane, hydrogen, ethanol, renewable diesel, and biodiesel fuels; and new vehicles technologies such as electric, hybrid electric and fuel cell vehicles are being considered to be the solution to reduce the greenhouse gas emissions, the petroleum use, and improve air quality in the U.S [76]. It is clear that in order to confront these problems, the electric and the transportation sectors are moving to “green” electric resources while at the same time electrifying the transportation sector [77].

According to [78] in order to reduce the GHG emissions and the dependence on foreign oil, the electrification of the transportation sector holds significant potential for the future system. However, the transition to these new fuel and vehicles alternatives technologies will take time. Based on [77] these new alternatives and renewable energy technologies will require considerable capital investment and will take years to build, therefore a long-term assessment is needed in order to select from among of them. Also, these new technologies are being used to create a highly interconnected system that integrates the electric and transportation infrastructures which creates interdependency between them [11].
For example, use of hydrogen as alternative fuel for the transportation sectors will lead to additional electric demands that will influence the structure, operation and emissions in the electric sector [79]. Furthermore, hydrogen would interact with and influence the electricity grid in several ways; some examples taken from [79] and [80], follow:

- **Feedstock:** Both energy carriers can be generated from the same primary energy resource that will result in a competition between them. Also, any change in the feedstock cost will play a large role in the price of these energy carriers. Furthermore, both will compete for renewable energy and low carbon resource to reduce the GHG emissions that will impact the trends in carbon intensity.

- **Co-production:** This refers to the production or generation of multiple useful products. Hydrogen and electricity can be produced in the same facility due to the fact that both can be generated from the same resource. This offers benefits for the overall energy efficiency and economics similar to that which combined cycle plants do. Some of these benefits are: flexibility in meeting demands, increased utilization, increased efficiency, lower emissions and carbon capture, and lower costs.

- **Convergence in H₂ and electricity delivery:** Starr and others in [79] and [81] have proposed an interesting and innovative idea for using these two energy carriers together by simultaneous co-delivery of the hydrogen and the electrical energy in a supergrid. The supergrid will transmit the electricity by using superconducting transmission, cooled by liquid hydrogen (at 20°K) in pipes that will surround the lines with the objective of cooling the conductors to enable superconductivity and minimize transmission losses.
• **Interconversion:** This refers to the use of one energy carrier to address weaknesses associated with the other energy carrier. The interaction between hydrogen and electricity is beneficial because both are complementary energy carriers. Examples of possible applications are: renewable variable electricity storage, off-peak electrolysis, central hydrogen production and electricity generation, central hydrogen production and distributed electricity production, central hydrogen production and distributed electricity production. These two energy carriers will converge and co-evolve as they address the challenges of reducing GHG emissions, petroleum dependence, and improve air quality [79].

However, it is difficult to know how, when, and where these technological options that exist and are still in development will be implemented and at what cost. In addition, there is a significant number of attributes that need to be taken into consideration for the evolution of the overall energy systems. For instance, cost, sustainability and resiliency are attributes that must be considered in the assessment of future technologies. Also, the lifetime associated to these technologies is crucial [77].

Hydrogen has been promoted as an alternative carrier for the transportation sector that will address the energy security and environmental issues associated with the petroleum systems. However, the major challenges that hydrogen is facing at the moment is the lack of an existing infrastructure for producing, delivering and refueling the fuel to the consumers.

In the last decades, significant research has been dedicated to every aspect of the hydrogen pathways, from feedstock, production technologies, delivery systems, refueling stations, until fuel cell vehicles. However, “*what are the energy efficient, environmentally benign and cost effective pathways to deliver hydrogen to the consumer?*” this results in a
large number of potential supply pathways [6]. For instance: cost, operability, environmental impacts, safety and social implications are some performances that need to be analyzed when assessing future commercial hydrogen as viable long-term alternative solution.

A long term assessment is necessary to assess the value of using hydrogen in the future. Nevertheless, there are a significant number of new alternative technologies similar to hydrogen that may play a role in future energy and transportation systems. The project NETSCORE 21, introduced in Chapter 1, address these issues.

NETSCORE 21 project goal is to identify optimal infrastructure designs in terms of future power generation technologies, energy transport and storage technologies, and hybrid-electric transportation systems to achieve desirable balance between sustainability, costs, and resiliency. As a result, the project has been able to develop a tool called NETPLAN that is able to analyze a long-term investment and operation model for the transportation and energy system. This chapter describes the tool NETPLAN, the mathematical formulation, the use of NETPLAN to assess hydrogen as an alternative fuel, and analysis results.

6.2 NETPLAN

In NETPLAN, the main objective is to be able to simultaneously evaluate different portfolios for those critical infrastructures (electric and transportation sectors) and search for the best ones in terms of sustainability, resiliency and cost [11]. The innovative nature of this tool is that it performs a long-term assessment for the electric/transportation infrastructure design at a national level while accounting for their interactions and interdependencies. The orientation is better captured in Figure 42 [10].
As seen in Figure 42, NETPLAN considers a long-term assessment planning for the two systems where it must represent the energy network responsible to supply energy demand to different subsystems shown in the upper portion of the figure. This energy network includes not only the electric network but also the natural gas and liquid fuel networks. At present, most liquid fuel is dominated by petroleum systems. The bottom portion is the transportation sector which consists of the movement of passengers and freight that occurs via different forms of transportation. Some of these two forms of transportation are captured in Figure 42 by electrification of vehicles and, rail.
NETPLAN considers both conventional and non-conventional energy systems that rely on a diverse resource portfolio with multiple conversion and transportation paths; system components fall into the following categories: source, conversion, transportation, storage, and end-use [10]. NETPLAN is developed to perform assessments over extended time periods, on the order of 40 or more years, in comparison to the traditional 20-30 year planning horizon required by most state and federal regulatory bodies today. NETPLAN has been applied in several studies; results of representative studies are reported in [82, 83, 84].

6.2.1 Modeling framework in NETPLAN

At the present time, the operation and the investment of the transportation and energy infrastructure are independent. For instance, the transportation sector is mainly driven by the petroleum, and the electric system is mainly driven by the use of raw bulk energy sources (e.g. coal or natural gas for the thermal power plant), uranium for nuclear, water for hydro, and wind, solar, and biomass for these renewable energy forms. At the operational level, with the existing infrastructure, both systems need to satisfy their own demand and the cost of meeting those demands will impact on the final price for both systems [11]. Nevertheless, there is very great potential for these two systems to become more interdependent, and as they do, it will require investment in new capacity which will in turn determine the behavior of the highly interconnected systems.

The modeling associated with NETPLAN is conceptually captured in Figure 43. At the operational level (inside the loop), the figure illustrates that the energy system loads the transportation systems and the transportation systems loads the energy system, i.e., each one loads the other. At the bottom and outside the inner box, the investment or planning level is captured which directly determines the evolution of these two systems. Thus, the energy and
transportation infrastructure systems interact at both the operational and the investment or planning levels. The NETPLAN model captures this interaction, to be explained more fully in the following sections.

![Proposed model that integrates the energy and transportation systems at two levels](source [11])

### 6.2.2 Energy Modeling

In order to model the energy systems, a generalized network flow transportation model is used. The energy system network analyzed by NETPLAN is captured in Figure 44. Here, a single commodity is flowing from sources to sink through the systems called “energy”. This energy commodity must satisfy the energy demand in the form of energy carrier such as electricity, natural gas or refined gasoline and must take in consideration the production and transportation of the primary energy (e.g. pipeline systems and transmission...
and their conversion (power plants, wind farms, and refineries) and ultimate form of consumption [11].

In order to invest in new infrastructure, the energy flow limits act as the capacity of the different infrastructure “links;” they are included as decision variables so that the model can explore investment in the systems [11].

<table>
<thead>
<tr>
<th>PRIMARY ENERGY</th>
<th>ENERGY TRANSPORT</th>
<th>ENERGY CONVERSION</th>
<th>DELIVERY ENERGY</th>
<th>END USE TECHNOLOGY</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crude Oil</td>
<td>Pipeline</td>
<td>Oil Refinery and Distribution System</td>
<td>Motor Gasoline</td>
<td>Automobile</td>
</tr>
<tr>
<td>Coal</td>
<td>Rail</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Natural Gas</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nuclear</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 44: Energy commodity flows from source to sink for energy modeling in NETPLAN (Source [35], [85], [86], [87])

To capture the energy modeling where a single commodity, energy, flows through the system, NETPLAN categorizes each pathway by applying the network structure as described in Table 23 [10].
Table 23: Network structure applied to the energy system in NETPLAN (Source [11])

<table>
<thead>
<tr>
<th>Network Structure</th>
<th>Definition</th>
<th>Types</th>
<th>Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Nodes</strong></td>
<td>Nodes are used to represent the points in the system where the conservation of energy (or flow) is enforced. A node is defined to represent both a geographical region and a type of energy.</td>
<td><strong>Sources:</strong> Represent the production of raw materials.&lt;br&gt;<strong>Transmission:</strong> are those that all the incoming energy leave the node&lt;br&gt;<strong>Storage:</strong> are those that are interconnected in time and allow the flow of energy between consecutive points in time.&lt;br&gt;<strong>Demand:</strong> where physical demand of energy like electricity or natural gas is enforced.</td>
<td>The difference between energy coming in and out of the node is the most important parameter associated with demand of energy.&lt;br&gt;Storage and Transmission nodes the demand is usually zero.&lt;br&gt;Source nodes are the source of the energy that is consumed for the systems so no demand is defined.</td>
</tr>
<tr>
<td><strong>Arcs</strong></td>
<td>Arcs are used to connect nodes and represent the available routes for flows. They are defined by the origin and destination nodes and can have costs and capacities associated to them.</td>
<td><strong>Two types of arcs:</strong>&lt;br&gt;- Transmission line, natural gas or petroleum pipeline are example of arcs that represent the transmission of energy geographically and at the same time belong to the same systems of sources.&lt;br&gt;- Electric generators, electrolysis facilities or refineries are example of arcs for NETPLAN because they conduct the conversion between energy types. The two types of arcs explained above will hold the following attributes:&lt;br&gt;- Arcs that result from the same source of nodes are assigned maximum extraction rate (MBtu/month) and extraction cost ($/MBtu).&lt;br&gt;- Conversion and transportation are endowed with: capacity (MBtu-capacity/month), efficiency (%), operational cost ($/MBtu-flow/month), investment cost ($/MBtu-capacity/month), component sustainability metrics, and component resiliency (e.g., reliability).</td>
<td>These parameters are associated to each arc, however not all of them apply in each case:&lt;br&gt;- Minimum flow. Usually is zero, but could be positive to represent situations such as electric transmissions contracts.&lt;br&gt;- Maximum flow or arc capacity. It is a combination of the initial capacity (which can be set to gradually decrease as initial capacity is retired) and new investments.&lt;br&gt;- Investment cost, per unit of capacity added to the flow&lt;br&gt;- Minimum investment&lt;br&gt;- Maximum investment&lt;br&gt;- Cost, per unit of flow&lt;br&gt;- Efficiency parameter, which is a multiplier that is applied to the flow. It serves to represent, for example, losses in gas transportation and electric transmission. It can be used to transform units from one subsystem to another.</td>
</tr>
<tr>
<td><strong>Flows</strong></td>
<td>Flows are the representation of energy moving along the system of arcs</td>
<td>Single Commodity (Energy)</td>
<td>Different units are used for different subnetwork: million short tons for coal, million cubic feet for natural gas, millions of gallons for the petroleum network, and GW-hours for electricity, for the only single commodity flowing in the system.</td>
</tr>
</tbody>
</table>
6.2.3 Transportation Modeling

In NETPLAN, a multicommodity flow network is used for modeling freight transportation systems where the flows are in the units of tons of each major commodity. The model considers the movement of goods around the country, and it analyzes five commodities. The first four commodities analyzed for the model are the four types of coal. For these four types of coal, the model accounts for production costs, heat content, sulfur and ash content. The fifth commodity analyzed for the model includes the rest of the commodities that do not have a direct relationship with the energy system, e.g., cereal grains, food-stuffs, gasoline and aviation fuel, chemicals, gravel, wood products, and base metals [11].

NETPLAN provides that each commodity may be transported by more than one mode (rail, barge, truck). It also models the infrastructure over which the commodity movements occur (rail, lock/dams, road, ports) and the corresponding fleets (trains, barges, trucks), and there may be different kind of fleets for each mode (e.g. diesel train or electric trains) [11].

In order to capture the flow into an ordinary network problem, NETPLAN represents the types of infrastructure as well as the different types of available fleets as illustrated in Figure 45.
6.2.4 Summary of the systems

Table 24 shows the summary of the different networks modeled within NETPLAN, which is represented by a single linear programing minimization cost model. The table lists the networks, and for each one of them, the following information is specified: network flow type, commodities transported, units used, infrastructure, fleets, and where the node is specified [11].
Table 24: Summary of modeled systems [11]

<table>
<thead>
<tr>
<th>Network</th>
<th>Flow</th>
<th>Commodities</th>
<th>Units</th>
<th>Infrastructure</th>
<th>Fleet</th>
<th>Demand</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy</td>
<td>Single Commodity</td>
<td>Electric</td>
<td>MWhr</td>
<td>Electric</td>
<td>N/A</td>
<td>Nodes</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Natural Gas</td>
<td>Kg/hr</td>
<td>Pipeline</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Petroleum</td>
<td></td>
<td>Pipeline</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Hydrogen</td>
<td></td>
<td>Pipeline</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Energy</td>
<td>Multicommodity</td>
<td>Bituminous</td>
<td>Tons</td>
<td>Rail</td>
<td>Diesel,Ele.</td>
<td>Nodes</td>
</tr>
<tr>
<td>(coal)</td>
<td></td>
<td>Subbituminns</td>
<td></td>
<td>Barge</td>
<td>Diesel</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Lignite</td>
<td></td>
<td>Highway</td>
<td>Diesel, Hybrid</td>
<td></td>
</tr>
<tr>
<td>Freight</td>
<td>Multicommodity</td>
<td>Grains</td>
<td>Tons</td>
<td>Rail</td>
<td>Diesel,Ele.</td>
<td>Arcs</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Chemicals</td>
<td></td>
<td>Barge</td>
<td>Diesel</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Gravel,etc.</td>
<td></td>
<td>Highway</td>
<td>Diesel, Hybrid</td>
<td></td>
</tr>
</tbody>
</table>

The single commodity called “energy” is expressed in energy units (e.g., GWhr); where capacity infrastructure in enforced on the arcs and nodal demand is specified. The freight transportation uses a multicommodity formulation where the demand is determined by arcs. Also, in this formulation, the infrastructure and fleets are principal components that determine the maximum flows across the arcs.

The energy commodities share some characteristics with both energy (single commodity) and freight transportations (multicommodity). Here, the demand is defined by the nodes that behave like freight transportation where a multicommodity flow is used to represent the infrastructure and fleet.
6.2.5 General cost minimization formulation

The optimization problem can be conceptually described by:

\[
\min \ CostOp + CostInv
\]

subject to:

- Meet energy demand,
- Meet transportation demand,
- Capacity constraints,
- Power flow constraints on electric transmission

This formulation leads to a linear program that minimizes the present value of the combined systems: energy and transportation infrastructure investment and operational cost over a period of time (40 years), subject to constraints related to meeting demands on energy and transportation while satisfying the networks capacity constraints [11]. The investments cost of the energy and transportation infrastructures, the cost of primary energy extraction at the sources, the operational costs of power plants including labor and maintenance (O&M costs), and the operational costs of the transportation sector are taken into account in the objective function.

The capacity investments in energy infrastructure, transportation infrastructure, and transportation fleets (such as trains, heavy-duty trucks, and LDVs), and operational flows of energy and freight are the decision variables that are analyzed.

6.3 Description of Data

The data needed for the implementation of hydrogen with in NETPLAN come from the US National Research Council Committee report on hydrogen energy [19, 87].
The data used is referred to current technology. It is based on technologies that could in principle be implemented in the near future. According to [19], no fundamental technological breakthrough would be needed to achieve satisfactory performance or cost, although normal processes of design, engineering, construction, and systems optimization might be needed to achieve costs as low as those estimated in this analysis.

In the present work, 5 technologies for hydrogen production were represented, taking into considerations the feedstock and whether or not sequestrations of carbon dioxide is considered at the facilities [19] as shown in Table 25.

The principal supply options for hydrogen production include in this analysis are: coal, natural gas and water as a primary energy source. The reasons for the selection of these resources were explained in section 2.3.1 and 2.3.2.

**Table 25: Hydrogen Pathways Analyzed**

<table>
<thead>
<tr>
<th>Scale</th>
<th>Primary Energy Source</th>
<th>Production Method Options</th>
<th>Options for Carbon Capture</th>
<th>Abbreviation</th>
<th>Delivery Systems</th>
</tr>
</thead>
<tbody>
<tr>
<td>Central Station (GH2)(^a)</td>
<td>Natural Gas</td>
<td>Steam Methane Reforming</td>
<td>NO</td>
<td>CS-SMR</td>
<td>Pipeline</td>
</tr>
<tr>
<td>Central Station (GH2)(^a)</td>
<td>Natural Gas</td>
<td>Steam Methane Reforming</td>
<td>YES</td>
<td>CS-SMR-CCS(^c)</td>
<td>Pipeline</td>
</tr>
<tr>
<td>Central Station (GH2)(^a)</td>
<td>Coal</td>
<td>Gasification</td>
<td>NO</td>
<td>CS-CG</td>
<td>Pipeline</td>
</tr>
<tr>
<td>Central Station (GH2)(^a)</td>
<td>Coal</td>
<td>Gasification</td>
<td>YES</td>
<td>CS-CG-CCS(^c)</td>
<td>Pipeline</td>
</tr>
<tr>
<td>Central Station (GH2)(^b)</td>
<td>Electricity (Grid)</td>
<td>Electrolysis of water</td>
<td>NO</td>
<td>CS-GE</td>
<td>Pipeline</td>
</tr>
</tbody>
</table>

\(^a\) GH2 = gaseous H2.
\(^b\) CCS = carbon capture and sequestration.
We focus on implementing hydrogen via a central station approach. Rationale behind this is that this approach would more likely yield attractive economies of scale.

For each station the production, delivery and dispensing segments are taken into account as shown in Figure 46. The following points describe the characteristics of each station:

1. **Central Station (for Coal and Natural Gas as a feedstock):** The maximum production capacity is 1,200,000 kg of hydrogen per day and operates with 98% annual load factor. It will be able to fuel more than 2 million fuel cell vehicles via four main transmissions pipelines of 150 km and 438 dispensing stations.

2. **Central Station (Water as a feedstock):** The maximum production capacity is 150,000 kg of hydrogen per day and operates with 90% annual load factor. It will be able to fuel more than 225,844 fuel cell vehicles via four main transmissions pipelines of 150 km and 411 dispensing stations.
Figure 46: Central plants for production, delivery and dispensing hydrogen into FCV

The economics parameters for the central plant are summarized in Table 26 and Table 27 [19]. These tables show the economics parameters needed for NETPLAN to simulate the hydrogen pathways. The investment cost is separated into 3 components: production cost (cost including production and storage onsite), transmissions and distribution cost (cost of transporting hydrogen by pipeline), dispensing cost (cost of compressing and storing hydrogen at the filling station and cost of dispensing hydrogen into fuel cell vehicles) as it is shown in Figure 47.
Figure 47: Investment cost (millions $/kg/hr) of the pathways analyzed

Figure 47 show that production of hydrogen from grid electrolysis involves a considerable capital investment for the production and transmission of hydrogen. In the case of the production, the high capital cost of the electrolyzer is one of the attributes that contribute to the high capital cost (~ $3,000/KW).

Figure 47 also shows that the investment cost of transmissions in all of the pathways is similar to the investment cost of the productions. The reason for this is the high capital investment that involves the use of the pipeline. However, the advantages of this type of transportation options are significant, since a large volume can be transmitted at high efficiency; it also offers storage and buffering capacity, low variable cost, and a longer useful life [88].
Figure 48 illustrates the levels of CO2 emissions corresponding to the pathways analyzed. Here, two pathways require carbon capture and sequestration for the production of hydrogen from coal and natural gas. Figure 48 also shows that the production of hydrogen from water through electrolysis process is not the best option when electricity is taken from the grid because of the greenhouse gas emissions that can be generated per kilogram of hydrogen produced due to the generation technologies used. Conversely, the electricity generation using renewable or nuclear energy technologies, separate from the grid, is a possible option for hydrogen production via electrolysis.

For each station and their respective segments, 5% and 1% of the total capital investment was assumed to represent fixed operating cost and variable non-fuel cost. The efficiency was taken from [87] and [88]. The electricity consumptions, the plant life and the CO2 emissions of the process were taken from [19].
Figure 48: Shows the CO2 Emissions to Atmosphere for Central Stations
<table>
<thead>
<tr>
<th>Central Station, Transmissions, Distributions and Dispensing</th>
<th>Capital Investment, (Millions $)</th>
<th>CS-Size Plant Design Maximum Capacity, (kg/hr H2)</th>
<th>Fixed Cost, (Millions $)</th>
<th>Total Investment Cost, (Millions $)</th>
<th>Variable Operating Cost, (Millions $/kg)</th>
<th>Efficiency, Electric Consumption (GWh/kg H2) Compressor</th>
<th>Short Tone CO2/kg H2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Central sized Hydrogen with Steam Methane Reformer</td>
<td>453.39</td>
<td>50000</td>
<td>23</td>
<td>476.39</td>
<td>0.0095278</td>
<td>1.03E-08</td>
<td>5967 kg H2/MMCF</td>
</tr>
<tr>
<td>Central size Hydrogen with SMR with CO2 CCS</td>
<td>624</td>
<td>50000</td>
<td>31</td>
<td>655</td>
<td>0.0131</td>
<td>1.42E-08</td>
<td>5967 kg H2/MMCF</td>
</tr>
<tr>
<td>Central size Hydrogen with coal gasification</td>
<td>1152</td>
<td>50000</td>
<td>58</td>
<td>1210</td>
<td>0.0242</td>
<td>2.74E-08</td>
<td>116338 kg H2/Thous and Short Ton</td>
</tr>
<tr>
<td>Central size Hydrogen with coal gasification with CO2 CCS</td>
<td>1177</td>
<td>50000</td>
<td>59</td>
<td>1236</td>
<td>0.02472</td>
<td>2.74E-08</td>
<td>116338 kg H2/Thous and Short Ton</td>
</tr>
<tr>
<td>Central size Hydrogen via Grid Electrolysis</td>
<td>566</td>
<td>50000</td>
<td>28</td>
<td>594</td>
<td>0.09504</td>
<td>1.03E-07</td>
<td>19051 kg H2/GWhr</td>
</tr>
</tbody>
</table>
Table 27: Hydrogen Pathways Economics Parameters for Delivery and Dispensing Units [20]

<table>
<thead>
<tr>
<th>Delivery and Dispensing Units</th>
<th>Capital Investment, (Millions $)</th>
<th>CS-Size Plant Design Maximum Capacity (kg/hr H2)</th>
<th>Fixed Cost (Millions $)</th>
<th>Total Investment Cost (Millions $)</th>
<th>Total Investment Cost (Millions $/kg/hr)</th>
<th>Variable Operating Cost (Millions $/kg)</th>
<th>Efficiency</th>
<th>Electricity Consumption (GWh/kg H2) Compressor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transmission</td>
<td>724.75</td>
<td>50000</td>
<td>36</td>
<td>760.75</td>
<td>0.015215</td>
<td>1.60E-08</td>
<td>0.98</td>
<td>0.000011</td>
</tr>
<tr>
<td>Distribution</td>
<td>1.63</td>
<td>114</td>
<td>0.048939</td>
<td>1.678939</td>
<td>0.01472754</td>
<td>8.16E-08</td>
<td>0.96</td>
<td>0.000002</td>
</tr>
<tr>
<td>For a Grid Electrolysis Central Station</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Transmission</td>
<td>603</td>
<td>6250</td>
<td>30</td>
<td>633</td>
<td>0.10128</td>
<td>1.15E-07</td>
<td>0.98</td>
<td>0.000011</td>
</tr>
<tr>
<td>Distribution and Dispensing (1 Station)</td>
<td>0.52</td>
<td>1.96E01</td>
<td>0.015496</td>
<td>0.535496</td>
<td>0.02734913</td>
<td>3.03E-08</td>
<td>0.96</td>
<td>0.000002</td>
</tr>
</tbody>
</table>
6.3.1 Cost of the Fuel Cell Vehicles

At the present time, hydrogen fuel cell vehicles are more expensive than conventional gasoline vehicles and currently exist only as demonstration and research vehicles. According to [89] fuel cell vehicles must and can be affordable by the time they reach the marketplace. The Department of Energy projects the cost of a fuel cell vehicle engine at $225 per kilowatt in mass production, based on the current best technology. The industry ultimate goal is $30 to $50 per kilowatts [89] as it shown in Figure 49.

![Figure 49: Cost of a fuel cell through the years (Source [89])]()

According to [90], in 2002 Toyota presented the first semi-commercial hydrogen fuel cell vehicle for demonstration purposes at $10,000 per month on a 30-month lease. If this leasing price fully covers the vehicle production cost, it would imply that a *fuel cell systems cost* around $300,000 based on a 75 KW system that cost around $4,000/ KW.
However, fuel cell vehicles could be introduced if the government subsidies lower the fuel cell price as is the case in the current promotional strategy for compressed natural gas vehicles [91]. Fortunately, the rapid cost declines are not an unreasonable assumption, as cost reductions due to technology and process improvements have been taking place in the past for a wide variety of new technologies [90]. Hydrogen vehicles will require fervent and sustained commitment by hydrogen producers, transporters, and retail vehicles manufacturing, consumers and governments in order to achieve success in the transportation sector [92].

According to [91] in 2015, the fuel cell vehicles price is expected to range between US $49,850 and US $60,750. The price of the fuel cell vehicle selected in this study is US $60,750 for all the years. It is assumed that the FCV has a lifespan of 10 years and each vehicle consumed 185 kg H2/ year.
6.4 Hydrogen Modeling Approach within NETPLAN

The implementation of hydrogen within NETPLAN is captured in Figure 50. The life cycle for hydrogen is comprised of production, delivery and dispensing into the fuel cell vehicles. This life cycle is represented by a set of nodes and arcs that are endowed with a large number of parameters in order to model their behavior.

![Figure 50: Hydrogen Network analyzed into NETPLAN](image)

The production, delivery and dispensing of hydrogen were represented geographically using the Census Bureau Divisions as presented in Table 28. These geographical divisions were used to facilitate a comparison to results presented in the National Energy Modeling System (NEMS)H2 [93]:
Table 28: Regional Representation for Hydrogen Economy into NETPLAN.

<table>
<thead>
<tr>
<th>Regions</th>
<th>States</th>
<th>Zone</th>
</tr>
</thead>
<tbody>
<tr>
<td>New England</td>
<td>NH, VT, ME, MA, RI, CT</td>
<td>1</td>
</tr>
<tr>
<td>Middle Atlantic</td>
<td>NY, PA, NJ</td>
<td>2</td>
</tr>
<tr>
<td>East North Central</td>
<td>WI, IL, MI, IN, OH</td>
<td>3</td>
</tr>
<tr>
<td>West North Central</td>
<td>ND, SD, NE, KS, MN, IA, MO</td>
<td>4</td>
</tr>
<tr>
<td>South Atlantic</td>
<td>WV, VA, DE, MD, DC, NC, SC, GA, FL</td>
<td>5</td>
</tr>
<tr>
<td>East South Central</td>
<td>KY, TN, MS, AL</td>
<td>6</td>
</tr>
<tr>
<td>West South Central</td>
<td>OK, AR, TX, LA</td>
<td>7</td>
</tr>
<tr>
<td>Mountain</td>
<td>MT, ID, WY, NV, UT, CO, AZ, NM</td>
<td>8</td>
</tr>
<tr>
<td>Pacific</td>
<td>WA, OR, CA, AK, HI</td>
<td>9</td>
</tr>
</tbody>
</table>

Therefore, the production, transmission, distribution and dispensing of hydrogen fuel is analyzed in 9 zones. These zones supply the demand of vehicles among the regions defined by NETPLAN as shown in Figure 51.
Figure 51: Hydrogen Supply Region into NETPLAN

The modeling assumptions and data reported in [11] for the energy and the transportation sector are used in this analysis without any modification. In the case of coal and natural gas, no investments or improvements are considered. Also, the same can be said for electric transmission lines; the existing petroleum network is simplified assuming a single node connected to an unlimited supply due to the lack of publicly available data. A summary of the system network model is shown in Table 29 [11].
Table 29: Node and Arcs by subsystems (Source [11])

<table>
<thead>
<tr>
<th>Subsystem</th>
<th>Type</th>
<th>Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal</td>
<td>Production</td>
<td>24 Nodes</td>
</tr>
<tr>
<td></td>
<td>Demand</td>
<td>46 Nodes</td>
</tr>
<tr>
<td>Natural Gas</td>
<td>Production</td>
<td>25 Nodes</td>
</tr>
<tr>
<td></td>
<td>Demand</td>
<td>50 Nodes</td>
</tr>
<tr>
<td></td>
<td>Pipelines</td>
<td>108 Arcs</td>
</tr>
<tr>
<td></td>
<td>Import Pipelines</td>
<td>9 Arcs</td>
</tr>
<tr>
<td></td>
<td>Storage</td>
<td>30 Nodes</td>
</tr>
<tr>
<td>Electricity</td>
<td>Generation</td>
<td>168 Arcs</td>
</tr>
<tr>
<td></td>
<td>Demand</td>
<td>13 Nodes</td>
</tr>
<tr>
<td></td>
<td>Transmissions Lines</td>
<td>19 Arcs</td>
</tr>
<tr>
<td></td>
<td>Import Transmission</td>
<td>8 Arcs</td>
</tr>
<tr>
<td>Petroleum</td>
<td>Gasoline</td>
<td>13 Nodes</td>
</tr>
<tr>
<td></td>
<td>Diesel</td>
<td>13 Nodes</td>
</tr>
<tr>
<td>Freight</td>
<td>Transportation</td>
<td>95 Arcs</td>
</tr>
<tr>
<td>LDV</td>
<td>Demand</td>
<td>13 Nodes</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>Generations</td>
<td>469 Arcs</td>
</tr>
<tr>
<td></td>
<td>Transmissions</td>
<td>45 Arcs</td>
</tr>
<tr>
<td></td>
<td>Distribution and</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Dispensing</td>
<td>45 Arcs</td>
</tr>
</tbody>
</table>
6.5 Hydrogen Assumptions Analysis and Results into NETPLAN

In order to become economically attractive for the transportation sector, hydrogen needs to overcome the challenges that are facing at the present time, for example:

- The construction of a supporting fuel infrastructure (chicken and egg problem)
- The ability to achieve economies of scale in production;
- The reduction on the cost of fuel cell and the storage systems in the fuel cell vehicles;
- The reduction on the cost of the hydrogen production from renewable energies
- The reduction on the cost of the hydrogen refueling stations

However, it is difficult to know how options which include significant use of hydrogen pathways will be implemented, and at what cost, when there is a lot of uncertain in the technology, as is the case at the present time. According to [92], if the technology goal of the Department of Energy related to fuel cell vehicles and infrastructure research are met, a sustainable transition to hydrogen appears to be achievable, but only if strong policy is deployed which induces the early transition of the market penetration of large number of fuel cell vehicles.

Based on these perspectives, assumptions are presented here which focus on the deployment of fuel cell vehicles. The following scenarios were analyzed:

1. **Determination of FCV purchase price for FCV to become economically competitive with gasoline-fueled vehicles:** The objective here is to identify the FCV purchase price to allow it to successfully compete with gasoline-fueled vehicles, given the price of gasoline is $4/gallon. In this scenario, we assume the PHEV is significantly more expensive than the gasoline-fueled vehicle.
2. **Determination of gasoline price necessary to for FCV to become economically competitive with gasoline-fueled vehicles:** The idea here is to set a value of investment cost ($60,750) on FCV and then determine the price of gasoline at which the FCV becomes the economically preferred choice. For this scenario, it is assumed that the PHEV becomes a very expensive option as a result of either high electricity prices or as a result of high PHEV manufacturing costs due to, for example, the unavailability of lithium.

3. **Determination of CO2 cost that results in FCV investment:** The objective here is to set the value of PHEV at ($38,935) and the FCV at ($60,750); so search for a price in the gasoline when the implementation is taking place in NETPLAN when we assigned a value of $30/metric ton and $100/metric ton, to the generations portfolios, the hydrogen generations portfolios and the vehicles that emits significant amount of CO2.

The following table 30 shows outline the assumptions mention above.

**Table 30: Shows the assumption taking into account in NETPLAN**

<table>
<thead>
<tr>
<th>Gasoline Price ($/gallon)</th>
<th>Gasoline Vehicle Cost</th>
<th>PHEV Cost</th>
<th>Fuel Cell Vehicles Cost</th>
<th>CO2 Emissions ($/metric ton)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>$22,651</td>
<td>$38,935</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>X</td>
<td>$22,651</td>
<td>$200,000</td>
<td>$60,750</td>
<td></td>
</tr>
<tr>
<td>X</td>
<td>$22,651</td>
<td>$38,935</td>
<td>$60,750</td>
<td>30</td>
</tr>
<tr>
<td>X</td>
<td>$22,651</td>
<td>$38,935</td>
<td>$60,750</td>
<td>100</td>
</tr>
</tbody>
</table>
6.5.1 Results

The following graph shows the results obtained from NETPLAN due to the above assumptions.

1. Determination of FCV purchase price for FCV to become economically competitive with gasoline-fueled vehicles

Here the investment cost of the FCV was reduced considerably compared to its actual price; and the value of $4/gallon was set for the operational cost of the gasoline vehicles. The value of the PHEV was set to $38,935 but it was not selected by NETPLAN during the simulation.

A series of simulations were performed in order to obtain results for the implementation of FCV in supplying the demand of vehicles in NETPLAN as it is shown in Figure 52. It can be noted that the penetration of FCV began to take place when the price was set to $32,000 and continued to increase when the cost was reduced until it reached the same price of the gasoline vehicles. Figure 53 shows the deployment of gasoline vehicles by zone into NETPLAN.

The technology selected by NETPLAN for the production of hydrogen was Steam Methane Reformer central station without CCS. The use of the natural gas as the feedstock for hydrogen production is due to the fact that this technology presents the low investment cost and the operational cost compared with the others technologies. The rest of the technologies correspond to: Steam Methane Reformer with CCS, Coal Gasification with and without CCS and Electrolysis of water using grid electricity.

On the other hand, the hydrogen supply node is based on the Census Region Divisions that it will supply hydrogen to the fuel cell vehicles needed by the 13 zones defined
by NETPLAN. The objective to select this allocation is a future comparison with the work that it is been conducted by National Energy Modeling System (NEMS) relate to hydrogen systems. It can be observed that 3 zones present considerable levels of investment for FCV such as: Zone 1 (ECAR), Zone 5 (MAPP) and Zone 10 (SPP). The reason is that in these zones is found more than two production nodes of natural gas that it is analyzed by NETPLAN.

Figure 52: Investment of Fuel Cell Vehicles (Millions Vehicles vs. Millions $/ Thousands of Vehicles)
It is important to note that in order to implement FCV in NETPLAN, it was required to first invest in the hydrogen production, transmission, and dispensing infrastructure first. Figure 54 shows the Hydrogen Infrastructure Capacity required by NETPLAN in order to supply the demand of vehicles when the price was set to $25,000. Here, the investment was allowed to begin in year 6. This assumption is made because hydrogen does not present an infrastructure at the present time.
Figure 54: Hydrogen Infrastructure Capacity needed for NETPLAN

For Figure 55, different investment cost for FCV were taking into account in NETPLAN over time (from 32 to 21 Millions $/Thousand of Vehicles) and the value of $4/gallon was set for the operational cost of the gasoline vehicles. Here we can note significant investment in year 17, 31 and 37 of FCV. NETPLAN invest in FCV due to that it results a better economic option instead of gasoline vehicles in these years. However, NETPLAN invest in FCV but the investment are restricted to the maximum investment that it is allow in these arcs for FCV in these years. Therefore, gasoline vehicles need to compensate the demand that is imposed by the system as it is showed in Figure 56. For these reason, gasoline vehicles does not present a decrease in the investment over the years when the FCV are implement in the system.
Figure 55: FCV Investment due to different FCV prices

Figure 56: Gasoline Vehicles Investment during the years due to different FCV prices.
Lastly, CO2 emissions can be emitted to the atmosphere when hydrogen is produced if the appropriate carbon capture and sequestration (CCS) have not been taken into account. Two types of sources can throw CO2 emissions to the atmosphere when hydrogen is produced:

- If the feedstock is non-renewable energy
- If the electricity needed for hydrogen production comes from the grid

These two types of CO2 emissions source are taken into account in NETPLAN when hydrogen is produced. The pathway that is selected by NETPLAN for hydrogen production is the Central Size Steam Methane Reformer. In this case, a substantial amount of CO2 is emitted per kilogram of hydrogen produced to the atmosphere (0.01016 short tons of CO2/Kg H2 produced).

This behavior is captured in Figure 57 when the investment cost of FCV is reduce. Here, FCV supply the demand of vehicles. The increment in the investment of FCV contributes to increase the CO2 thrown to the atmosphere because more hydrogen is needed to supply the demand of FCV.

The opposite can be observed from Figure 58. This figure presents the CO2 emissions from all light-duty vehicles (LDV). Here, the demand of vehicles has been supplied by gasoline vehicles and FCV. Therefore, due to the increment on investment of FCV, a considerable reduction of CO2 is observed because FCV does not emit GHG, they only produce vapor water.

This scenario helps us to analyze the impact of the CO2 emissions that can be emitted to the atmosphere due to the use of hydrogen as alternative fuel if it comes from non-renewable energy resources or when CCS is not implemented. Figure 59 shows CO2 emissions as a function of FCV investment cost for both scenarios explained above.
Figure 57: CO2 Emissions from the Electric Power Plants due to different investment cost of FCV

Figure 58: CO2 emissions from all light-duty vehicles (LDV) due to different investment cost of FCV
Figure 59: CO2 Emissions from Electric Power and Passenger Vehicles due to different investment cost for FCV

2. Determination of gasoline price necessary to for FCV to become economically competitive with gasoline-fueled vehicles

For this task, we began to increase the price of the gasoline at which FCV becomes a choice for NETPLAN as it is showed in Figure 60. Here the price of purchase a FCV is $60,750. It can observe that when the price of the gasoline was set to $9/gallon, the investment in FCV began to take place in NETPLAN in order to satisfy the demand of vehicles. When the price was between (12-16) $/ gallon, the investment in FCV increased considerable in most of the zone. However, zone 7 (NE) and zone 3 (MAAC) the investment was low compare with the others zone. The reason could be the lack of natural gas production node in these zones. Therefore, not considerable investment is taking into account into these zones.

Here, the PHEV does not play a role into NETPLAN. It is assumed that the PHEV becomes a very expensive option as a result of high PHEV manufacturing costs due to, for
example, the unavailability of lithium. According to [94], the electric vehicle industry has recently come for reliance on lithium (Li) based batteries; some experts argue that there is plenty while other experts suggest there is not. This brings concern about replace one dependency-oil for the transportation sector with another, in this case lithium.

![Investment of Fuel Cell Vehicles due to different price of gasoline](image)

**Figure 60: Investment of Fuel Cell Vehicles due to different price of gasoline**

From Figure 61 and 62, the same conclusion can be made for the CO$_2$ emissions thrown to the atmosphere due to the investment of FCV that was analyzed from point 1. The high price of gasoline shift the demand of gasoline vehicles to FCV. Therefore, carbon capture and sequestration techniques are required in order to reduce the emissions to the
atmosphere when hydrogen is produced from non-renewable energies. However, the FCV investment can reduce significantly the CO2 emission as it is showed in figure 62.

Figure 61: CO2 Emissions from Electric Power Plant due to different gasoline price

Figure 62: CO2 Emissions from Ligh-duty Vehicles due to different gasoline price
3. **Determination of CO2 cost that result in FCV investment**

The objective was search for a price in the gasoline when the implementation of FCV is taking place in NETPLAN when we assigned a value of 0$/ metric ton, $30/metric ton and $100/metric ton to the generations portfolios that emits significant amount of CO2 to the atmosphere.

The generations portfolios that were applied this incremental cost were: pulverized coal, integrated gasification combined cycle, natural gas combined cycle, oil and geothermal. The extra cost was added to the variable non-fuel operating cost based on the value mentioned above and their respective thrown to the atmosphere for the case of the generations portfolios (mlns $/GWh).

Figures 63, 64 and 65, show the investment in FCV due to different price of gasoline when a value of $0/metric ton, $30/metric ton and $100/metric ton was added to the operational cost of the generation portfolios that emitted significant amount of CO2. From these figure we can observed that the investment of FCV began when the price of the gasoline is around 8-10$/ gallon for the $0/metric ton scenario. Contrary to figure 64, the investment of FCV began at the price of $10/gallon; for both, the FCV investment increase when the price of gasoline increment. However, from figure 65, we can observed that when we assigned 100$/metric ton to the operation cost of the generations portfolios mention above, the investment of FCV is not as huge compare with the others two scenarios. The reason can be that the electricity needed for hydrogen production is very expensive compare with 0 and 30 $/metric ton.
Figure 63: FCV Investment due to different price of gasoline at 0$/metric ton

Figure 64: FCV investment due to different price of gasoline at 30$/metric ton
Figure 65: FCV investment due to different price of gasoline at 100$/metric ton

From figure 66 to 71, we plotted the emissions that were generated due to the above scenarios. We analyzed the electric power plants CO2 emissions and the Light-duty vehicles emissions during the 40 years of analysis for different prices gasoline and the investment that we obtained for FCV. The following can be observed:

- From figure 66, when there is not cost ($/metric ton) applied to the generation portfolios that emit CO2, the short ton from the power electric plant increase when the price of gasoline growth. Therefore, more FCV are been invested in the system in order to supply the demand of vehicles. However, this behavior is not worthy because we observed the CO2 increase when the hydrogen is produced because the electricity needed for this process increment the CO2 in the systems. The opposite can be observed from figure 67, the short tons generated from the LDV due to the investment in FCV are less compare with
the CO2 from the electric power systems. For example, when the price of gasoline is $12/gallon, the CO2 emission from the power electric plants is 82,744 short ton and the LDV is 44168 short ton.

![CO2 Emissions from Electric Power Plants](image)

**Figure 66: CO2 Emissions from Electric Power Plants due to different gasoline price at 0$/metric ton**
Figure 67: CO2 Emissions from Light-duty vehicles and Electric Power Plants due to different gasoline price at 0$/metric ton

- From figure 68 and 69, we can observe that when we add the price of $30/metric tone in the systems, the CO2 emissions from the Electric Power Plants were less compared with the CO2 emissions from the LDV for the price of $8/gallon and $10/gallon for the gasoline. However, when the price increased from 12 to 16 $/gallon, the electric power plant emitted more CO2 than the LDV. More investment in FCV is applied.
Figure 68: CO2 Emissions from Electric Power Plants due to different gasoline price at 30$/metric ton

Figure 69: CO2 Emissions from Ligh-duty vehicles and Electric Power Plants due to different gasoline price at 30$/metric ton
Form Figure 70 and 71, the CO2 from the LDV were more than the electric power plant due to the investment in FCV were less compare when the others two scenarios mention above. However, when the price hit the $16/gallon, NETPLAN invest more in FCV. Therefore, less CO2 are being generated by the systems due to the FCV.

**Figure 70: CO2 Emissions from Electric Power Plants due to different gasoline price at $100$/metric ton**
Figure 71: CO2 Emissions from Light-duty vehicles and Electric Power Plants due to different gasoline price at 100$/metric ton

- From figure 72 to 74, we can observe the FCV investment through the years due to different gasoline price. When the value of 0$/metric ton was applied, more FCV were invested in the systems. The opposite can be observed when the price was set to 100 $/metric ton.

Figure 72: FCV investment at 0$/metric ton
The investment in PHEV for all the scenarios mentioned above was the same. NETPLAN, invest in the maximum amount of vehicles allow per years when the gasoline hit a high price (more than 8$/gallon). Figure 75, shows the investment on PHEV at the price of 30$/metric ton during the years for different price of gasoline.
Figure 75: PHEV investment at 30$/metric ton
CHAPTER 7. CONCLUSION AND FUTURE WORK

7.1 Conclusions

The present work presented the assessment of using hydrogen as alternative fuel in U.S. The evaluation of economics, performance, and environmental impact of large-scale hydrogen deployment was analyzed in this study. Moreover, the identification of the potential resource available in the U.S for the production of hydrogen is presented.

NETPLAN, a computational model tool, was used in this analyzed. It is able to model and analyze long-term investment (e.g., 40 years) strategies for the transportation and energy systems that account for interdependencies between them. NETPLAN has been used to perform such an evaluation for the hydrogen systems, where performance has been assessed in terms of overall economics and carbon dioxide emissions associated with both the light-duty vehicle and the electric power generation sectors.

Different scenarios were analyzed in order to search for the implementation of fuel cell vehicles. The results obtained from these scenarios show that the development of FCV in the national energy and transportation systems will contribute mitigate the energy security and environmental issues associated with petroleum dependence if the feedstock used it for hydrogen production come from renewable energy and CCS techniques are applied but improve in the economic scale need to be implemented. In addition, the high price of gasoline can play a significant role for shift from our light-duty vehicles that are gasoline-fueled based system to pluggable hybrid electric and fuel cell LDVs.

Finally, it is clear that hydrogen systems can contribute to mitigate the issues mention above through the use of fuel cell driven light-duty vehicles (LDV) in the transportation sector. In our analysis, we are assuming technology success and high oil price that can be
apply in the future. However, the need for strong policy for the implementation of hydrogen as alternative clean fuel is a reality.

7.2 Future Work

Future research, we propose the following directions:

- Analyze the hydrogen as “energy commodity” (multicommodity): Hydrogen can be transport by truck. The early transition of hydrogen, as alternative fuel, will be by using this type of transportation systems. It is clear that the oil consumption for transport hydrogen is an attribute that will play a role that need to be account for the interdependence between transportation and the energy systems.

- Analyze the hydrogen for electricity production: This secondary carrier would interact with and influence the electricity grid in several ways, for example, the competition between the feedstock.

- Analyze the hydrogen production from renewable energies resource: The production of hydrogen from renewable energies resource requires storage systems due to this types of energies varies during the day but, hydrogen can be store an used it later when the power production is low or peak demand. Contrary to electricity, hydrogen can be stored and used later to generate electricity.

- Analyze the hydrogen from biomass: Biomass is an abundant, clean and renewable resource that will play an important role in initiating use of hydrogen. One of the principal attributes of biomass is that during its growth, removes approximately the same amount of CO$_2$ as it releases when it is used for energy production. However, no commercial technology of biomass for hydrogen production is available at the present time.
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