Synthetic Fuel Production via Carbon Neutral Cycles with High Temperature Nuclear Reactors as a Power Source

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Abstract

This paper analyzes a number of carbon neutral cycles, which could be used to produce synthetic hydrocarbon fuels. Synthetic hydrocarbons are produced via the synthesis of Carbon Monoxide and Hydrogen. The cycles considered will either utilize Gasification processes, or carbon capture as a source of feed material. In addition the cycles will be coupled to a small modular Nuclear Reactor (SMR) as a power and heat source. The goal of this analysis is to reduce or eliminate the need to transport diesel and other fossil fuels to remote regions and to provide a carbon neutral, locally produced hydrocarbon fuel for remote communities. The technical advantages as well as the economic case are discussed for each of the cycles presented.

1. Introduction

The production of synthetic fuels via carbon neutral cycles could prove to be an important technology to control the current trend of increasing atmospheric carbon dioxide levels. This paper analyzes potential pathways to a carbon neutral cycle and discusses how a small nuclear power plant could prove useful in these cycles. Various carbon neutral cycles that utilize a small modular Reactor (SMR) are analyzed and compared. In this study Generation IV High Temperature Gas Reactors (HTGR) will be considered as the nuclear power source. In comparison to classic Gen III reactor designs these reactors output significantly higher temperature gas from the reactor core. Higher temperature gases are useful for hydrogen production and other process uses.

2. A Biomass Carbon Neutral Cycle

Biomass Gasification cycles are a leading method of producing synthetic fuels with a carbon neutral, or nearly carbon neutral, fuel production cycle. In simple terms gasification of biomass occurs when the feed material (biomass) is reacted with a limited amount of oxygen. This reaction results in the incomplete combustion of the hydrocarbons in the feed and the production of hydrogen and carbon monoxide. The gasification reaction can be defined as follows [1]:

$$C_n H_m + \frac{n}{2} O_2 \leftrightarrow nCO + \frac{m}{2} H_2 \quad (1)$$

Depending on the type of process and feed the ratio of CO to H_2 produced by the gasification of biomass will vary. For the purposes of this study it is assumed, in reference to existing biomass gasification processes, that the product will have an H_2: CO ratio of 0.5. The required ratio of the two gasses will be largely dependent on the desired product fuel, as well as the type of synthesis reactor used. For the purpose of this study it is assumed that the ratio of hydrogen to carbon

monoxide required for fuel synthesis will be 2:1 [2]. In order to adapt the product from a CO rich stream to a hydrogen rich stream one of two methods is commonly used.

Water Gas Shift: The water gas shift converts carbon monoxide and water to hydrogen and carbon dioxide, via the following relationship [1]:

$$CO + H_2O \rightarrow H_2 + CO_2 \quad (2)$$

Steam Methane Reforming: The reforming of natural gas with steam produces carbon monoxide and hydrogen via the following reaction [1]:

$$CH_4 + H_2O \rightarrow 3H_2 + CO \quad (3)$$

These two processes while effective at producing additional hydrogen, also introduce waste carbon into the system. This is an issue as the cycle can no longer be considered carbon neutral.

To rectify this issue a proposal is made for a nuclear hydrogen production source that could be used to produce the hydrogen emissions free, via electrolysis. This plant would involve a nuclear small modular reactor and electrolysis equipment to produce hydrogen. Due to the use of electrolysis it is anticipated that the cost of hydrogen production will be high and as such the economics of this scenario will be hampered. This design will be considered in line with carbon and hydrogen electrolysis/capture cycles introduced in following sections.

3. Carbon Dioxide Capture and Electrolysis Hybrid Cycles

Several cycles that combine carbon dioxide capture and Hydrogen produced by electrolysis have been proposed in research. Some of these technologies such as the Audi E-diesel are reported to be near commercialization [3]. The common factor between these cycles is the usage of captured carbon dioxide as a feed material, and the combination of this feed material with hydrogen to form synthetic fuels.

3.1 Challenges to Carbon Dioxide Capture

The capture of CO_2 is the first major technical challenge to any hybrid electrolysis cycle. CO_2 capture from plant output, particularly natural gas, is in practice at various locations around the world. CO_2 has rarely been captured from the air, and never on a large scale [4]. Technologies such as that designed by Canadian company Carbon Engineering are moving towards a commercialized carbon capture plant [5]. The invention of a large scale carbon capture, from air, plant coupled to a small modular nuclear hydrogen producer, would remove the geographical limits on a synfuel plant and allow production to take place anywhere nearby the fuel demand.

3.2 Electrolysis

Electrolysis is a process that utilizes electrical potential to separate a molecule. 3 Types of electrolysis are relevant to the cycles. Each is discussed below:

1) Water is electrolyzed into hydrogen and Oxygen. This is a well proven technology and is the lowest cost however it requires large amounts of input electricity.
2) Steam is electrolyzed into hydrogen and oxygen. This technology is nearing commercialization and while it will be more expensive than conventional electrolysis, the electrical requirement will be significantly reduced as thermal energy assists in the splitting of the water molecule.
3) Steam and Carbon Dioxide are directly split into Hydrogen, Carbon Monoxide and Oxygen. This method of production is the furthest from commercialization and would be the most expensive to commercialize. It will present savings in the quantity of hydrogen that must be produced via electrolysis. In both options 1 and 2 above the reverse of the water gas shift reaction (introduced in section 2) is used to produce carbon monoxide, requiring an excess of hydrogen.

3.3 Synthetic Diesel Production

Synthetic Diesel can be produced from a Syngas product with the correct ratio of H_2 to CO in the presence of an appropriate catalyst. Fischer-Tropsch reactor vessels are used to facilitate this fuel synthesis [1]. The produced diesel may require some additional processing for compliance with environmental regulations, but for the most part could be used as a fuel in any diesel operated internal combustion engine.
The reaction taking place in a Fisher-Tropsch reactor is characterized below [1]:

$$(2n+1)H_2 + nCO \rightarrow C_nH_{(2n+2)} + nH_2O \quad (4)$$

In the above n is typically 10-20 and the formation of methane (n=1) is unwanted.

3.4 Synthetic Methane Production

The Syngas mixture of Carbon Monoxide and Hydrogen gas can also be synthesised into methane. Methane being the largest component of natural gas can be used to serve domestic or industrial natural gas needs, or as a fuel for natural gas vehicles. The methane formation reaction is called the Sabatier reaction, and was developed over 100 years ago. The reaction takes two forms, hydrogen reacting with carbon dioxide or hydrogen reacting with carbon monoxide. The equations for these reactions are presented below. It can be seen from the below that the advantage of utilizing carbon monoxide over carbon dioxide is the decreased hydrogen requirement [6]:

$$3H_2 + CO \rightarrow CH_4 + H_2O \quad (5)$$

$$4H_2 + CO_2 \rightarrow CH_4 + 2H_2O \quad (6)$$

4. Use of a Small Modular Reactor

This paper suggests the use of a small modular reactor for the following reasons:

- All Electricity is provided to the process free of CO_2 emissions
- Hydrogen as well as carbon monoxide will be produced at a high purity; the syngas will require less treatment than conventional processes.

- Equipment required for the process is minimized.
- The High Temperature Gas reactor produces high temperature steam. The steam can be used to greatly improve the efficiency of electrolysis.
- Small scale installations can be completed at a lower capital cost allowing the production of fuels in a shorter timeframe.
- Nuclear plants require infrequent refuelling and have high operability factors. This helps to enable the business case for the use of these systems in remote areas, where grid connections are not available.
- Fuels can be produced locally in hard to access locations. Reducing the difficulty of transportation and the associated cost.

5. Comparison of Proposed Cycles

In the sections that follow the product requirements and economics of each of the cycles is considered. The carbon capture / hydrogen electrolysis cycles are assessed in section 5.1, and the proposed hybrid gasification cycle is assessed in section 5.2. Figure 1 below illustrates the different cycles leading to synthetic hydrocarbon fuels, as an example.

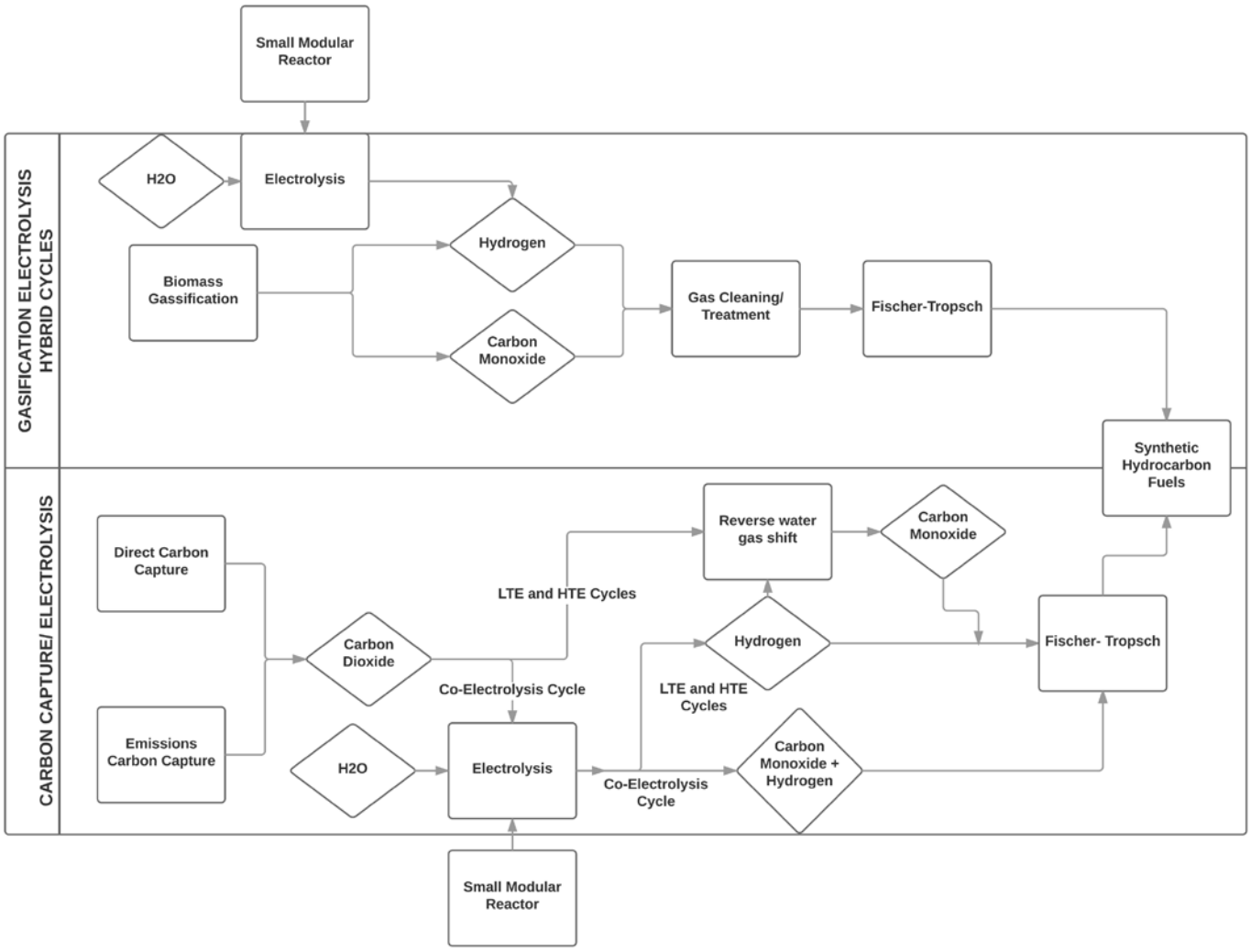

Figure 1: Flow Chart for Analyzed Cycles

5.1 Carbon Capture / Hydrogen Electrolysis Cycles

5.1.1 Reaction Reagent Requirements

The common factor between all of the technologies is the usage of hydrogen and carbon monoxide as reagents to produce the output fuel. The quantity of hydrogen and Carbon Dioxide required in each scenario is assessed below using mass balance. An output of 1kg of the subject fuel is considered.

5.1.1.1 Sabatier Reaction Mass Balance

In order to produce methane the Sabatier reaction is used. As discussed above the reaction takes two forms. A mass balance is completed for each, to determine the required mass of reagent gases required to produce 1kg of methane. The quantities of each species required are detailed in Table 1.

Table 1: Mass Balance for Sabatier Reaction

$3H_2 + CO \rightarrow CH_4 + H_2O$			
Variable	Methane	Carbon Monoxide	Hydrogen
Mass	1 kg = 1000g	1746.3 g = 1.75kg	377.8 g = 0.38 kg
Molar Mass	16.04 g/mol	28.01 g/mol	2.02 g/mol
Moles	62.34	62.34	187.03
$4H_2 + CO_2 \rightarrow CH_4 + 2H_2O$			
Variable	Methane	Carbon Dioxide	Hydrogen
Mass	1 kg = 1000g	2743.6g = 2.74kg	503.7 g = 0.5 kg
Molar Mass	16.04 g/mol	44.01 g/mol	2.02 g/mol
Moles	62.34	62.34	249.36

5.1.1.2 Fischer-Tropsch Reaction Mass Balance

In order to produce hydrocarbon fuels the Fischer-Tropsch process is used. To assess the effect the n value has on the reagent masses required scenarios for n=12 and n=18 will be analyzed. Diesel Fuel would correspond to a value of n=10-15. As discussed above 1kg of the synthetic fuel is the desired product. The quantities of each species required are detailed in Table 2.

Table 2: Mass Balance for Fischer-Tropsch Reaction

N=12	$25H_2 + 12CO \rightarrow C_{12}H_{26} + 12H_2O$		
Variable	$C_{12}H_{26}$	Carbon Monoxide	Hydrogen

Mass	1 kg = 1000g	1973.02g = 1.97 kg	296.4 g = 0.3 kg
Molecular Weight	170.335 g/mol	28.01 g/mol	2.02 g/mol
Moles	5.87	70.44	146.75
N=18	$37H_2 + 18CO \rightarrow C_{18}H_{38} + 18H_2O$		
Variable	$C_{18}H_{38}$	Carbon Monoxide	Hydrogen
Mass	1 kg = 1000g	1981.02g = 1.98 kg	293.6 g = 0.29 kg
Molecular Weight	254.49 g/mol	28.01 g/mol	2.02 g/mol
Moles	3.93	70.73	145.4

5.1.1.3 Reverse Water Gas Shift Mass Balance

The reverse of the water gas shift reaction can be used to convert captured CO_2 to CO, which can then be synthesised with hydrogen to produced synthetic hydrocarbon fuels by the Fischer-Tropsch process discussed above. In this case the required carbon monoxide of 1.98 kg calculated above is used as the value for required output. The quantities of each species required are detailed in Table 3

Table 3: Mass Balance for Reverse Water Gas Shift Reaction

$H_2 + CO_2 \rightarrow CO + H_2O$			
Variable	Carbon Monoxide	Carbon Dioxide	Hydrogen
Mass	1.98 kg = 1981g	3111.5 = 3.11 kg	142.8 g = 0.14 kg
Molecular Weight	28.01 g/mol	44.01 g/mol	2.02 g/mol
Moles	70.7	70.7	70.7

5.1.2 Levelized Cost of Components

In order to accurately compare all costs, levelized cost of production in kg will be used for each sub component of the systems. The components of the electrolysis plant are considered below in Table 4. It is assumed that the levelized cost of electricity provided to each system is provided at a constant value of 16 ¢/kWh [7]. The cost of other equipment in the system was estimated as discussed in the table.

Table 4: Cost of Electrolysis Components

Equipment	Levelized Cost/kg of product	Source
Standard Electrolysis Unit	$0.36/kg	produced using capital cost, operating cost, and production metrics from the paper by Saur et al, and assuming a 40 year lifetime, a 7 year replacement period, and an a 8% discount rate [8]
High temperature Steam Electrolysis Unit	$0.43/kg	Estimated 20% increase in cost above standard electrolysis
Co-Electrolysis Unit	$0.54/kg	Estimated 50% increase in cost above standard electrolysis (additional material handling costs beyond high temperature electrolysis)
CO_2 Capture Unit	Direct = 0.66USD/kg Emission capture = 0.088USD/kg	Values obtained from [4] Table 2.5

The Electrolysis units for Low Temperature and the High Temperature units are assumed to have the efficiencies presented in Table 5.

Table 5: Effective efficiency of Various electrolysis mechanisms

Equipment	Efficiency (kWh/kg)	Source
Standard Electrolysis Unit	50	[8]
High temperature Units Electrical hydrogen	35	[9]
High temperature Units Thermal hydrogen	8	[9]
High temperature Units Electrical Carbon Monoxide	6	Estimated Value based on a comparison of the Gibbs free energies of Hydrogen splitting reaction and of the CO_2 to CO reaction.
High temperature Units Thermal Carbon Dioxide	2	Conservative Estimated value based on the percentage relationship between electrical and thermal for hydrogen.

5.1.3 Cost Comparison of Electrolysis Cycles

The study used to reference the cost for a standard electrolysis unit assumed a unit throughput of 50,000 kg/day; this translates to an electric requirement of 104 MW [8]. This will be larger than the reactor required in this application however with a larger nuclear reactor the levelized electricity cost would decrease while the cost of the electrolysis device scales fairly linearly, so the present study will provide a conservative result.
The levelized cost of electricity provided to the electrolysis unit is added to the levelized cost of the electrolysis unit to calculate the levelized cost of the assembly/ kg of hydrogen produced.

In order to estimate the cost of different methods of carbon capture the estimate that is provided in the direct air capture manual is modified with the actual cost of electricity which instead of being $71/MWh will be estimated as $160/MWh for the higher levelized cost of electricity for an SMR. This changed the total cost from $80/ton CO_2 for off gas capture and $610 for direct capture to $110/$CO_2$ ton and $650/$CO_2$ ton respectively.

5.1.3.1 Methane Production

The conditions for this scenario are provided in Table 6 below.

Table 6: Conditions for Methane Production Scenarios

Variable	Low Temp Electrolysis	High Temp Electrolysis	Co-Electrolysis Cell
Levelized Cost of Electricity	16¢/kWh	16¢/kWh	16¢/kWh
Effective Levelized cost of heat		9¢/kWh	9¢/kWh
Electrolysis Efficiency hydrogen (elec)	50 kWh/kg	35 kWh/kg	35 kWh/kg
Electrolysis Efficiency hydrogen (heat)		8 kWh/kg	8 kWh/kg
Electrolysis Efficiency Carbon Dioxide (elec)			6 kWh/kg
Electrolysis Efficiency Carbon Dioxide (heat)			2 kWh/ kg
Electrolysis Unit Cost	$0.36/ kg	$0.43/ kg	$0.54/ kg
Direct Air Capture Cost	$0.65/ kg	$0.65/ kg	$0.65/ kg
Emissions Capture Cost	$0.11/ kg	$0.11/ kg	$0.11/ kg
Hydrogen Gas Required	0.5 kg	0.5 kg	0.38 kg
CO_2 Required	2.74 kg	2.74 kg	2.74 kg

The costs of Hydrogen production is calculated by summing each of the separate $/Kg costs. The results for each calculation are presented in Table 7

Table 7: Cost for all Methane Scenarios

CO_2 Capture Method	Low Temp Electrolysis	High Temp Electrolysis	Co-Electrolysis Cell
Direct Capture	$6/kg	$5.2/kg	$4.8/kg
Emissions Capture	$4.5/kg	$3.7/kg	$3.3/kg

5.1.3.2 Hydrocarbon Fuel Production

The conditions for this scenario are provided in Table 8 below.

Table 8: Conditions for General Hydrocarbon (n-=12-18) Production Scenarios

Variable	Low Temp Electrolysis	High Temp Electrolysis	Co-Electrolysis Cell
Levelized Cost of Electricity	16¢/kWh	16¢/kWh	16¢/kWh
Effective Levelized cost of heat		9¢/kWh	9¢/kWh
Electrolysis Efficiency hydrogen (elec)	50 kWh/kg	35 kWh/kg	35 kWh/kg
Electrolysis Efficiency hydrogen (heat)		8 kWh/kg	8 kWh/kg
Electrolysis Efficiency Carbon Dioxide (elec)			6 kWh/kg
Electrolysis Efficiency Carbon Dioxide (heat)			2 kWh/kg
Electrolysis Unit Cost	$0.36/kg	$0.43/kg	$0.54/kg
Direct Air Capture Cost	$0.65/kg	$0.65/kg	$0.65/kg
Emissions Capture Cost	$0.11/kg	$0.11/kg	$0.11/kg
Hydrogen Gas Required	0.43 kg	0.43 kg	0.29 kg
CO_2 Required	3.11 kg	3.11 kg	3.11 kg

The costs of Hydrogen production is calculated by summing each of the separate $/kg costs as was done above in section 5.1.3.1. The results are presented in Table 9 below.

Table 9: Costs for all Hydrocarbon Fuel Scenarios

CO_2 Capture Method	Low Temp Electrolysis	High Temp Electrolysis	Co-Electrolysis Cell
Direct Capture	$5.6/kg	$5/kg	$4.4/kg
Emissions Capture	$4/kg	$3.2/kg	$2.7/kg

5.2 Consideration of the Gasification Hydrogen Electrolysis Hybrid Cycle

The cost of a biomass plant is dependent on many factors including: the quality of the feed, the required process, and the desired output fuel. For the purpose of this study the cost analysis work completed by Swanson is used [10]. From the results presented in this paper a reference cost of 4 – 8 $/GGE, will be used to estimate the cost of a standard biomass to synthetic fuel gasification process. The GGE refers to the gasoline gallon equivalent this is a unit used to describe the amount of alternative fuel required to

equal the energy content of a gallon of gasoline. The conversion from gallons of diesel to GGE is 1.140 Gal diesel =1 GGE [11].
To estimate the cost of the proposed Gasification Hydrogen Electrolysis Hybrid Cycle the cost of producing supplemental hydrogen via electrolysis is considered. Referring to the mass balance exercise complete in 5.1.1.2 it is assumed that 1.97Kg of carbon monoxide and 0.3 Kg of hydrogen are required to produce 1Kg of synthetic hydrocarbon fuel. The amount of hydrogen produced from gasification is then calculated and the required amount supplied from electrolysis can be estimated. The results are indicated in Table 10.

Table 10: Cost of Electrolysis Gasification Hybrid

Carbon Monoxide Produced from Gasification	1981.02g
Moles of Carbon Monoxide	(1981.02g)/(28.01 g/mol) = 70.7 mol
Moles of Hydrogen Produced	35.35 mol
Mass of Hydrogen from Gasification	(35.35mol)*(2.02 g/mol)=71.4g
Mass of Hydrogen required from Electrolysis	300-71 =229 g =0.23kg

In an accompanying paper the cost of hydrogen production was estimated to be $8/kg [12]. This equates to an added cost of $1.85/kg of synthetic fuel produced. The total GGE cost including the biomass to fuel and nuclear hydrogen production is estimated to be $9.1-13.1/GGE. It should be noted that the use of electrolysis would also produce oxygen which could be used as a feed for the gasification process; this will reduce the cost required for air separation. Furthermore the use of pure hydrogen produced from electrolysis of H_2O will reduce the requirements for syngas cleaning. The above factors will reduce the effective cost of the synthetic fuel production however it is not anticipated that they will incur a substantial reduction in the cost of the produced fuel per GGE. A larger effect will be incurred by the fact that a water gas shift reactor or a steam reformer is no longer required. As these cost savings are dependent on a number of factors it will be assumed that the cost could reach the lower end of the range at around $9-10/GGE.

5.3 Cost Summary

The costs per kg above are converted to Gasoline gallon equivalent in order to compare to the estimated cost of production via gasification.
A brief analysis of Canadian diesel and natural gas purchase prices was conducted to determine the economic feasibility of synthetic fuels in general. It was found that northern Canada experiences the highest fuel costs with an estimated diesel cost of $1.3/L ($4.92/Gal) or $4.32/GGE[13]. Natural gas costs are significantly lower currently about 20% of the diesel cost for the same energy content [14]. In Table 11 below the lowest cost scenarios are compared.

Table 11: Lowest Cost Scenarios for Fuel Production

Scenario	Cost	Density	Cost	GGE conversion	GGE cost
Co-electrolysis methane production (Emission Capture)	$3.3/kg	0.656 kg/m3	$2.16/m 3	3.587m3=1GGE	$7.8/GGE
Co-electrolysis hydrocarbon fuel Production (Emission	$2.7/kg	0.8kg/L 3.03 kg/Gal	$8.2/Gal	0.9 G = 1GGE	$7.4/GGE

Capture)					
Gasification Plant producing diesel					$4-8/GGE
Nuclear Gasification plant Hybrid Cost					$9-10/GGE

Current natural gas prices are at such a level that it would not be possible for synthetic natural gas to be produced at a competitive cost. Diesel costs may be an achievable metric in future; especially considering the cost of diesel is expected to rise in coming years. As such all diesel cost scenarios are considered below in Table 12.

Table 12: Diesel Cost Scenarios ($/GGE)

	LTE	HTE	Co-Electrolysis	Gasification	Nuclear Gasification Hybrid
Emission Capture	11	8.7	7.4	4-8	9-10
Direct Capture	15.3	13.7	12	4-8	9-10

6. Discussion of Results

The cost figures above for the electrolysis/capture cycles do not include the cost of the Fischer-Tropsch synthesis reactor, which would be required to synthesise the fuel from the syngas. Referring to the paper by Swanson an estimated levelized cost of a Fisher-Tropsch unit was estimated to be $0.02/Kg [10]. Considering the high level of uncertainty for the cost estimates made in this study this cost will have a negligible effect on the results.

Comparing carbon neutral cycles based on the results of section 5.3 it is noted that the cost of fuel production using capture/ electrolysis processes is lower than the carbon neutral cycle using a nuclear/ gasification hybrid plant as long as emissions capture is used. The two primary factors that will decrease the cost per GGE for the product fuels are the levelized cost of electricity and the efficiency of the electrolysis equipment. Both of these parameters remain uncertain quantities, as the technologies are in their infancy and have not yet been commercialized on a large scale. Regardless of the uncertainty in the values the results indicate that significant improvements in levelized cost of energy from an SMR and electrolysis efficiency would need to be realized in order to make a viable business case. As the cost of diesel fuel rises in future and with any government incentives designed to restrict fossil fuel usage these technologies could be economically comparable to the shipping of fossil fuels. It should also be noted that the use of an SMR and small size equipment, while producing less throughput allows for a smaller initial capital investment. This may be of value if some upfront funds are available to initiate a project and quick fuel production is desired.

Due to the ease of dispatching diesel or natural gas fuels it is possible that the proposed cycles could be used as energy storage mechanisms when linked to a grid powered by a nuclear reactor. In this concept the synthetic fuel production cycle would be engaged when the power supplied by the reactor exceeded the communities demand, the fuel produced is easily stored or transported with equipment that is well commercialized. When the load demand rises above the capacity of the nuclear generation, supplementary electricity would be generated by burning fuel, produced in low demand periods. The by-product carbon dioxide from the combustion of this fuel could be captured and re-circulated for use in producing more fuel in low demand periods. Hydrogen has frequently been proposed for grid storage; however the storage of hydrogen and electric recovery in a fuel cell is not as developed as the storage and combustion of diesel fuels. The cost of hydrogen production versus the cost of synthetic

diesel fuel production is very comparable per GGE. The efficiency of a fuel cell exceeds that of an internal combustion engine, but depending on the end use and the difficulty of storage, transportation, and dispatch for hydrogen the conversion to a diesel fuel may prove more economic in some cases.

7. References

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