Techno-Economic Analysis of Ammonia Production in the Presence of Uncertainty

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Abstract

This work aimed to model the costs of ammonia production comparing three hydrogen input technologies (SMR, pyrolysis, & electrolysis) while accounting for irreducible uncertainties within the calculation framework. This was accomplished through the use of Monte-Carlo simulations both in @RISK and with proprietary Python scripts producing CNPV distributions for each design under various carbon tax and discount rate conditions. It was determined that pyrolysis was the most consistently cost effective hydrogen technology option in the production of ammonia while incorporating uncertainties.

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Nomenclature

ASL	Ammonia Synthesis Loop	**NPV**	Net Present Value
ASU	Air Separation Unit	**OC**	Operating Cost
CCS	Carbon Capture & Storage	**PC**	Product Costs
CF	Cash Flow	**PE**	Purchased Equipment
CNPV	Cost-Net Present Value	**PEM**	Polymer Electrolyte Membrane
CTM	Carbon Tax Multiplier	**PFD**	Process Flow Diagram
CEPCI	Chemical Engineering Plant Cost Index	**PS**	Production Scale
DR	Depreciation Rate	**PSA**	Pressure Swing Adsorber
FCI	Fixed Capital Investment	**SMR**	Steam Methane Reforming
FO&M	Fixed Operating & Manufacturing Cost	**TCI**	Total Capital Investment
GE	General Expenses	**TPC**	Total Product Cost
GPV	Gross Present Value	**VO&M**	Variable Operating & Manufacturing Cost
IRS	Internal Revenue Service	**WC**	Working Capital
MACRS	Modified Accelerated Cost Recovery System	**WUC**	Water Utility Cost
MCS	Monte Carlo Simulation	$\boldsymbol{\theta_{fs}}$	Federal and State Taxes
MM	Maintenance & Material Cost	$\boldsymbol{\Psi}$	Tax Shield

Executive Summary

As global energy consumption increases rapidly, compounded by a growing concern with regard to climate change, alternative energy vectors are highly desirable. Current technological limitations in long term energy storage mean that renewable energy, such as wind, solar, and hydroelectric power, are often impractical or prohibitively expensive [5]. Hydrogen is a promising alternative energy source, producing no CO_2 at point of use via a hydrogen fuel cell. Hydrogen requires extreme conditions to transport or store, which makes long term hydrogen storage expensive and impractical. Ammonia is a potential solution to this, as it can be stored under much more favorable conditions and could serve as a hydrogen transportation mechanism.

An alternative energy source such as ammonia requires economic favorability to see widespread uptake. A discounted cash flow model is often used to evaluate the profitability of a project through calculating its net present value (NPV). However, this analysis does not take into account the many uncertain aspects of a system, resulting in the "flaw of averages;" the average value of an economic parameter over time is not truly indicative of the variance and impact of that parameter, leading to mischaracterization of the parameter, its trends, and its performance [11]. To overcome the "flaw of averages," Monte Carlo simulations (MCS) are used by creating distribution profiles for uncertain inputs and sampling them numerous times (for the purposes of this paper, 10,000) to create a distribution profile of the analyzed output metric(s). This equips the decision maker with additional insight into cost probabilities, as well as the impact of each uncertain parameter on the simulation outcome thus allowing a more informed decision about the risks associated with the project.

For the purposes of this paper, a cost-net present value (CNPV) will be considered. This is similar to an NPV, but removes the revenue stream to evaluate only the distribution of associated project costs. This leaves the complex assessment of market value of the product to the decision maker to determine profitability, and allows this paper to compare competing technology options without directly assessing profitability.

The three technology options for ammonia production considered by this paper are steam methane reforming (SMR), methane pyrolysis, and electrolysis. SMR is the catalytic separation

of hydrocarbons (coal) in the presence of carbon capture and storage technology (CCS), representing the most carbon-intensive process considered. Methane pyrolysis is a newer technology which separates methane into hydrogen and solid carbon. While this does not produce CO_2 on its own, this process is often powered by fossil fuel combustion and thus produces CO_2, but to a lesser degree than SMR. Electrolysis involves the decomposition of water into hydrogen and oxygen. Notably this produces no CO_2, but has considerably increased costs of purchased equipment and energy than the other options considered.

This paper uses MCS to analyze a discounted cash flow model with uncertain inputs. A full breakdown of the CNPV framework of equations can be found in section 2.1, and a table of all uncertain inputs can be found in section 2.2. @RISK (a software by Palisade) was used as a computational platform for performing MCS.

One of the other important endeavors of this work was to replicate the functionalities of the @RISK software in a suite of proprietary Python scripts, written to conduct the MCS. Further description of these efforts can be found in sections 1.3 and 2.3. The results of the CNPV simulations conducted using our Python scripts showed appreciable congruence with the results procured from @RISK within the same order of magnitude. We can say with a high degree of certainty the Python scripts used to carry out the simulations presented in this report are consistently and accurately replicating the @RISK software, and furthermore serve as proof of concept for the implementation of MCS into higher level platforms.

Below are the pertinent CNPV results describing the base case where the discount rate (r) was set to 0.16 and the Carbon Tax Multiplier (CTM) was set to 0. Given the significantly higher PE and OC of electrolysis, its resultant CNPV distribution was of much greater magnitude than the other technologies. While the PE and OC of SMR and pyrolysis were comparable in magnitude, SMR remains slightly more cost effective in the absence of significant regulation or tax on carbon emissions.

Table i: Pertinent results for base case: r = 0.16, CTM = 0

	Electrolysis	Pyrolysis	SMR
PE ($)	1.96×10^9	9.33×10^8	9.37×10^8
OC ($)	3.90×10^9	8.09×10^8	6.23×10^8
Carbon Intensity (metric tonne/day)	0	1141.6	4246.75
P_5	5.82	1.69	1.55
P_{95}	6.90	2.18	2.04
STDEV*	3.29	1.47	1.47
AVG	6.33	1.93	1.78

***All STDEV are $\$x10^9$ and all other costs are $\$x10^{10}$**

As the CTM was increased over the course of multiple simulations, the impact of carbon intensity was realized as the SMR distribution shifted far more than did pyrolysis. As CTM was increased the shifted SMR distribution approached that of electrolysis, thus making electrolysis a comparatively attractive hydrogen technology option for ammonia production in high carbon regulation environments. Overall, pyrolysis showed to be the most consistently attractive technology option in the widest variety of economic situations. Figure (i) depicts CTM sensitivity analysis findings as described above.

A sensitivity analysis on the discount rate was performed, analyzing rates between 10% and 20%. This analysis shows that as the discount rate increases, the average CNPV, P_5, P_{95}, and standard deviation decrease for all technology options. As the associated costs are lower for a higher discount rate, consideration of a higher discount rate could be seen as the risk-tolerant choice. However, given that the standard deviation also decreases as discount rate increases, a lower discount rate could be seen as the risk-averse choice, as it narrows the possibilities of CNPV outcomes. Ultimately, a decision maker must consider both of these aspects in defining their risk tolerance with regard to discount rate.

A logical extension of this work is to evaluate revenue streams for the considered technologies in the presence of uncertainty to generate NPV distribution profiles, which would give the decision maker information about the profitability of the plant instead of purely comparative cost evaluations.

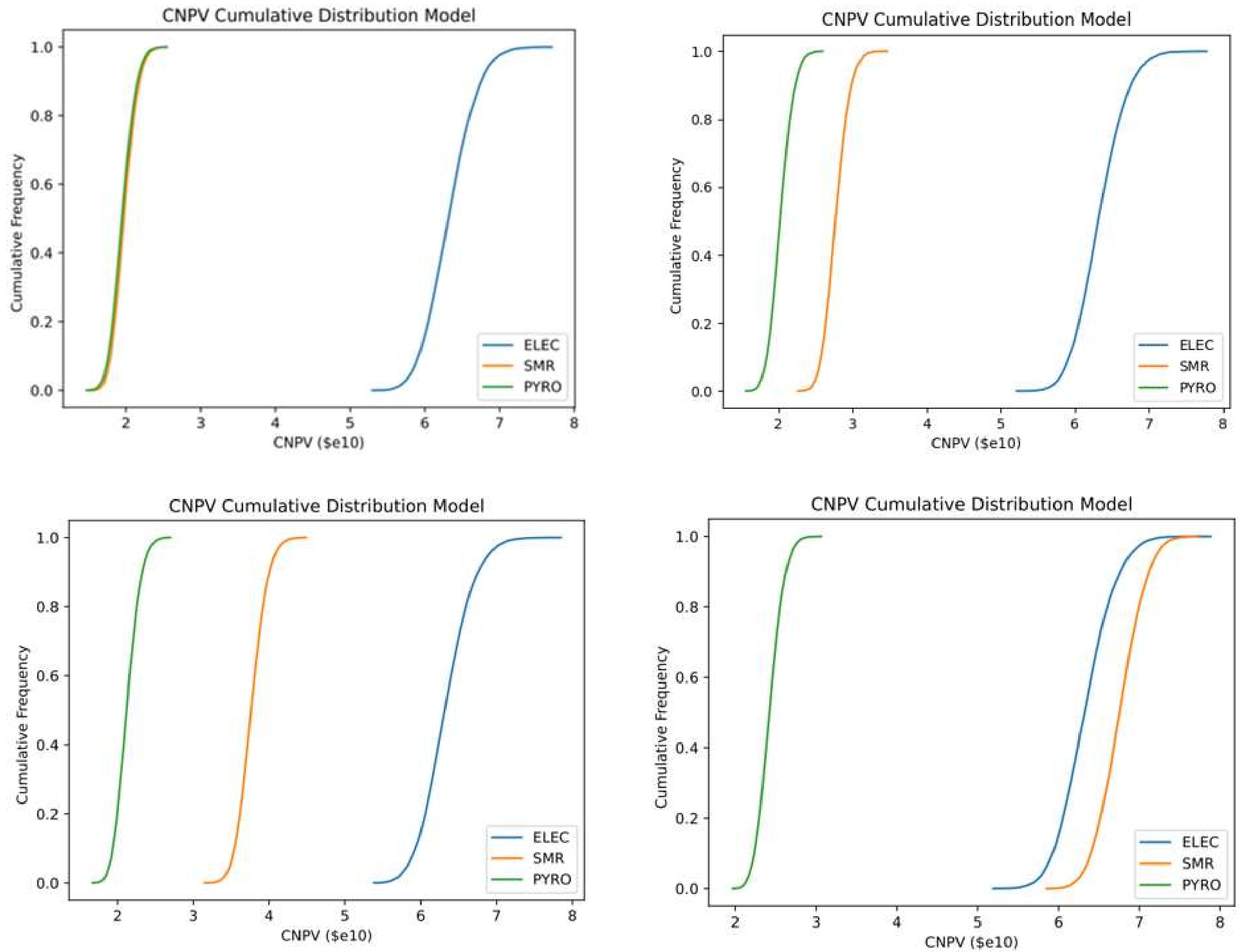

Figure i: Cumulative CNPV Distributions for all process designs under different carbon tax conditions

Top Left: CTM = 1, Top Right: CTM = 5, Bottom Left: CTM = 10, Bottom Right: CTM = 25

1: Introduction

1.1: Preliminaries

The world has undergone tremendous revolutions in technological advancement, urbanization, and industrialization in the past few decades, while sustaining an ever growing population. Central to this rapid development is the energy that powers our homes, businesses, and way of life. Global energy consumption has increased by 46% in the last 20 years, with 80% of energy being produced from oil, gas, and coal [1][2]. At the current rate of consumption, it is predicted that all fossil fuels will be exhausted by the year 2090 [3]. Compounded with the growing concerns over climate change and carbon emissions, development of alternative energy production vectors has never been more pertinent.

The primary interest in fossil fuel alternatives is renewable energy, namely hydroelectric, wind, and solar power. These production vectors provide purely renewable energy without the need for consuming limited natural resources or producing carbon dioxide. However, they have some limitations as a permanent replacement to fossil fuels. The primary issue faced by these processes is their intermittency; energy production is limited to current conditions and is not available to meet dynamic energy needs [4]. Compounding this issue, large scale energy storage is currently too expensive and impractical to see widespread use [5]. This is what makes fossil fuels so desirable; energy is physically stored as oil, gas, or coal that can be burned on demand to meet consumption needs.

Another growing area of interest in the field of energy is hydrogen. From 2000 to 2018, global demand for hydrogen increased by 46%, as shown in Figure 1 [6]. Its primary use is as an energy storage vector in the form of hydrogen fuel cells; hydrogen gas reacts exothermically with oxygen to produce water, making carbon-free energy at point of use. Because of this property, it has been postulated that hydrogen can be used as a storage mechanism for renewable energy to eliminate the intermittency problem completely carbon-free. However, energy

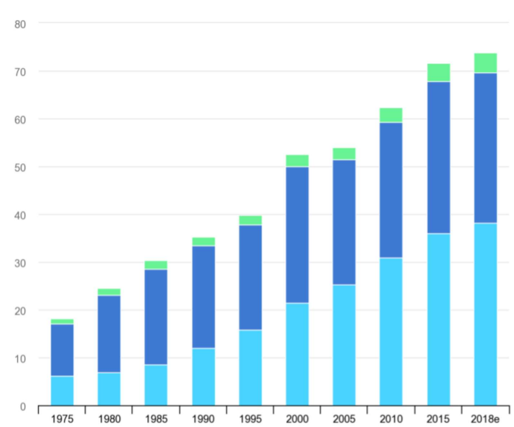

Figure 1: Global hydrogen demand [6]

losses in this process are presently too great for renewable energy storage through hydrogen to see widespread use [7]. Hydrogen has applications beyond renewable energy storage - it can be produced from coal and natural gas to centralize the carbon production where its impacts can be mitigated through carbon capture and storage (CCS) systems. Refer to section 1.4 for detailed descriptions of these hydrogen production pathways. Hydrogen-based energy is a promising transitional pathway from fossil fuels to renewable energy.

Despite its potential, hydrogen has some logistical problems as a widespread energy source. Hydrogen is a highly volatile and flammable gas that requires extreme conditions to transport and store. Gaseous hydrogen storage requires vessels up to 700 bar, while liquid hydrogen storage requires cryogenic conditions of -253 °C [8]. The energy required to maintain these conditions makes hydrogen storage impractical in the long term. One solution to this is to use ammonia as a hydrogen carrier. Ammonia is gaseous at room temperature, but only requires conditions of 10 bar or -33 °C to be liquefied. Additionally, ammonia has a higher volumetric energy density at 14 MJ/L, compared to 10 MJ/L and 6 MJ/L for liquefied and gaseous hydrogen respectively [8]. Ammonia can be combusted directly for fuel, or hydrogen can be re-evolved from it, but these processes both induce an energy loss. This energy loss must be weighed against the high storage and transport costs of hydrogen. Ammonia has added industrial use aside from the energy sector. Ammonia is used in explosives, refrigeration, textiles, plastics, and commercial cleaners, with 150 million metric tons being produced worldwide in 2022 [9]. Its primary industrial use is in fertilizers, accounting for 80% of global ammonia consumption, as shown in Figure 2 [10]. Ammonia is a multi-faceted product that shows promise as a hydrogen-carrier for energy production as well as its industrial applications.

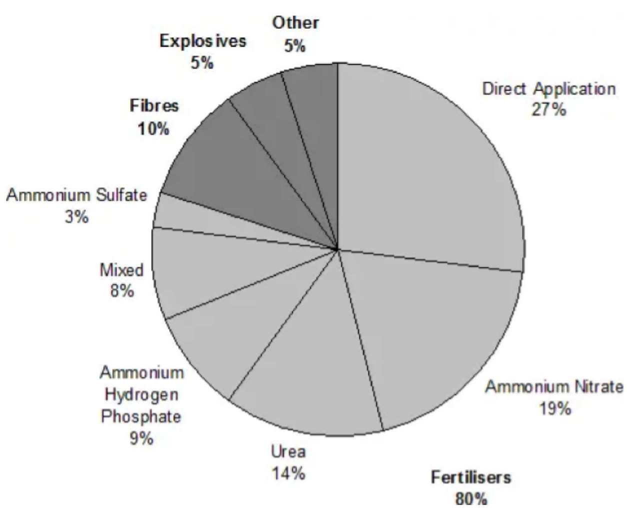

Figure 2: Industrial uses of ammonia [10]

1.2: Pertinent Economic Modelling Techniques

In order for an energy production vector such as ammonia to see widespread uptake, it must have economic favorability over its competitors. As such, a standardized model for comparing and quantifying profitability is needed. The commonly used model for this is discounted cash flow analysis. This method incorporates the time value of money with a discount rate to generate a net present value (NPV), or the sum of the discounted difference between cash flows in and out over the lifetime of the plant. For a detailed description of the framework of equations used in this analysis, see section 2.1. Discounted cash flow analysis is extremely popular for its simplicity which allows it to be easily modeled in any computational platform such as Excel.

While discounted cash flow analysis is a widely accepted, simple method for comparing and evaluating economic performance, it has many limitations in the assumptions that must be made to arrive at an NPV. Many aspects of the plant are uncertain in nature; from the market dependent cost of raw material, selling price of product, labor costs, tax rates, and many more, the actual NPV of the plant can vary drastically if these potential variances are not accounted for. From this stems the "flaw of averages" - the idea that the average value of an economic parameter over time is not truly indicative of the variance and impact of that parameter. This in turn may lead to mischaracterization of the parameter, its trends, and its performance [11]. Discounted cash flow analysis may find that the average NPV of a project is positive, but this is far from a guarantee of profit. The potential NPVs of the project could extend far into the negatives, meaning a seemingly profitable project has a substantial chance to actually lose money over its lifetime. The reverse can also be true; a seemingly mediocre project may have the potential for sizable profit if its full range of potential NPVs are considered.

To overcome the "flaw of averages," uncertain model inputs must be accounted for in the discounted cash flow analysis instead of single point estimates. This is accomplished by representing the uncertain parameters of the model with distributions of potential values. These distributions consider reasonable ranges of the values determined by experience in the field, or by sampling historic data. The NPV can then be calculated iteratively, sampling random values from the distributions of uncertain inputs. Once the desired number of iterations has been reached (for the purposes of this paper, 10,000 iterations), an NPV distribution profile can be generated that gives more insight into the likely possibilities for the NPV of the project. This process is known as a Monte Carlo simulation (MCS). The NPV profile can be used to make decisions about the project that appeal to the decision maker's risk tolerance. For instance, a risk-tolerant decision maker may value the top 5% of profit possible, or the 95th percentile of the distribution (P_{95}), while a risk-averse decision maker may be more interested in the bottom 5% of potential profit (P_5). Additionally, these simulations can be used to analyze the sources of uncertainty in the model to locate potential cost saving measures or focus resources for optimization. The use of Monte-Carlo simulations arms the decision makers with the probabilistic data needed to make a well informed decision, effectively overcoming the "flaw of averages."

This paper will utilize a metric that is similar to NPV, but removes the revenue. This leaves a distribution profile depicting only the associated costs of the project. This metric is referred to as the cost-net present value (CNPV). This is given as a positive number, which notably reverses the risk profile; the P_5 is now the value at risk, depicting the lowest 5% of costs, and the P_{95} is the value at opportunity, depicting the highest 5% of costs. When different production vectors have equivalent production scales, revenue is the same, so CNPV is able to compare production methods without directly analyzing profitability. Ammonia selling price fluctuates greatly according to market conditions. The ammonia market has been particularly volatile in the last

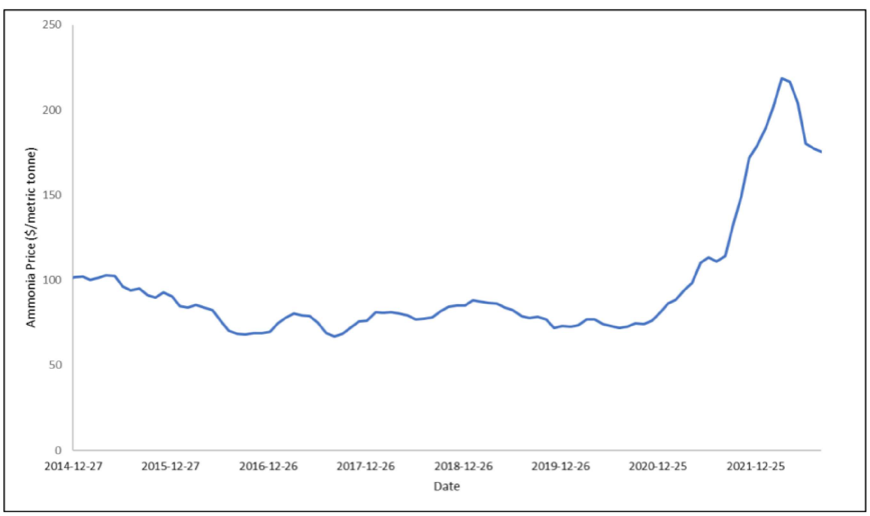

Figure 3: Historic ammonia pricing [12]

few years, as shown in Figure 3. Ammonia price has shown a large increase in 2021, over doubling its previous peak [12]. These volatile conditions mean that a simple historic sampling of ammonia pricing is an incomplete metric for predicting future revenue. Predicting the market is a complex task that is highly individualized to the risk preferences of the decision maker, and is well beyond the scope of this paper. By presenting a CNPV, the decision maker is allowed to incorporate their own market predictions to achieve a better reflection of the profitability of the project.

1.3: Utilization of Python in Modern Data Analytics

While Excel remains a powerful and popular data analytics tool, it has its limitations in terms of efficiency when carrying out complex calculations similar to the aforementioned economic modeling techniques. The use of Python has become an immensely popular choice for performing advanced computational tasks or manipulating large datasets when efficiency and speed are of high importance[13]. Python has the added benefit of being significantly easier to automate than Excel, as well as being easier to integrate into other software. The diverse set of available modules, packages, and add-ons to the normal Python library make it an attractive alternative for a breadth of applications where automation and speed are necessary. For instance, there are modules for performing advanced statistical analyses on large datasets, graphing results in numerous ways, and saving those results as various file types. This level of automation while simultaneously performing advanced calculatory tasks would not be possible in Excel with the same level of efficiency. Also notable is that Python syntax errors are significantly easier to identify, interpret, and correct than they are in Excel, and in situations where security is of high importance Python offers more protection against hacking than does Excel [13].

One of the goals of this project was to create a suite of Python scripts to replicate the performance of @RISK by conducting MCS of the proposed process designs and graphically representing our findings as cumulative distributions. These efforts would serve as proof of concept for implementing MCS into higher level platforms with the goal of incorporating these scripts as supplementaries into commonly used process flow diagram softwares such as Aspen in future work.

1.4: Hydrogen Production Methods Incorporated into Ammonia Production

The following section will elaborate on the use of three different viable technology options in the production of hydrogen which will serve as the inputs to the proposed ammonia synthesis design. Descriptions of the functionality and governing chemical equations of each technology, along with process diagrams will be provided.

1.4.1: Steam Methane Reforming (SMR)

Steam reforming of natural gasses accounts for approximately 98% of worldwide hydrogen production, with reforming of methane specifically accounting for 48% [14][15]. Given the fact that it is readily available at relatively low cost, Methane remains an economically attractive hydrocarbon for use in these types of processes. Steam reforming produces significantly less CO_2 per unit H_2 produced than other more hydrocarbon intensive gasification methods [14]. In general, steam reforming to produce hydrogen involves the catalytic separation of hydrocarbons at high temperatures (700-900 °F) in the presence of both steam and specifically a metallic catalyst. This first catalytic splitting step results in a combination of carbon monoxide (CO) and hydrogen known as Syngas along with CO_2 and other byproducts of smaller side reactions. The reforming step enacts the general chemical equation described below:

$$C_nH_m + nH_2O \rightarrow nCO + (n + m/2)H_2$$

The Syngas is then sent through a series of gas-shift reactions in which the CO reacts with the steam present to produce CO_2 and H_2 as shown below.

$$CO + H_2O \rightarrow CO_2 + H_2$$

After a series of subsequent separation and purification steps (usually including a Pressure Swing Adsorption or PSA unit among others), the H_2 product is isolated with some of the product gas being recycled back to fuel the reactors earlier in the process. CO_2, CH_4, and other Non-Methane-Hydrocarbons are among the predominant emissions from SMR processes [14].

For the purposes of simulations in this report, the H_2 output from the SMR process would be the hydrogen input to the Ammonia Synthesis Loop (ASL). An air separation unit (ASU) would be used to isolate nitrogen gas from the air, and as mentioned, a PSA purifies and isolates the H_2 and both are fed into the ASL. A full SMR to NH_3 process flow diagram (PFD) can be found in Figure 4.

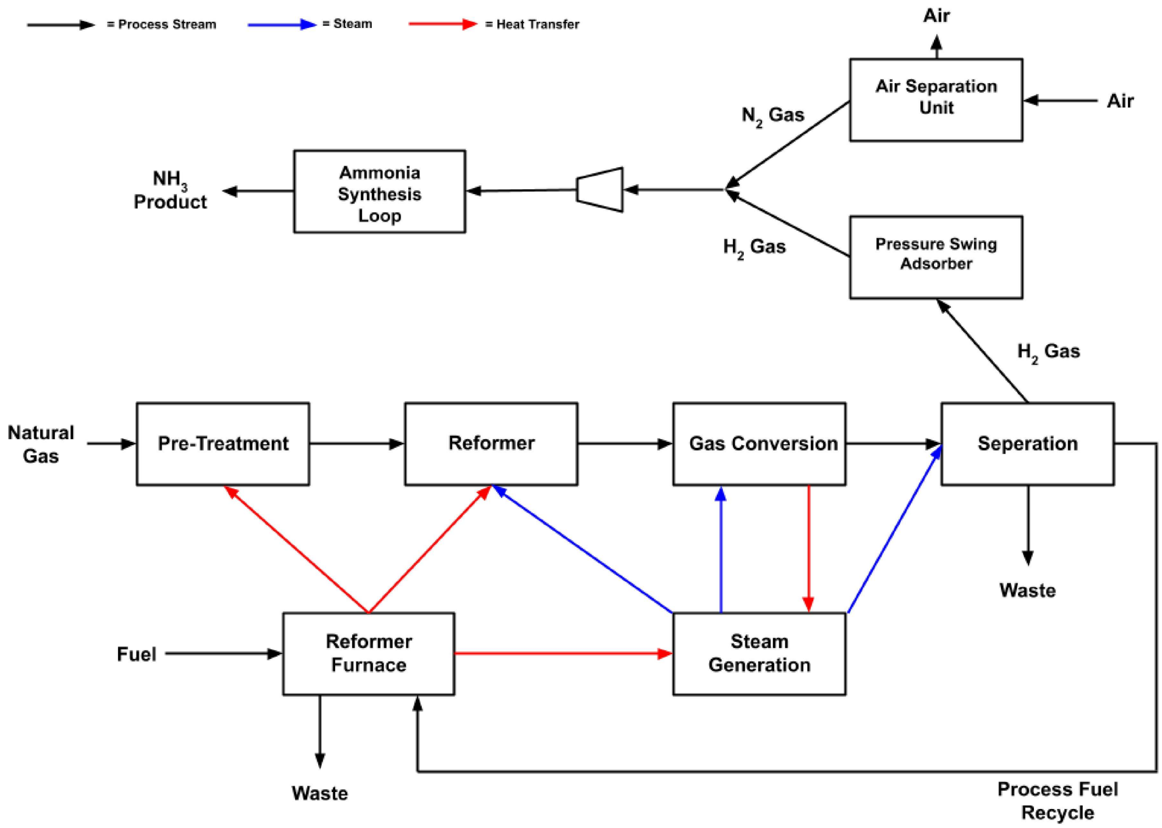

Figure 4: Process flow diagram of SMR ammonia production process (adapted from [15][16])

1.4.2: Methane Pyrolysis

As discussed in the previous section, while SMR produces considerably less greenhouse gas emissions than other gasification methods, it does still emit a considerable amount of CO_2 per unit H_2 produced. Thus, it can be inferred that in an increasingly carbon constrained environment, SMR could become considerably less cost efficient than other technologies. Methane pyrolysis is an emerging technology involving the production of H_2 from methane without directly producing CO_2. The chemical equation describing this process is shown below.

$$CH_4 \rightarrow C_{(S)} + 2H_2$$

It is often the case (and will be simulated as such in this report) that the pyrolysis process itself is powered by fossil fuels which brings about an equivalent CO_2 emittance for the technology option. However, that emittance is still significantly less than SMR and other gasification methods making it more attractive and competitive in the presence of regulatory actions on carbon release. Also worth noting is the solid carbon produced by this process can be sold in any number of forms offering another potential stream of revenue for this technology option [17]. However, one of the important caveats with pyrolysis is the management of the solid carbon produced, which if not correctly removed can more quickly degrade the catalyst(s) used and thus the efficiency of the process. Thus, operating costs associated with pyrolysis can vary with improperly handled carbon product.

Typically, pyrolysis works through the use of reactors containing molten metallic catalysts. This report will simulate a process containing a molten Ni-Bi alloy catalyst as described in the paper by Parkinson et al. [15], in which further description of the optimization process of reactor size and conditions to maximize yield while minimizing costs can also be found. After the reactor, a number of waste heat boilers, separation steps, and another PSA unit are used to isolate both the solid carbon and the H_2 gas, which as before will become the input to an identical NH_3 synthesis loop as previously described. A full pyrolysis PFD can be found in Figure 5.

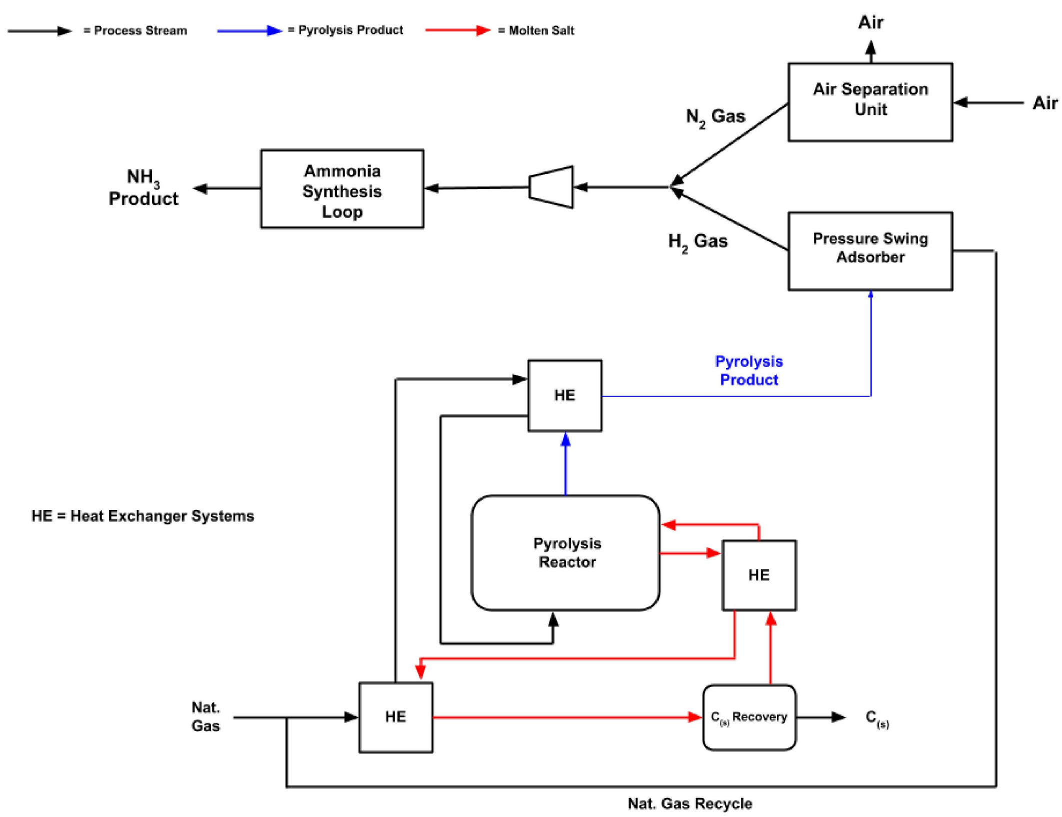

Figure 5: Process flow diagram of pyrolysis ammonia production process (adapted from [15][16])

1.4.3: Electrolysis

It is also worth investigating technology options in which no CO_2 is emitted at all in the production of hydrogen. Electrolysis of water is one such method and its governing chemical equation is shown below:

$$2H_2O \leftrightarrow O_2 + 2H_2$$

The notable tradeoff in the use of a technology option like this is that while the absence of emitted CO_2 is attractive, the required equipment is much greater than for other technologies thus increasing capital investment into the process to a much higher extent [18]. In general, electrolysis involves the splitting of water into its components, oxygen and hydrogen when electrical current is applied. Hydrogen yields are dependent on the strength of the applied current, which creates another interesting tradeoff as higher current strengths bring lower capital costs but higher operating costs and vice versa [15]. There are three prominent technology options for electrolysis, however, this report will specifically simulate the use of a polymer electrode membrane (PEM) electrolysis technique. Further information on the optimization of the PEM electrolysis costs can be found in the paper by Parkinson et al. [15]. The electrolysis process contains five key modules: water delivery systems, power electronics, electrolysis stacks, and postprocessing of both oxygen and hydrogen. As previously described, the hydrogen output from electrolysis becomes the input to the identical ammonia synthesis. A full electrolysis to ammonia PFD can be found in Figure 6.

A few final notes on electrolysis technologies: the power input to the process can come from any number of places, however this simulation will analyze electrolysis powered solely from renewable energy resources (wind, solar etc.). This is done to ensure the electrolysis process is truly carbon neutral, thus avoiding the impacts of carbon taxes or other regulatory measures. It is sometimes the case that surplus power is created beyond what is necessary to supplement the process or be held in the energy storage (if energy storage technologies are being implemented). In these situations there would be the added revenue stream associated with selling excess power back to the grid.

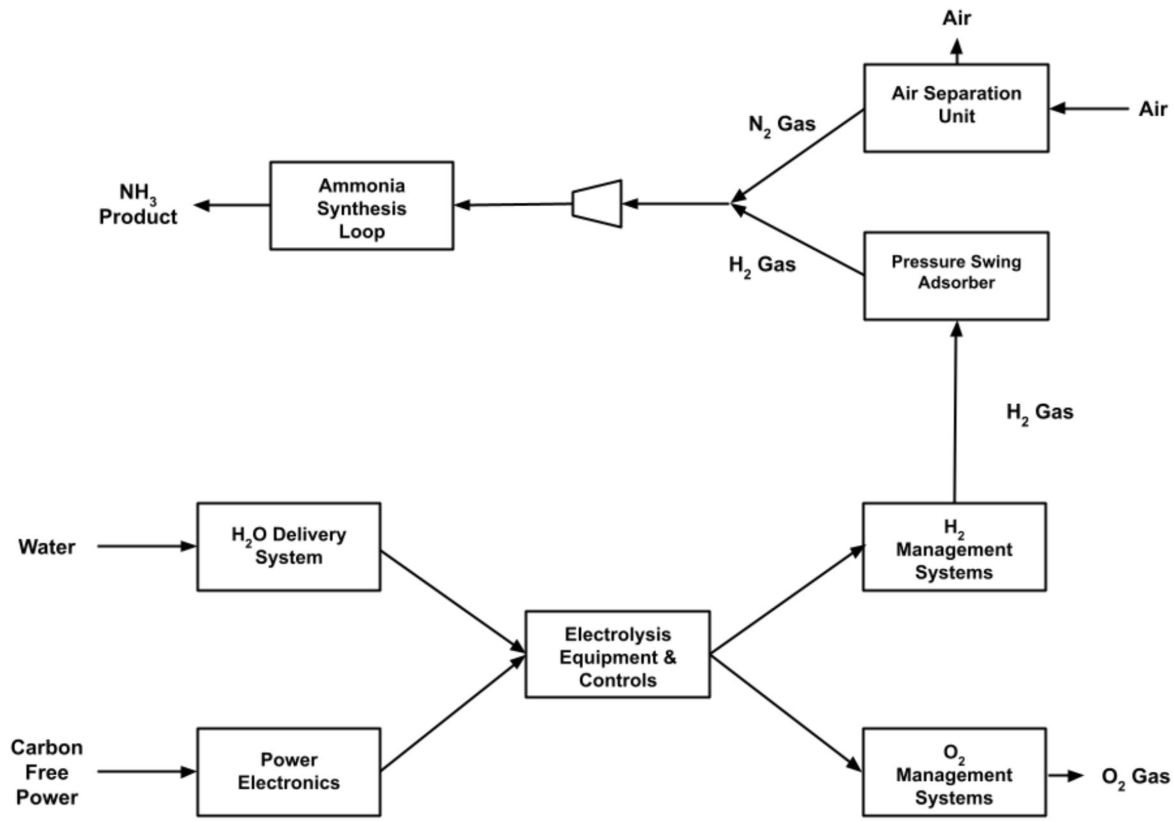

Figure 6: Process flow diagram of electrolysis ammonia production process (adapted from [15][16])

2: Methodology

The overall methodological approach to the Monte Carlo simulations performed in this paper is depicted in Figure 7 below. Additionally, one of the goals of our work was to replicate the performance of the MCS in Python in order to facilitate MCS in a higher level platform. This section details the methodology to accomplish each of these objectives.

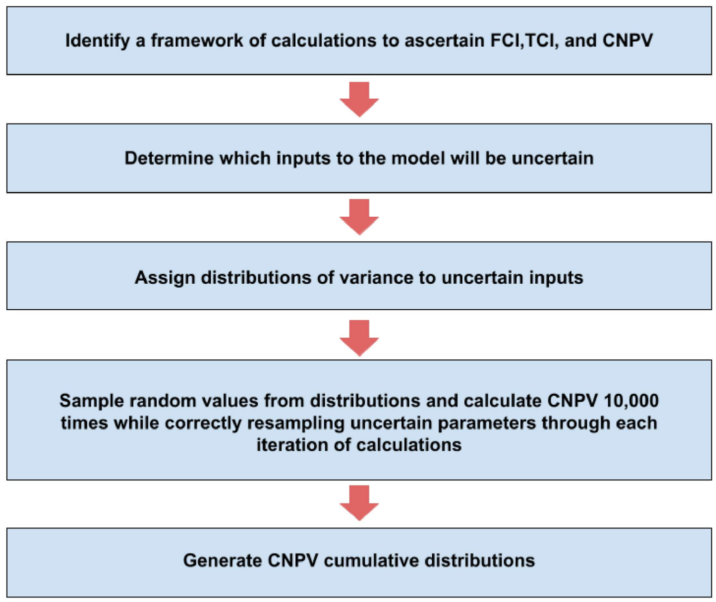

Figure 7: Procedural steps for implementation of Monte-Carlo Simulations

2.1: Cost Evaluation Framework

In order to analyze and compare the three ammonia production pathways considered, a sound framework of equations was needed to calculate the CNPV for each method. This framework was based upon discounted cash flow analysis. The basic model used here is dependent on many factors which in this paper are represented as a distribution of values rather than a fixed point using MCS. These parameters are further discussed and specified in section 2.2. The framework of equations introduced here will be written for the calculation of CNPV, but the calculation of NPV simply includes the addition of revenue where indicated in equation 10. CNPV is calculated by subtracting the initial fixed capital investment (FCI) from the gross present value (GPV), as shown in Equation 1 below:

$$CNPV = -(GPV - FCI) \tag{1}$$

The negative sign is introduced here to represent CNPV as a positive value, or a cost, rather than a negative cash flow. Note that this would not be necessary for the calculation of NPV. The GPV is a total of the discounted cash flows over the lifetime of the plant, discounted by the plant's nominal discount rate, as described by Equation 2:

$$GPV = \sum_{t=1}^{n} \frac{CF_t}{(1+r)^t} \quad (2)$$

where CF_t is the cash flow out (net cash flow for NPV) at year *t*, which is contributed to by the total product cost (TPC), depreciation, salvage value, working capital, and, in the case of NPV, revenue. *n* is the total lifetime of the plant in years, which is 30 for the purposes of this paper. *r* is the plant's nominal discount rate, the factor used to devalue money over time according to the time value of money. The nominal discount rate is determined by the project risks as well as the overall influence of the economy. For the baseline case in this paper, the discount rate was set at 16%. However, a sensitivity analysis on the discount rate was performed in section 3.2 to analyze its impact on the CNPV distribution profiles.

Total product cost is estimated as the sum of the production cost (PC) and general expenses (GE). Each of these expenses are comprised of several smaller expenses, many of which are a distribution of fractions of a set expense such as TCI. PC is the total of operating cost (OC), CO_2 transport and storage costs (CTSC), carbon tax (CT), insurance (INS), patents and royalties (PR), and plant overhead costs (POC). General expenses are the sum of administrative costs (AC), marketing costs (MC), research and development costs (RDC), and financing interest costs (FIC). The distributions used for each of these is shown in Table 1. The calculations for PC and GE are described below in Equations 4, 5 and 6:

$$TPC = PC + GE \quad (4)$$

$$PC = OC + CTSC + CT + INS + PR + POC \quad (5)$$

$$GE = AC + MC + RDC + FIC \quad (6)$$

Product cost may include other expenses, such as the delivery cost of the product. In the case of ammonia, transport does not require extreme pressure or refrigeration conditions (as is the case with hydrogen), so this expense was assumed to be negligible.

Depreciation of assets is also factored into the cash flow. Over the course of their lifetime, assets lose value. In this case, the plant is assumed to have fully depreciated at the end of the recovery period, 20 years, as is typical for a project such as this. The loss in value due to depreciation is tax exempt, and thus serves as a tax shield (Ψ), calculated by Equation 7:

$$\Psi_t = DR_t \cdot FCI \cdot \theta_{fs} \tag{7}$$

where DR_t is the depreciation in year *t* according to standard convention used by the Internal Revenue Service, FCI is fixed capital investment, and θ_{fs} is the sum of federal and state taxes. The depreciation method used to determine DR_t is the Modified Accelerated Cost Recovery System (MACRS). The DR_t terms are available from the IRS publication 946 [19]. This method is used over a simpler method such as straight line depreciation as it leverages the time value of money, depreciating assets more earlier in their lifetime when the value lost is worth more. θ_{fs} is dependent on plant location, and will vary over time. As such, it is represented by a distribution and can be found in Table 1.

The salvage value is the money recuperated through resale of the plant at the end of its lifetime. This is dependant on the market and book value of the plant, as well as federal and state taxes, as described below in Equation 8:

$$SV = MV - (MV - BV)\theta_{fs} \tag{8}$$

where SV is the salvage value of the plant, MV is the market value, BV is the book value, and θ_{fs} is the sum of federal and state taxes as previously described. As the plant is assumed to be fully depreciated at the end of the recovery period, the book value of the plant is zero at the end of the plant's lifetime. As such, the equation reduces as follows in Equation 9:

$$SV = MV(1 - \theta_{fs}) \tag{9}$$

The cash flow incorporates the TPC, Ψ_t, and SV as well as revenue and federal and state taxes as described in Equation 10:

$$CF_t = \begin{cases} (R_t - TPC_t)(1 - \theta_{fs}) + \Psi_t & t \neq 30 \\ (R_t - TPC_t)(1 - \theta_{fs}) + \Psi_t + SV & t = 30 \end{cases} \tag{10}$$

where CF_t is the cash flow in year *t* and R_t is the revenue in year *t*. For the calculation of CNPV, R_t is 0 for all years. For the calculation of NPV, revenue would be calculated using Equation 11:

$$R_t = SP_t \cdot CF_t \cdot PS \tag{11}$$

where SP_t is the selling price of product in year *t* in dollars per metric tonne, CF_t is the capacity factor in year *t*, and PS the production scale of the plant in metric tonnes per year. The capacity factor is a metric that is often used in these types of economic analyses; it is a percent of the maximum capacity of the plant at which the plant operates. This may be used to decrease production when demand is lower, or to simulate lower production during plant start-up. Because this paper analyzes CNPV, capacity factor is not applicable. The production scale is relevant to this analysis, as although it does not contribute to revenue, it does have implications in carbon production, equipment sizing, and raw material cost. The production scale for this analysis was set to 3850 metric tonnes of ammonia per day.

The fixed capital investment (FCI) is comprised of direct and indirect costs. Direct cost (DC) is the sum of purchased equipment (PE); installation; instrumentation & controls (I&C); piping (PIP); electrical (ELEC); buildings, process, and auxiliary (BPA); service facilities and yard improvements (SFYI); and land. Indirect cost (IC) is the sum of engineering and supervision (E&S), legal expenses (LE), construction & contractor fee (CCF), and contingency (CONT). These calculations are detailed below in Equations 12, 13, and 14:

$$FCI = DC + IC \tag{12}$$

$$DC = PE + INST + I\&C + PIP + ELEC + BPA + SFYI + LAND \tag{13}$$

$$IC = E\&S + LE + CCF + CONT \tag{14}$$

Purchase equipment excepted, all of these expenses are distributions of fractions multiplied by either PE, DC, or FCI, as detailed in table 1. Notably, this creates the need for circular references, as contributions to FCI are multiplied by FCI. This is handled natively in Excel, but FCI can be solved for algebraically if circular calculations are not supported by the computational platform.

Purchased equipment is the total of the bare module costs (as installation is accounted for by the INST distribution) of the major equipment in the plant. The purchased equipment cost was adapted from the hydrogen techno-economic analyses by Parkinson et al. and modified for the production of ammonia using case studies from a report by the DOE [15][16]. The adaptation of these costs required scaling for both inflation over time and production scale. Scaling for inflation was accomplished using the Chemical Engineering Plant Cost Index (CEPCI), a value published by industry experts each year to represent how plant process and construction costs vary over time [20]. The calculation is executed according to Equation 15 as follows:

$$C_1 = \frac{CEPCI_1}{CEPCI_0} C_0 \tag{15}$$

where C_1 is the cost at the present year, C_0 is the cost at the original year, $CEPCI_1$ is the CEPCI at the present year, and $CEPCI_0$ is the CEPCI at the original year. For the purposes of this paper, the present year was taken to be 2021.

Additionally, the costs needed to be adjusted for the production scale of the plant. This is not as simple as a linear scale, as the economies of scale dictate that as size increases, costs will increase more slowly. The industry standard for compensation for production scale is the six-tenths rule, as shown in Equation 16:

$$C_1 = \left(\frac{PS_1}{PS_0}\right)^{0.6} \cdot C_0 \tag{16}$$

where C_1 is the cost at the present year, C_0 is the cost at the reference year, PS_1 is the desired production scale, and PS_0 is the reference production scale. As previously mentioned, the production scale for this paper is 3850 metric tonnes of ammonia per day.

The operating cost of the plant was taken to be the sum of raw material costs (RM), fixed operating and manufacturing costs (FO&M), and variable operating and manufacturing costs (VO&M). FO&M includes expenses such as operating labor, maintenance labor, administrative costs, and property taxes. VO&M includes maintenance material costs (MM), water utility costs (WUC), and recurring chemical costs for the consumed catalysts (CHEM). These calculations are shown in Equations 17 and 18 below:

$$OC = RM + FO\&C + VO\&C \tag{17}$$

$$VO\&C = MM + WUC + CHEM \tag{18}$$

The FO&M and RM were adapted from the paper by Parkison et al., adjusted for inflation as previously described. However, these costs do not benefit from economies of scale like equipment costs do. As such, these costs were scaled linearly with production scale, rather than using the six-tenths rule. MM is a fixed percent of FCI, and WUC and chemical costs were adapted from the DOE report case studies on ammonia production [16].

Lastly, the the TCI is the sum of the FCI and working capital (WC), as described by Equation 19:

$$TCI = FCI + WC \tag{19}$$

Working capital is an initial investment of raw material and supplies necessary to start running the plant. It is assumed that the working capital is recovered at the end of the plant's lifetime; for example, the last purchase of raw material is not necessary, as current supplies will be used up instead. This is why when calculating CNPV, FCI is subtracting instead of TCI; the cost is recovered at the end of the plant's lifetime. In this paper, working capital is a distribution of fractions multiplied by TCI, as outlined in Table 1.

2.2: Use of @RISK for Monte-Carlo Simulations

The framework of equations described in section 2.1 allows for an estimation of CNPV for a set of single-point estimations of parameters. As previously discussed, this type of analysis is often susceptible to the "flaw of averages;" this type of model with average single-point inputs often gives unsatisfactory or misleading results. To eliminate the "flaw of averages" and better represent the possible range of inputs and outputs, Monte Carlo simulations are used with uncertain model inputs represented as a distribution of values. For the CNPV distributions, the primary benchmarks calculated are the average CNPV, the 5th percentile, the 95th percentile, and the standard deviation. The P_5 represents the lowest 5% of costs predicted by the model, representing the risk-tolerant cost, or "value at opportunity." The P_{95} represents the highest possible 5% of costs according to the model, representing the risk-averse cost, or "value at risk." Note that these metrics are inverted from an NPV model. The standard deviation gives an indication of the breadth of the data, or how far the data strays from the mean. A large standard deviation means that costs are less concentrated

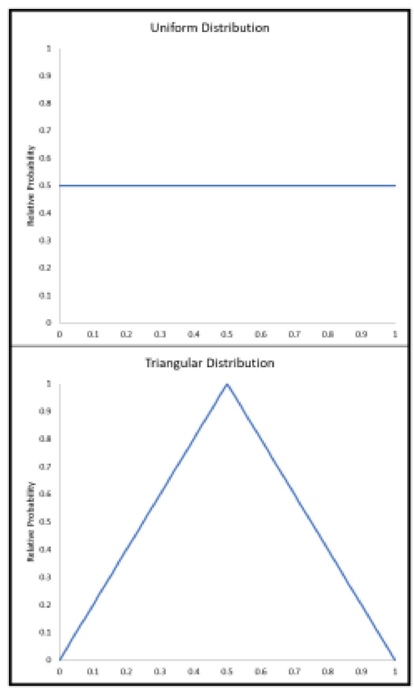

Figure 8: Uniform and triangular distribution profiles

around the average CNPV and are more likely to be further from the average than for a distribution with a smaller standard deviation. All of these metrics are important for the decision maker to consider, and are lacking in the fixed-point estimation model.

There are two types of distributions used in the MCS in this paper: uniform and triangular, as shown in Figure 8. Uniform distributions have an equal chance of choosing any point within its bounds. These distributions only require two arguments to be fully defined: the two endpoints of the distribution. This is the most commonly used distribution type in the model described in this paper, and is used when there is no indication of bias towards the center or any specific point in the distribution. Triangular distributions have a concentration towards the mode of the distribution. Thus, points closer to the mode of the distribution are more likely to be sampled. This distribution requires three arguments to be defined: the two endpoints and the mode. This type of distribution is used when there is an indication that points closer to the mode of the distribution are more likely.

@RISK (a software by Palisade) is a powerful tool for performing MCS. @RISK is an extension of Excel, which allows for intuitive definitions of distributions and generation of distribution profiles for outputs such as CNPV in a computational platform that many people are already familiar with. @RISK was used in this report to set up the framework of equations, define distributions, run MCS, and analyze results. The distribution profiles used in the framework of equations are generally agreed upon by industry experts to accurately represent the range of potential costs for each entry. All of the distributions used throughout the simulation are detailed below in table 1.

Table 1: Distribution profiles for uncertain model inputs [21]

Uncertainty Driver	Symbol	Dist. Type	Minimum	Mode	Maximum	Based on
CO_2 Transport & Storage Cost ($/metric tonne)	CTSC	Triangular	9	10	11	-
CO_2 Tax Rate (year 1) ($/metric tonne)	CT	Triangular	27	30	33	-
Annual CO_2 Tax Growth Rate	-	Triangular	5.4%	6.0%	6.6%	-
Combined Federal and State Taxes	θ_{fs}	Triangular	0.0%	6.4%	9.5%	-
Ratio for Market Value of the plant after 30 years	MV	Uniform	13.5%	15%	16.5%	FCI
Ratio for Installation	INST	Uniform	25.0%	-	55.0%	PE
Ratio for Instrumentation & Controls	I&C	Uniform	8.0%	-	50%	PE
Ratio for Piping	PIP	Uniform	10.0%	-	80.0%	PE
Ratio for Electrical	ELEC	Uniform	10.0%	-	40.0%	PE
Ratio for Buildings, Process, and Auxiliary	BPA	Uniform	10.0%	-	70.0%	PE
Ratio for Service Facilities & Yard Improvements	SFYI	Uniform	40.0%	-	100.0%	PE
Ratio for Land	LAND	Uniform	4.0%	-	8.0%	PE
Ratio for Engineering & Supervision	E&S	Uniform	5.0%	-	30.0%	DC
Ratio for Legal Expenses	LE	Uniform	1.0%	-	3.0%	FCI
Ratio for Construction & Contractor's Fee	CCF	Uniform	10.0%	-	20.0%	FCI
Ratio for Contingency	CONT	Uniform	5.0%	-	15.0%	FCI
Ratio for Insurance	INS	Uniform	0.4%	-	1.0%	FCI
Ratio for Working Capital	WC	Uniform	10.0%	-	20.0%	TCI
Ratio for Financing Interest Costs	FIC	Uniform	6.0%	-	10.0%	TCI
Ratio for Plant Overhead Costs	POC	Uniform	5.0%	-	15.0%	TPC
Ratio for Patents and Royalties	PR	Uniform	0.0%	-	6.0%	TPC
Ratio for Administrative Costs	AC	Uniform	2.0%	-	5.0%	TPC
Ratio for Marketing Costs	MC	Uniform	2.0%	-	6.0%	TPC
Ratio for Research and Development Costs	RDC	Fixed	-	5.0%	-	TPC

In the above table, please note the items related to CO_2 tax: the CO_2 tax rate in year one and the annual growth rate. The carbon tax in this simulation was modeled as a distribution of initial tax rates with a yearly compounding growth, which is also a distribution. This is of particular relevance as a sensitivity analysis was performed on the carbon tax, which emphasized the economic differences between the three ammonia production pathways. In performing the sensitivity analysis, the carbon tax for each year was scaled up by a fixed multiple, and the effects on the resultant distribution profiles are shown and analyzed.

<u>2.3: Integration of Monte-Carlo Simulations into Python scripts</u>

As previously described, one of the integral goals of this project was to replicate the functionalities of @RISK in Python as proof of concept for implementing MCS into higher level platforms with potential for future integration into other commonly used process modeling softwares. Among the important considerations to note, the most impactful to MCS implementation in Python were the following:

- As was the case in @RISK, calculations would need to be conducted iteratively to generate a distribution of CNPV results.
- Python and Excel handle circular references differently. Variables in Python and their values are parsed in the order they are assigned, and cannot be circularly defined in the same way they can in Excel. @RISK allows for circular references if the program settings are adjusted correctly, while Python will overwrite previous values resulting in incorrect variable values.
- The @RISK program understands when and how to resample distributions for new randomly assigned values throughout a simulation. In Python however, simply assigning a distribution to a variable and recalling that variable multiple times throughout a script *does not* produce a new randomly assigned value as would be expected.

The following section will describe how these and other intricate aspects of MCS implementation in Python were addressed, and will highlight the pertinent modules and add-ons that were amalgamated into our suite of scripts.

Each of the proposed design processes had a separate script written to independently find CNPVs for the given process. The structure of the Python files was the same for each process with different variable values for things like purchased equipment, operating costs, and Hydrogen production values found in literature and adapted for NH_3 production using DOE reports [15][16]. As was the case in @RISK, different effectuations of carbon tax were also considered as they were required for the particular process design. To ensure that parameters from distributions were correctly resampled throughout simulations, all uncertain variables were assigned by calling separate functions which referenced the corresponding distribution. Assigning distributions to variables directly in the simulation scripts *would not* return new random values with each new reference to the variable. The resampling functions were stored in a file called DistFunctions which was imported into each of the simulation files, thus giving them access to the resampling capabilities. Distributions were created in DistFunctions using the numpy and scipy.stats modules, with uniform and triangular being the most commonly used. Figure 9 shows an excerpted version of the DistFunctions file.

```
def CO2_Transport_FN():
    return np.random.triangular(9, 10, 11, 1)

def CO2_Tax_FN():
    return np.random.triangular(27, 30, 33, 1)

def CO2_Tax_Growth_FN():
    return np.random.triangular(0.054, 0.06, 0.066, 1)

def Combined_Taxes_FN():
    return np.random.triangular(0.0, 0.064, 0.095, 1)

def MV_Plant_FN():
    return np.random.triangular(0.135, 0.150, 0.165, 1)

def Installation_FN():
    return uniform.rvs(size = 1, loc = 0.25 , scale = 0.55 - 0.25)

def IC_FN():
    return uniform.rvs(size = 1, loc = 0.08 , scale = 0.50 - 0.08)
```

Figure 9: Excerpted DistFunctions file

The Python simulations were constructed similarly to how they were in @RISK, with direct costs (DC) and FCI being calculated as a function of purchased equipment costs (PE) first. Given the inability to circularly define variables in terms of their uncertain components, the equations for DC and FCI were algebraically rearranged to remove the need for circular references. Figure 10 shows the equations for DC and PE as they were in the literature [21] (which can be found more concisely in equations 13 and 14 above), and Figure 11 is excerpted code showing the rearrangement of these equations in terms of explicitly defined variables. Similar algebraic rearrangements were done throughout the cost evaluation framework to remove circular references and create an adapted set of equations Python could evaluate.

I. Direct costs
A. Equipment + installation + instrumentation + piping + electrical + insulation + painting
1. Purchased equipment
a. WGS reactor
b. HTS catalyst
c. Pd/Au alloy composite membrane
2. Installation (25–55% of purchased equipment)
3. Instrumentation and controls, installed (8–50% of purchased equipment)
4. Piping, installed (10–80% of purchased equipment)
5. Electrical, installed (10–40% of purchased equipment)
B. Buildings, process and auxiliary (10–70% of purchased equipment)
C. Service facilities and yard improvements (40–100% of purchased equipment)
D. Land (4–8% of purchased equipment)
II. Indirect costs
A. Engineering and supervision (5–30% of direct cost)
B. Legal expenses (1–3% of fixed capital investment)
C. Construction expense and contractor's fee (10–20% of fixed capital investment)
D. Contingency (5–15% of fixed capital investment)
III. Fixed capital investment (=I + II)
IV. Working capital (10–20% of V)
V. Total capital investment (=III + IV)

Figure 10: DC and PE from literature [21]

```
DC = purchasedEquipment * (
        1 + Installation_FN() + IC_FN() + Piping_FN() +
        Electrical_FN() + AUX_FN() + Facilities_FN() +
        Land_FN())

FCI = (DC * (1 + Supervision_FN())) / (1 - (Legal_FN() + Construction_FN() + Contingency_FN()))
```

Figure 11: Excerpted code showing rearrangement of PE and DC equations to remove circular references

Discounted cash flow analysis over the 30 year plant lifetime was accomplished through the use of for loops. TPC, and DCF was determined for each year of the plant's lifetime. Where applicable, carbon tax rates were incremented by the CO2_Tax_Growth() function at the end of each iteration of the loop occuring after year one. The use of the DistFunctions file, as previously discussed, ensures that uncertain parameters contributing to TPC were resampled correctly in each year of the loop. In the 30th year, salvage value of the plant was included in the cash flow analysis as was the case in @RISK. Given the desire for a CNPV distribution, no revenue was calculated or included in CF calculations. In compliance with the previously given definition of NPV, FCI was subtracted from the cumulative 30 year GPV term, and was multiplied by (-1) to get a CNPV for a given simulation.

With the ability to produce a single CNPV result for each of the three design options, the next step was to iteratively run simulations and graph results as cumulative distributions. The three independent files were subsequently imported into a MainSim file to streamline the simulation process and allow all three to be run simultaneously. Another for loop was used to conduct 10,000 simulations for each process design and append the results to their respective CNPV lists. Figure 12 is an import map of the Python files showing how they interact with and build off each other to produce results.

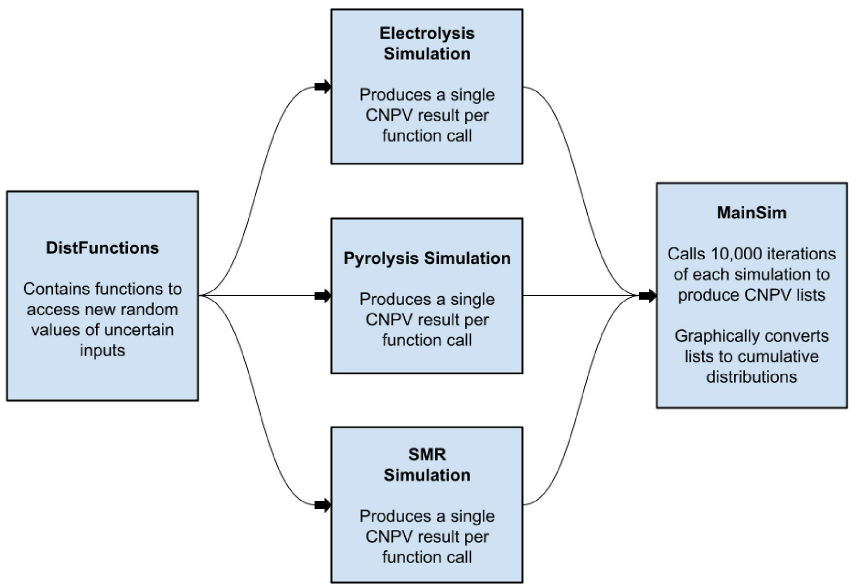

Figure 12: Import map of the integrated Python suite of scripts

After the simulations were complete, the CNPV lists were fed into a CreateCumulativeDist() function which was written to subdivide each list into a defined set of subranges and determine how many CNPV values were less than or equal to the maximum value in each range, thus creating a cumulative distribution of CNPV. Matplotlib. and pyplot. are modules that were imported and used to graph results and format the graphs as desired. Further information on the syntax of these modules can be found in their documentation [22]. Figure 13 shows the excerpted portion of the MainSim file which graphs and formats results. Variables a, c, and e represent the lists of x-values, while b, d, and f are the lists of y-values returned from the cumulative distribution function. These sets of values were then graphed using the built-in plot() method followed by axis and legend formatting. Consult the results section of this report to find the figures generated by these modules, and Appendix A to find a full version of the code.

```
numSubranges = 200

a,b = createCumDist_FN(elecNPVList, numSubranges, "")
c,d = createCumDist_FN(SMRNPVList, numSubranges, "")
e,f = createCumDist_FN(pyroNPVList, numSubranges, "")

plt.plot(a,b, label = "ELEC")
plt.plot(c,d, label = "SMR")
plt.plot(e,f, label = "PYRO")
plt.legend()
plt.xlabel("CNPV ($e10)")
plt.ylabel("Cumulative Frequency")
plt.title("CNPV Cumulative Distribution Model")
plt.show()
```

Figure 13: Excerpted MainSim file showing instantiation of graphs and formatting

3: Results and Discussion

3.1: Comparison between @RISK and Python

During the development and testing of the Python scripts, the values of important parameters (FCI, TPC, CNPV etc.) were compared to those of the @RISK simulations. Given the probabilistic nature of the models, an exact match among results was not expected. However, agreement within the same order of magnitude was desired. The base case analyzed was a discount rate (r) of 0.16, and a CTM of 1, with all uncertain inputs represented as described in Table 1. Table 2 compares the base case average CNPV results across both platforms and they show appreciable congruence within the same order of magnitude. Thus, we can say with a high degree of certainty the suite of Python scripts are accurately and consistently replicating the results of the MCS model as represented in @RISK software.

Table 2: Comparison of pertinent average CNPV results among simulations methods

CNPVs ($)	@RISK Result	Python Result
SMR	1.61×10^{10}	1.98×10^{10}
Pyrolysis	1.70×10^{10}	1.95×10^{10}
Electrolysis	5.27×10^{10}	6.33×10^{10}

Table 3 below gives simulation results for our base case where the discount rate (r) was held at 0.16, and the CTM was set to 0. Please recognize PE and OC were fixed input parameters (calculated from literature) and did not vary throughout the simulations [21][15][16]. As previously discussed, electrolysis has considerably higher PE and OC while maintaining no carbon intensity. SMR and pyrolysis have similarly lesser costs, while SMR has a considerably higher carbon intensity than pyrolysis. Values of P_5, P_{95}, STDEV, and AVG were the results from the Python simulations and were in close agreement with those of @RISK.

Table 3: Pertinent results for base case: r = 0.16, CTM = 0

	Electrolysis	Pyrolysis	SMR
PE ($)	1.96×10^9	9.33×10^8	9.37×10^8
OC ($)	3.90×10^9	8.09×10^8	6.23×10^8
Carbon Intensity (metric tonne/day)	0	1141.6	4246.75
P_5	5.82	1.69	1.55
P_{95}	6.90	2.18	2.04
STDEV*	3.29	1.47	1.47
AVG	6.33	1.93	1.78

***All STDEV are $\$x10^9$ and all other costs are $\$x10^{10}$**

3.2: Discount Rate Sensitivity Analysis

The discount rate is a parameter of the system that is especially difficult to predict. In general, it is the parameter used to devalue money over time according to the time value of money. In practice, this is difficult to assign a numerical value to, as it depends on the technological risks of the project and the state of the economy throughout the plant's lifetime. As such, it is often more useful to choose a fixed value for the discount rate, and analyze how the resultant distribution profile changes when the discount rate is varied over a reasonable range of values. In this analysis, the base case was a discount rate of 16%, and discount rates between 10% and 20% were analyzed. Results of this analysis can be found in Table 4:

Table 4: Results of sensitivity analysis of discount rate on CNPV of each process design

		Discount Rate (%)					
		10	**12**	**14**	**16**	**18**	**20**
Electrolysis	**P_5**	8.13	7.17	6.41	5.82	5.34	4.96
	P_{95}	9.45	8.39	7.55	6.90	6.36	5.93
	STDEV*	4.03	3.71	3.43	3.29	3.09	2.96
	AVG	8.77	7.74	6.95	6.33	5.83	5.43
SMR	**P_5**	2.42	2.13	1.90	1.74	1.60	1.50
	P_{95}	3.03	2.70	2.43	2.24	2.08	1.95
	STDEV*	1.86	1.72	1.60	1.50	1.43	1.37
	AVG	2.71	2.40	2.16	1.97	1.83	1.71
Pyrolysis	**P_5**	2.32	2.07	1.87	1.72	1.59	1.49
	P_{95}	2.93	2.62	2.39	2.20	2.05	1.94
	STDEV*	1.84	1.69	1.59	1.49	1.43	1.37
	AVG	2.61	2.33	2.12	1.95	1.81	1.70

***All STDEV are $\$x10^9$ and all other costs are $\$x10^{10}$**

The discount rate sensitivity analysis reveals that in general, CNPV decreases as the discount rate increases, which would indicate that a higher discount rate is beneficial. However, this is a slightly misleading result. As there is no revenue present in this model, a higher discount rate decreases the CNPV as it causes the money spent later on in the project to be worth less, according to the time value of money. In reality, a profit based model would reveal the opposite; a higher discount rate decreases the profit of the plant, as the money earned is also devalued over time.

Nonetheless, this analysis is beneficial in analyzing the magnitude of change induced in the model with each change to the discount rate. At either extreme of the range of analysis, the model shows a significant shift in CNPV, P_5, and P_{95}. When the discount rate increases from 16%

to 20%, the average CNPV, P_5, and P_{95} all decrease by approximately 13% for ammonia production pathways. Likewise, when the discount rate decreases from 16% to 10%, CNPV, P5, and P95 increase by approximately 35% for all pathways. In this respect, an increased discount rate could be viewed as incurring higher risks, as assuming a higher discount rate yields lower costs.

The standard deviation increases as the discount rate decreases. Notably, this is also true for an NPV analysis, as a lower discount rate increases the magnitude of the analyzed value, whether that be CNPV or NPV. As the distributions are primarily fractions of other costs, a greater magnitude of cost correlates with an increased standard deviation. This means that a lower discount rate widens the overall spread of the CNPV distribution, thereby further polarizing values at opportunity, and at risk, from the average CNPV. In this respect, a lower discount rate could be seen as incurring higher risk, as the assumption of a lower discount rate yields a greater standard deviation, and thus a wider range of possibilities.

This unearths an apparent discrepancy in the risk evaluation of discount rate; a higher discount rate yields lower costs, but a narrower distribution profile. Ultimately, this equips the decision maker with additional information. It is up to the individual whether they value the consistency of a smaller standard deviation at the risk of underestimating the cost, or the safer cost estimation in exchange for a greater variance in CNPV.

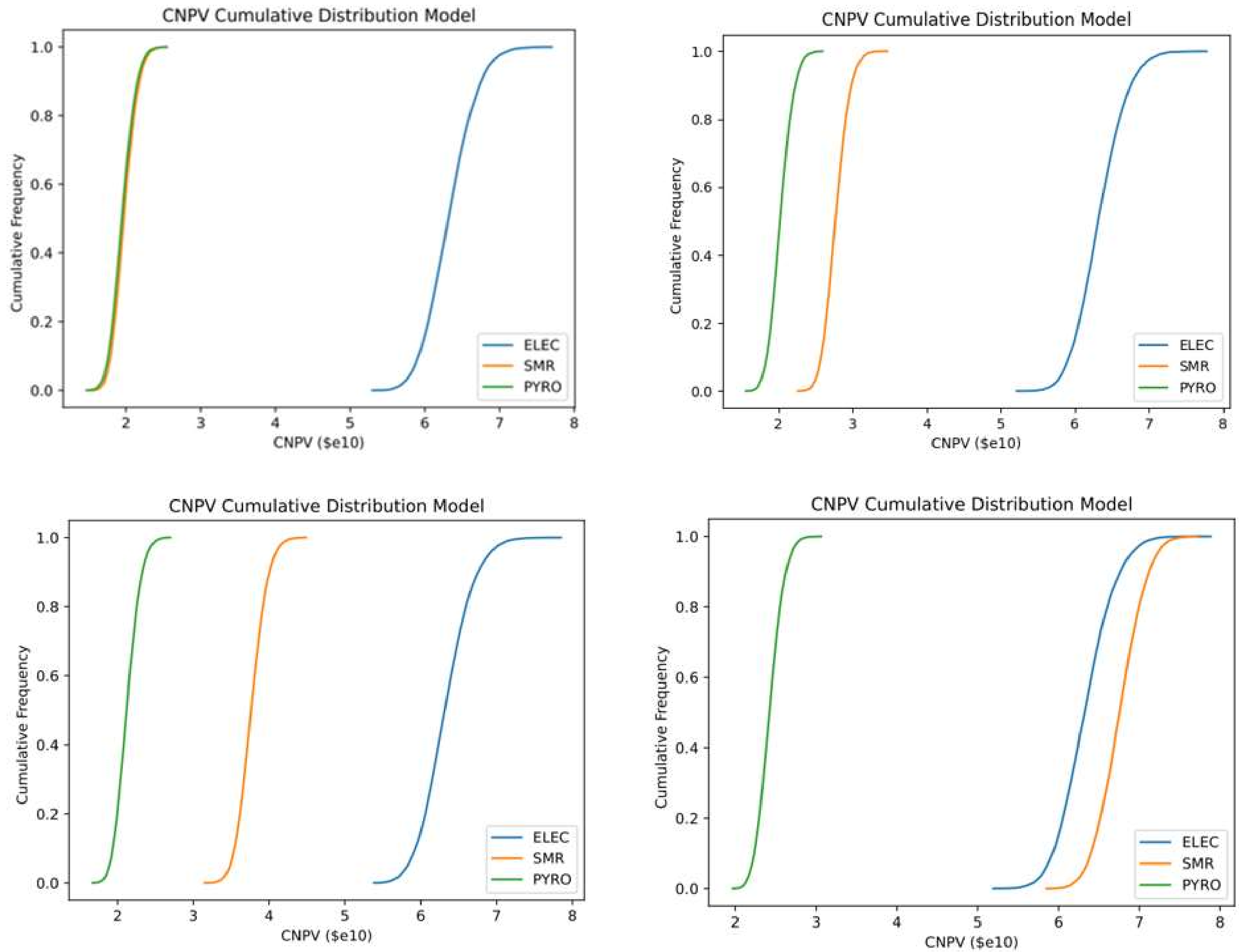

Figure 14: Cumulative CNPV Distributions for all process designs under different carbon tax conditions

Top Left: CTM = 1, Top Right: CTM = 5, Bottom Left: CTM = 10, Bottom Right: CTM = 25

Table 5: Pertinent results of sensitivity analysis on carbon tax (r held at 0.16)

		Carbon Tax Multiplier (CTM)					
		0	1	5	10	22	25
Electrolysis	P_5	5.82	5.82	5.83	5.83	5.81	5.82
	P_{95}	6.90	6.90	6.89	6.90	6.90	6.89
	STDEV*	3.29	3.29	3.22	3.27	3.29	3.25
	AVG	6.33	6.33	6.33	6.34	6.33	6.33
SMR	P_5	1.55	1.74	2.52	3.48	5.75	6.31
	P_{95}	2.04	2.24	3.05	4.07	6.58	7.22
	STDEV*	1.47	1.50	1.59	1.77	2.53	2.76
	AVG	1.78	1.97	2.77	3.76	6.16	6.76
Pyrolysis	P_5	1.69	1.72	1.79	1.89	2.13	2.18
	P_{95}	2.18	2.20	2.28	2.38	2.63	2.69
	STDEV*	1.47	1.49	1.48	1.47	1.51	1.52
	AVG	1.93	1.95	2.03	2.13	2.37	2.42

***All STDEV are $\$x10^9$ and all other costs are $\$x10^{10}$**

3.3: Carbon Tax Sensitivity Analysis

A sensitivity analysis was performed on the carbon tax rate using the previously described Carbon Tax Multiplier (CTM). The CTM was multiplied with the carbon tax distribution (as described in Table 1) and its effect on CNPV for each technology option was investigated. Our base case (Table 3) displays that in the absence of carbon tax, SMR is the most cost effective hydrogen technology option in the production of ammonia. SMR also has lower values at risk and opportunity than both other options. Worth noting in particular is that in the base case, SMR has a P_5 that is \$0.14 x 10^9 lower than pyrolysis and a P_{95} which is \$0.11 x 10^9 lower. While both technologies are comparable in costs, it would appear there is a larger difference in "values at risk" between the two. This trend holds true for increased CTM. Without the presence of carbon taxes and regulation, we would expect that SMR would be the least expensive option given its lower purchased equipment and operating costs (see Table3). Given that (under the same production conditions) SMR has a carbon intensity of 4246.75 metric tonnes per day, and pyrolysis of 1141.6 metric tonnes per day, we would expect SMR to be affected to a far higher magnitude by regulatory actions on carbon [15]. This suspicion is confirmed by Figure 14, where for CTM greater than 1, pyrolysis becomes the comparatively attractive and cost effective hydrogen technology option in the production of ammonia. In cases of extreme carbon tax (CTM greater than or equal to 25), SMR becomes the least economically feasible option and more expensive than electrolysis. Across the scope of our simulations we see pyrolysis is consistently the most cost efficient technology option, and in all situations is either the least expensive option, or within approximately 8.5% of the closest technology.

One of the benefits in the use of a probabilistic approach to CNPV calculations, and the determination of values at "risk" and "opportunity" is the ability for a more nuanced analysis of the data gathered. Further investigation of the P_5, P_{95} values for each technology under varying carbon tax conditions gives the decision maker an increased awareness of the potential cost outcomes of implementing each technology option under the economic circumstances being analyzed in the presence of irreducible uncertainty. For instance, in low carbon tax situations ($0.5<CTM<2$) it may be found that the values of P_5 and P_{95} for SMR and pyrolysis are similar in magnitude. The decision maker would need to determine whether the use of slightly more expensive, lower carbon intensity pyrolysis methods outweighs the use of less expensive, more carbon intense SMR. A similar inquiry arises in higher carbon tax environments (20<CTM<25) as the CNPV distributions, along with values at "risk" and "opportunity" for SMR and electrolysis approach similar magnitudes. The decision maker would need to determine in the presence of high or increasing carbon tax, if the slightly more expensive, carbon neutral electrolysis is more suitable than the carbon intense, less expensive SMR. This level of intricacy in the analysis of cost outcomes would not be possible with the use of single point estimates or average values over the analyzed time periods. The implementation of MCS and distributions to reduce economic uncertainties allows for an increased level of insight in the analysis of cost probabilities.

3.4: Impact Assessment of Uncertain Parameters on Total Capital Investment

The implemented framework of equations includes a wide array of uncertain parameters. However, it is unclear to what degree an individual parameter affects the resultant distribution from the parameter's distribution alone. To analyze these impacts, tornado diagrams can be generated, shown in Figures 15 through 17. These diagrams evaluate each parameter at its minimum and maximum to measure the maximum impact the parameter can have on the system. These analyses were performed to consider the parameters which had the greatest impact on the total capital investment of the project for each ammonia production pathway.

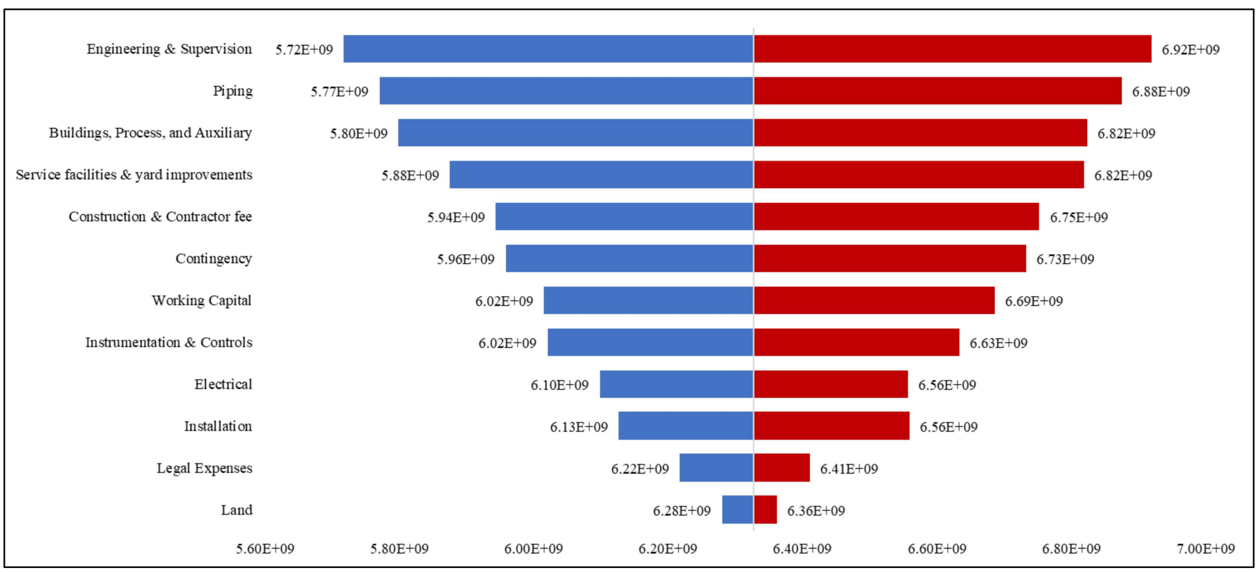

Figure 15: Tornado diagram for SMR TCI

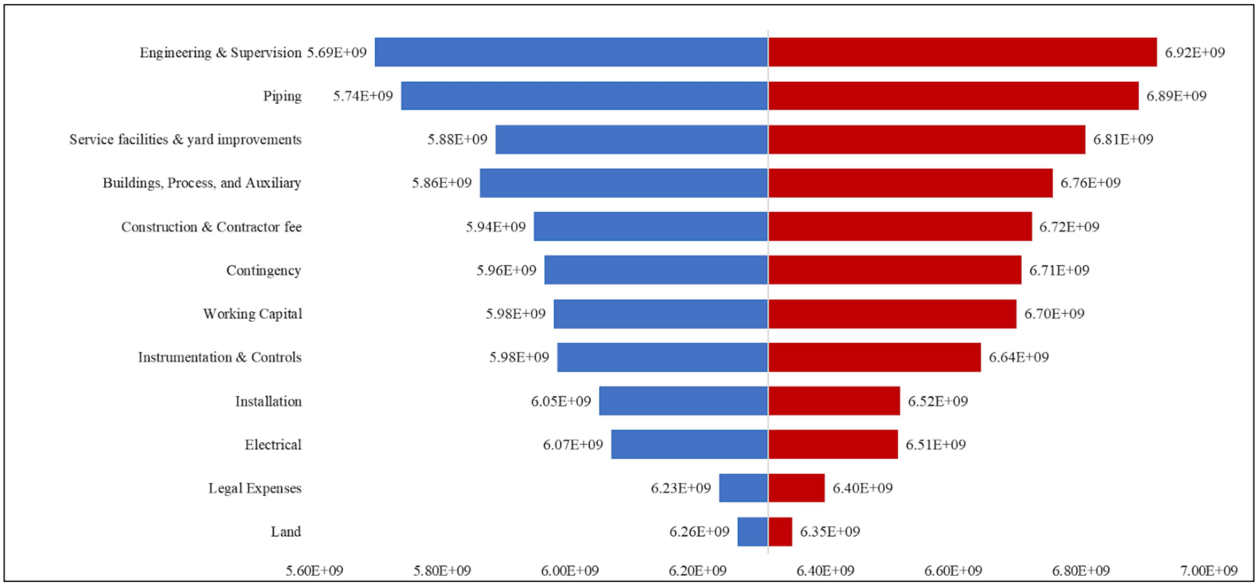

Figure 16: Tornado diagram for pyrolysis TCI

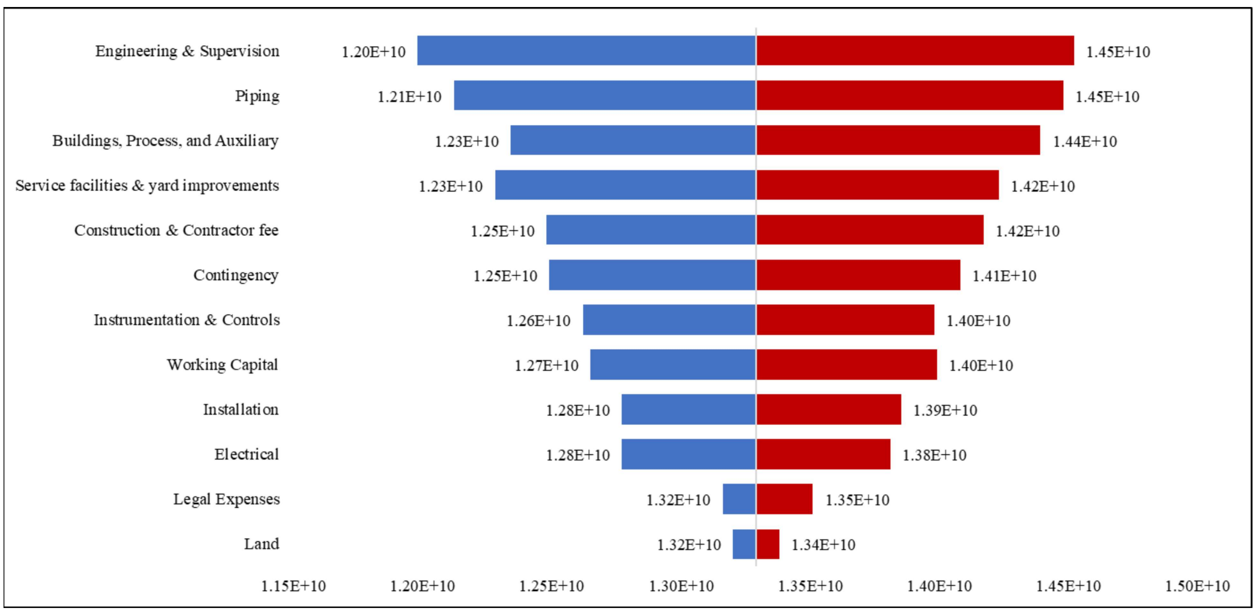

Figure 17: Tornado diagram for electrolysis TCI

These analyses reveal that all ammonia production pathways analyzed have similar large contributors to uncertainty. Namely, the largest four contributions for all cases are engineering & supervision; piping; buildings, process, and auxiliary; and service facilities & yard improvements. These distributions all either have a wide range of possible values or are multiplied by a large expense. In either case, this gives the decision maker the information needed to reduce the uncertainty of the system by further researching specifics of these categories and refining the range of possibilities in the distributions. For example, a decision maker could research current costs of piping, the amount of piping required for the plant, and the material of piping needed to hone in the estimation of piping cost, greatly decreasing its uncertainty and thus the uncertainty of the system. Additionally, the decision maker can devote additional resources to these expenses to drive them towards their minimum values, equipped with the knowledge that variance in these categories are the largest drivers of fluctuation of TCI.

4: Conclusions and Recommendations

4.1 Concluding Remarks

This work proposed the use of a MCS calculation framework to model the costs of ammonia production through various hydrogen inputs in the presence of uncertainty. Our framework was curated from an array of literature sources, and was first implemented in @RISK. Subsequent design of a suite of Python scripts was conducted with the effort of replicating the @RISK results in a more efficient manner. A number of challenges had to be overcome in the design and implementation of these scripts, including but not limited to addressing circular references of parameters, incorporating iterative calculations, and correctly resampling distributions used to model uncertain inputs. Rather than a single script, a series of interconnected, interdependent scripts were created and imported into each other to allow for distributions to be resampled and functions to be called iteratively to perform necessary calculations. The results of the calculations performed by the scripts were compared to those of @Risk. It was determined and shown that the simulation results of the scripts were in close agreement with those of the @RISK platform. Thus, the results presented herein are those of simulations conducted using these scripts.

The resultant CNPV distribution profiles were generated and analyzed under a variety of conditions. Firstly, the discount rate was varied across a range of reasonable values. An increase in discount rate correlated with a decrease in CNPV, and a decrease in standard deviation of the profile. This gives the decision maker additional information to decide on an appropriate discount rate for the specific project based on their personal risk preferences.

Next, the results were analyzed through a sensitivity analysis on the carbon tax. Each ammonia production pathway had a different carbon intensity, which meant that the carbon tax affected each method differently. Electrolysis produces no carbon, so an increase in carbon tax has no effect on its CNPV profile. However, for even very high carbon tax rates, the high purchased equipment cost prevents it from being competitive compared to the other two methods. SMR has the lowest purchase equipment cost, but has a high carbon intensity. Only for very low carbon tax scenarios (CTM <1) was SMR less expensive than pyrolysis, which has a slightly higher purchased equipment cost in exchange for a lesser carbon intensity.

Lastly, the major contributors to uncertainty of total capital investment were analyzed through generation of tornado diagrams. This analysis showed that all ammonia production pathways had the same major contributors to uncertainty of TCI: engineering & supervision; piping; building, process, and auxiliary; and service facilities and yard improvements being the top four. This allows decision makers to focus resources on these areas to reduce uncertainty and lower costs.

Within the broader context of research surrounding alternative energy technologies, Timmerberg, Kaltschmitt, and Finkbeiner have conducted a more detailed study comparing the same three hydrogen production avenues discussed herein, although without the implementation of MCS. Their study models the use of thorough CCS technologies in conjunction with hydrogen production and calculated levelized cost of hydrogen for each technology option. They determine that SMR substantially outperforms pyrolysis and electrolysis economically, with levelized costs of 1.0 to 1.2 €/kg H_2, 1.6 to 2.2 €/kg H_2, and 2.5 to 3.0 €/kg H_2 respectively [23]. This is contradictory to the findings of this paper, which found that for any reasonable present carbon tax, pyrolysis is more economically favorable than SMR. This further illustrates the point that these technologies are developing and changing rapidly, and there are numerous metrics to take into account when conducting a cost/risk analysis. As discussed, MCS better represents the uncertainties present in the system, which can offer an insightful alternative to other calculation frameworks. That said, uncertainties within a process are not the only important aspect to consider in an economic analysis, emphasizing the decision of which type of model best represents and characterizes the process in question. In the rapidly changing technological space, it is imperative to consider current information that best reflects the economic conditions in which technology options are being evaluated.

4.2: Implementation of Profit Based Analysis

The first logical extension of the work presented in this report is to consider various revenue streams and thus calculate an NPV distribution containing profit for all three technologies analyzed. As discussed, there are a number of potential revenue streams even beyond the selling of ammonia for each proposed process design; pyrolysis produces solid carbon products which can be sold in a number of different forms, and at times a portion of the hydrogen produced through SMR is sold directly to the market thus adding an additional revenue stream beyond the production of ammonia. It is also sometimes the case that electrolyzers are run at constant power and excess power is sent back to the grid, which creates another revenue stream [15]. Further research would be necessary to find reliable and meaningful distributions of selling prices for the various products, and revenue would be incorporated into the 30 year cash flow analysis as was shown in equation 11 above. The resulting distributions would be of NPV and would purport to describe the profitability of these process designs in the presence of uncertainty.

4.3: Incorporation of Design Flexibility in Ammonia Production Processes

Another facet of process design not considered in this report is design flexibility. As presented in the work by Liang-Chih Ma et al., such a flexibility consideration could involve selective use of CCS systems to minimize carbon related costs (whether those costs are sustained through taxes or CCS operation) by turing CCS off when its operational costs would be higher than the carbon taxes incurred for a given year of process CO_2 production [24]. In general, incorporating flexibility into the simulations allows for a more robust management of risks and opportunities through potentially value-enhancing operational adjustments, and retrofits to the plant throughout its lifetime. These transient adjustments to the process gives the decision maker more operational abilities to minimize incurred costs in response to uncertain carbon tax environments.

4.4: Further Considerations for MCS Python Scripts

4.4.1: Significance

Worth acknowledging further is the importance of the aforementioned success in replicating @Risk MCS performance and results in Python. The design, and successful implementing of these scripts should not be overlooked as it overcame a number of technical and program specific challenges and served as proof of concept for incorporating MCS into higher level platforms beyond Excel. Using Python not only allows multiple technology options to be simulated simultaneously (something not possible in @Risk), but also reduces simulation runtime in comparison to Excel. Furthermore, Python presents the prospect of converting our scripts to executable files designed to run in conjunction with other process modeling software not equipped with economic/risk analysis capabilities, thus further consolidating pertinent aspects of process design into a more succinct and mutable workflow. These advantages made Python an attractive alternative to an Excel based approach to MCS and risk incorporated economic analyses.

4.4.2: Further Script Optimization and General Improvements

Another advantage in the use of using Python as an MCS platform is that there is significantly more room for further optimization of the code's performance both from the perspective of runtime, and ease of use than there is in Excel. With specific regard to future improvements in runtime and efficiency, an effort should be made to find more built-in Python functions to accomplish some of the tasks within the scripts. Many of Python's built-in functions are actually written behind the scenes in C (another faster language). Thus, built-in functions complete a given task faster than an equivalent, purely Python method. For instance, the createCummulativeDist() function was written exclusively for the work in this report due to the absence of available built-in functionalities to create cumulative distributions. However, if a built-in functionality was to be found in further research, its amalgamation into our scripts could reduce runtimes. Likewise, the aforementioned numpy module has built-in data structures that are faster to search and iterate through which may offer an attractive alternative for storing and retrieving CNPV values from their respective lists. With regard to ease of use, an effort should be made to more diligently comment the code throughout the scripts such that their future readers can more quickly ascertain what each function or sequence of code aims to accomplish in the bigger picture of the program.

Another logical extension of the presented work is incorporating the ability to resample historical data representing relevant parameters into the Python scripts. @Risk contains built-in functionality to fit distributions to datasets and present a number of possible fits to the user who decides which of them most accurately represents the dataset in question. Our scripts do not currently have this capability as our research did not procure any viable built-in Python modules to accomplish this, thus leading to the need for a proprietary set of functions to incorporate similar capabilities.

A final note on the prospect of future work: if the scripts presented in this report were to be incorporated into aspen (and/or like softwares) they would likely be converted to an executable file, and when run, set to prompt the user to provide an input file for the software being used. Thus, it would be worth including a more in-depth error analysis system such as an error logger. Such a logger would contain code to present Python's console errors in a pop-up window with a more detailed “layman's terms” explanation of the error and possible solutions. Common errors may include an incorrectly formatted or type of input file, a corrupted or incomplete input file, and/or not completely specifying the type of simulation desired (NPV, CNPV, number of uncertain inputs, etc.). This would offer an easier point of entry to our scripts for users not familiar with Python, its functionalities, or coding in general. With the goal of future integration into other process modeling software in mind, optimizing runtimes and ease of use of these scripts will be important as the flow diagrams they are run on increase in size and complexity.

4.5: Limitations

It is worth acknowledging the limitations in the methodology and scope of this study. Firstly, there are some aspects of the construction of a plant that are not reflected by the framework of equations. For example, there is often a construction period and startup period associated with a plant as the infrastructure of the plant is developed, during which production is zero and limited respectively. While this would have larger impacts on a profit based NPV model, there are still effects that would manifest in the CNPV model in this paper. A decreased production scale in certain years would decrease the required raw materials, utilities, and overall operating cost in those years. Consideration of these factors would decrease the overall CNPV due to the potential for decreased cost during these years.

Additionally, some system inputs were treated as fixed, whereas consideration of the range of potential values could more accurately reflect the associated costs. Most notably, the raw material costs were considered fixed for all three ammonia production technologies. In reality, this is a relatively large expense, and could contribute substantially to the systems' uncertainties. Raw material costs are market dependent, and thus could vary unpredictably, even if historical price data were resampled. Additionally, the different technology options use different raw materials in different quantities. As a result, consideration of probabilistic raw material costs may disproportionately affect the standard deviations of some technology options. Likewise, uncertainty in operating cost was also not considered. Operating cost includes similar market and location dependance in factors such as labor cost and property taxes. The incorporation of uncertainty in these factors would again increase the standard deviation of the technology options. In the development of a functional model for a prospective project, it may be useful to account for these uncertainties once a site location is decided, as a more accurate distribution of values based on local costs could be used.

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Appendix A: Full Python Code

For a full version of the proprietary Python code used in this report, please see the attached GitHub link:

pjasmin1046/Monte-CarloSimulationFrameworkForEconomicRiskAnalysisOfChemicalProcesses: Suite of scripts written to perform a Monte-Carlo simulation of a proposed ammonia plant design evaluating three different hydrogen inputs in the presence of uncertainty. (github.com)

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