A Simulation of the Costs and Firm Level Incentives in Alkanolamine Flue Gas Carbon Capture

By

Mack J. S. Murphy

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Approved by the Thesis Supervisor

Dr. Justin Beaudoin Date

Approved by the Head of the Department

Dr. Andrew Davis Date

Approved by the Chair, Senate Honours Committee

Dr. Matthew McSweeney Date

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Abstract

This thesis quantifies the firm-level incentives and describes the capital and operating costs of implementing alkanolamine-based flue gas carbon capture systems designed to capture 100 metric tonnes of carbon dioxide (100 % of carbon dioxide generated) per day in a coal-fired power plant. Determining the costs and the areas where firms could be incentivized to engage with alkanolamine flue gas carbon capture systems are both important in assessing the economic viability of this carbon dioxide emission mitigation technology. This thesis takes a simulation approach, assessing the viability of four of the most prevalent alkanolamine molecules currently being used for carbon carpture: monoethanolamine, diethanolamine, methyl diethanolamine, and aminomethyl propanol. Each of these four chemicals are simulated independently in the same conceptual flue gas carbon capture process. Simulating the process with a consistent layout across all four alkanolamines permits a more reasonable direct comparison of the cost and incentive differences arising from the properties unique to each chemical.

Component prices and operating parameters were determined based on available data, with a focus on the chemical and engineering implications associated with all components, parameters, and chemicals involved. Where data was not available, various ad hoc methods were used to derive a given cost. Capture process operation parameters

were varied to suit the requirements dictated by the specific chemical properties of each alkanolamine.

The results indicate that monoethanolamine, the most pervasive alkanolamine currently in use for carbon capture, was the least expensive from a capital and operating cost standpoint. Diethanolamine was the second least expensive by capital costs, and third least expensive by operating costs. Aminomethyl propanol was the third least expensive by capital costs, and second least expensive by operating costs. Methyl diethanolamine was the most expensive by capital and operating costs. The degree to which a firm would be incentivized to implement a flue gas carbon capture system was not consistent across all four alkanolamines. In all simulations, firm level incentives were subject to specific prices and parameters, with solvent circulation rate improvements or coal subsidies offering the greatest potential for incentive impacts.

1. Introduction

In recent decades, climate change resulting from greenhouse gas emissions has been identified as a crucial issue facing humanity. An extensive body of literature has consistently found that the current level of greenhouse gas emissions on a global scale is unsustainable, and without substantial changes to infrastructure, agriculture, and many other greenhouse gas emitting sectors, significant damages will be incurred (Wigley, 1995) (Nordhaus, 2017). The topics of greenhouse gas emissions and mitigation methods have given rise to entire journals dedicated to their study. Areas of research pursuing greenhouse gas emission mitigation include industry-specific mitigation techniques, the invention of more energy efficient technology, and the development of direct atmospheric capture technologies/methods, be they biological or mechanical. While all these areas of research hold their own merit, from the perspective of a profit-maximizing firm, if the costs of these methods outweigh the benefits garnered from their use, the firm is unlikely to engage with them unless adequately incentivized or compelled. It is in this spirit that the topic of this thesis was conceptualized. This thesis seeks to model the specific cost structure and examine under which conditions a firm operating a coal fired power plant can be incentivized to implement and alkanolamine flue gas[1] carbon capture system. Another element that should also be taken into account is the notion that some

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[1] Flue gas is a term used to describe the exhaust gas inherent to industrial combustion-driven processes, and is often used in the context of fossil fuel power generation.

firms may not be pure profit-maximizers, and their incentives may include an ethical component (however dubious this may seem for a petrochemical-adjacent sector), thus this thesis also incorporates external and social costs in the analysis. The external and social costs can also be conceptualized in terms of government regulations. While it is impossible to know exactly how lawmakers may impose a cost of emissions on firms in the future, the use of the social cost of carbon dioxide provides a reasonable base to incorporate a cost resembling regulation into these models.

In 2021, power generation comprised nearly 37.7 percent of global carbon dioxide emissions, making it the largest CO_2 emitter by sector (Tiseo, 2023). This was a major motivating factor for this thesis topic, as the notion of providing a cost analysis of a technologically feasible, potentially incentive-congruent carbon dioxide mitigation technique was made more meaningful by the fact it could directly impact the single largest carbon-emitting sector. The capture techniques proposed in the simulations here are not limited to this sector either; any process in which carbon dioxide-containing flue gas is emitted could theoretically implement these techniques.

This paper takes an interdisciplinary approach to the cost analysis by carefully considering the chemical and engineering implications of alkanolamine flue gas carbon capture. It also considers the associated chemical nuances involved with the use of different alkanolamines in the process, then presents results in an economic benefit context. Where data about specific parameters pertaining to the alkanolamines were unavailable, other known properties were used to calculate an estimate of the missing values in order to make as accurate of a cost assessment as possible. The cost analyses are conducted by the simulation of a flue gas capture process employing four different alkanolamines (monoethanolamine, diethanolamine, methyl diethanolamine, and aminomethyl propanol), assessing their necessary operational requirements, and determining costs based on these requirements in terms of capital and operating costs. Simulation results show that the cost of a process is heavily dependent on the necessary solvent circulation rate in the process, and the price of each alkanolamine. What is also shown is that the net internal (private), external, or social costs/benefits are heavily subject to assumptions about the process or prices of components/resources.

The presentation of this thesis is as follows: Section 2 details the historical development of the literature pertaining to the engineering and costs of flue gas carbon capture, as well as the chemical literature discussing alkanolamines, and the development of carbon capture systems involving their use. Section 3 discusses the methodological approach of the simulations in greater detail, and outlines the assumptions made in its construction. Section 4 describes the methods used in cost determination of all simulation components, quantification of the simulation's parameters, and the limitations pertaining to both, followed by the simulation results in Section 5. The final portion, Section 6, summarizes all simulation results, and presents arguments for methodological and process design improvements, as well as potential policies which would create a greater incentive to engage with this technology.

2. Literature Review

2.1 Flue Gas Carbon Capture Process: Models, Empirics, and Costs

The notion of employing methods to mitigate carbon dioxide emissions from large scale industrial emitters is relatively new in the pure sciences. Publications detailing methods by which carbon dioxide can be recovered from the flue gas of coal combustion began to emerge in the late 1970s and throughout the 1980s. Their contributions, however, were almost entirely limited to technical feasibility, with no mind paid to the construction, implementation, and upkeep (operational)[2] costs of such an endeavour. To their credit, many of the publications identify that attacking the problem at the source, the emitters themselves, would be more efficient than attempting to extract carbon dioxide directly from the atmosphere, which still holds true today in terms of cost efficiency, despite the vast difference in available technology (Albanese and Meyer, 1980). Furthermore, these early publications posit the use of the (currently) most prevalent alkanolamine, monoethanolamine, as a solvent for use in flue gas carbon capture, though, they estimate the capture efficiency to be significantly lower than what has been experimentally proven to be possible today. Moreover, they offer no

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[2] Upkeep costs or operational costs are terms that are used interchangeably throughout this thesis. They both refer to the costs a firm pays per day to sustain capture process operation. Economically, they can be thought of as variable costs, however, due to the simulations' assumptions, they do not vary over time in a given alkanolamine's capture process.

contributions in terms of precisely how a capture process would operate from an engineering perspective.

As time progressed, and social and political pressures mounted over concerns about global warming caused by greenhouse gases, the field of study that is flue gas carbon capture gained momentum. Wilson et al (1992), a collaboration between the S*askatchewan Provincial Ministry of Energy and Mines*, *Shell Canada*, and the *Amoco Canada Petroleum Company,* details the operation of a capture plant capable of capturing four tonnes of carbon dioxide per day, using monoethanolamine. It served as a pilot program intended to prove the technical feasibility for the actively developing basis of engineering requirements for such a plant. Booras and Smelser (1991), is perhaps one of the first publications to provide an economic analysis of flue gas carbon capture with increased attention given to the engineering nuances. Their result, however, proved lackluster. Although they approximate the capture efficiency of monoethanolamine more in line with what is consistently seen in its use today, they posit that the cost of implementing the capture process on a national scale would be so prohibitively high as to make it non-viable. Instead, they suggest optimizing fuel contents, or opting for renewable or nuclear power generation over coal combustion as means of mitigating carbon dioxide emissions in the near term. This is perhaps a result of the higher costs associated with a somewhat novel technology, which could not yet leverage an economy of scale, making the aforementioned alternatives appear more feasible.

Both Wilson et al (1992) and Booras and Smelser (1991) enlist the services of the *Fluor Daniel* corporation (hereafter referred to as *Fluor,* which did eventually become the firm's name following restructuring efforts) in the development of their studies. *Fluor* is a multinational, multidisciplinary engineering firm operating primarily in the petrochemical and construction industries. It is particularly noteworthy here, as it acquired a method of flue gas carbon capture, dubbed *FG Econamine*, from the *DOW Chemical Company* in 1989. This process uses a proprietary solvent containing monoethanolamine, among other constituents. Wilson et al (1992) and Booras and Smelser (1991) both utilize the *Econamine FG* process in their capture plants. *Fluor* continued to improve the process throughout the subsequent years. The *Econamine FG* process, or as *DOW* had called it, *Gas/Spec FT-1*, appears to have existed as early as 1980, according to a cursory reference in Lytle and Marchant (1980) which sought to use the process in the capture and resale of various gaseous products arising from coal combustion. Unfortunately, however, information about the process' early-stage development is not publicly available, supposedly due to corporate confidentiality constraints, according to a brief phone conversation this thesis' author had with *Fluor*'s director of process engineering, John Gilmartin.

It would not be until the late 1990s that engineers at *Fluor* would begin to publish studies outlining the process and its associated costs in any real depth. The content of Mariz (1998) and Sander and Mariz (1992) prove remarkably illuminating in this sense, each with numerous subsequent citations in papers published in moderate impact journals such as *The Chemical and Engineering Journal, The Journal of Membrane Science,* and *The Journal of Energy Conversion and Management.* These publications tend to explore some element or derivation of flue gas carbon capture by means of the *Econamine FG* process or similar such processes. Mariz (1998) provides elements of the engineering foundation the model in this thesis uses. It outlines in nuanced detail the precise operation of the capture plant, considering parameters such as the carbon dioxide concentration in flue gas, alternative alkanolamines to monoethanolamine, and specific areas in the capture process where the costs of such an operation could theoretically be reduced. Additionally, it provides a cost function in the form of USD per tonne of CO_2 captured, and breaks down the individual plant components that contribute to the total cost, though it provides no basis upon which the individual costs were determined, making the use of this function in an academic cost study such as this questionable. Chapel, Mariz, and Ernest (1999) build off of Mariz (1998), offering the same cost breakdown nearly verbatim, but also providing several equations necessary to calculate component dimensions and parameter values, several of which aided in the formulation of this thesis' parameter calculations.

Throughout the early 2000s and 2010s, many studies detailing theoretical models and real-world proof-of-concepts would be published. Chang and Shih (2007), Schach et al (2010), and Abu-Zahra et al (2006) all provide theoretical models of flue gas carbon capture using *Econamine FG* or some variation of it, and attempt to optimize, in an engineering sense, various aspects of the process' operation. Chang and Shih (2007) and

Schach et al (2010) also attempt to offer some degree of cost analysis, but again, fall short in their conveyance of the determination of the costs included in their study. Reddy et al (2017), and a paper contributed to by John Gilmartin (Gilmartin et al, 2014) are publications by *Fluor* providing engineering analyses of the improved *Econamine FG Plus* process in use, further establishing the feasibility of the carbon capture method in various settings, and indicating the process can be further developed with newer solvent technologies and more advanced machinery. Many of the more recent publications in this field seek to contribute to the development of *Fluor's* method in a similar spirit: by modifying the components, solvents, or operating conditions. However, less effort is directed towards constructing rigorous cost models, creating a significant deficit in terms of publicly available information in related literature. While the proprietary nature of *Econamine FG* introduces inherent uncertainty into external attempts to develop cost models using data pertaining to it, it is an area that warrants study.

To date, there is very little literature pertaining to the markets for the relevant alkanolamines in this study, making establishing their costs more difficult. The small body of literature that does exist tends to have been conducted by research firms, and is thus not entirely publicly available. A useful piece of information that can be extracted from the preliminary summaries of these reports, however, is a consensus that the amine markets, and by association, the alkanolamine markets, are expected to grow in the coming decade. This is primarily a result of these chemicals' use in other sectors that are forecasted to experience growth, such as personal care, surfactants, water treatment, and crop protection (Grandview Research, n.d.). On an aggregate level, the chemical manufacturing industry has been well-established to be a sector that benefits from economies of scale at a plant level. Aside from isolated examples of more complex molecules, generally speaking, firms see increasing returns to scale in the manufacture of chemicals (Lieberman, 1987). This leads to decreased costs to the consumer agent by virtue of the competition arising from the oligopolistic nature of bulk chemical markets. Therefore, as the market for a particular chemical grows, so does the manufacturing output, leading to diminished marginal costs of production, and thus, lower prices. Based on this reasoning, the prices of the alkanolamines presented in this study can reasonably be expected to decrease in nominal terms over the coming years.

A particularly notable gap in the literature pertaining to flue gas carbon capture, and cost models of such systems is a disregard for the social impacts of carbon dioxide emissions. To date there are no widely available studies which incorporate the external costs of carbon dioxide emissions in the context of flue gas carbon capture. In the planning phase of this thesis, it was determined that this literature gap would be a meaningful one to begin to fill. To this end, Nordhaus (2017), known for his work in the study of the social cost of carbon emissions, was used to quantify the external benefit of the carbon captured in the simulations. In essence, Nordhaus' social cost of carbon is an estimate of the present value of future damages resulting from one additional tonne of carbon dioxide emitted. In other words, the marginal social cost of carbon dioxide emissions. The future damages are quantified as a cost in dollar terms, and include aspects such as reduced agricultural productivity, damage to infrastructure, and increased healthcare costs. Though the validity of the cost established by Nordhaus is impossible to determine until enough time has passed to conduct empirical analyses, it can still be argued to be the one of the best estimates available at this time. Nordhaus identifies several elements which incorporate a greater degree of uncertainty into the estimate than others:

- The degree to which carbon dioxide directly influences atmospheric temperature. Given the Earth's atmosphere is a complicated, enormous physical system, it is likely impossible to control for the impacts of other gases in the atmosphere to determine carbon dioxide's direct temperature impact.
- The energy demand of society in the future is difficult to estimate. Additionally, the methods by which the energy will be produced, and the associated carbon dioxide emissions resulting from energy production are uncertain.
- The discount rate chosen in the present value calculation has a significant impact on the social cost estimate, and is also practically impossible to estimate with a great degree of certainty.

There are several other aspects of the social cost model presented by Nordhaus that introduce uncertainty. In the pursuit of knowledge, explicitly detailing and exploring the implications of all factors contributing to the estimate of the social cost of carbon would be valuable, but for the purposes of this thesis, it would be redundant. The most important takeaway is that Nordhaus' estimate is inherently uncertain. That being said, the primary estimate proposed by Nordhaus (2017) and the value used in these simulations is discussed in Section 3.4.

2.2 Alkanolamines and Their Properties in a Carbon Capture Context

Alkanolamines, by definition, are molecules which contain a hydroxyl functional group (R-OH, where R is some substituent), and an amine functional group (NH_3, where one or more hydrogen atoms is replaced by some substituent). The chemical and engineering literature pertaining to carbon capture by use of this variety of molecule has an extensive and colourful history. Alkanolamine carbon capture systems were not born in the spirit of environmental protection, rather, early sources suggest they were developed as a means to remove unwanted acid gases (CO_2, H_2S) from natural gas for the extraction of helium (Storrs and Reed, 1942). The *Girbotol Process*, developed in 1928, appears to be one of the first patented processes capable of achieving this goal. It details a method not dissimilar to *Econamine FG*, in which carbon dioxide is captured from various gas mixtures and used in the production of dry ice. Furthermore, a particularly interesting piece of literature, written in August 1960 by *The Aerospace Medical Division* of *The United States Air Force*, details a smaller scale alkanolamine-based carbon capture system designed to control carbon dioxide concentrations in space-faring vessels, and allow for the oxygen content of carbon dioxide to be recycled (Hsu and Schwartz, 1960). This publication appears before the first manned space mission, making it a captivating piece of history. Unfortunately, exploring the lengthy history of alkanolamine carbon capture in any serious depth is outside the scope of this study, and is also not particularly relevant to the simulations beyond what has already been mentioned. Nonetheless, a salient observation to make is that while pollution mitigation literature employing these methods begins appearing relatively recently, the technology itself predates it by several decades, further establishing its technical feasibility.

The alkanolamines presented in this study are some of the most pervasive in the context of flue gas carbon capture, with an extensive body of literature detailing their characteristics and use. The vast majority of such publications include monoethanolamine, such as Abu-Zahra et al (2006), Chang and Shih (2007), and Schach et al (2010). Others include diethanolamine (Saeed et al, 2019), methyl diethanolamine, and aminomethyl propanol (Li et al, n.d.) (hereafter referred to as MEA, DEA, MDEA, and AMP respectively). There exist very few studies which analyze the characteristics of all four molecules in carbon capture under identical conditions, aside from Aroonwilas and Veawab (2004) and Sakwattanapong, Aroonwilas, and Veawab (2005). The two aforementioned publications prove immensely useful in the sense of providing relative absorption efficiencies and regeneration energy requirements. These two studies, and several others, also evaluate the carbon capture potential of blended solvents, which contain more than one type of alkanolamine, though these solvents are beyond the scope of this thesis. Li et al (n.d.) and Xue et al (2017) provide the heat (enthalpy) of the reaction of the four relevant alkanolamines with carbon dioxide, and Davis and Rochelle (2009), Saeed et al (2019), Closmann and Rochelle (2011), and Huang et al (2014 provide comprehensive analyses of the rates at which the molecules degrade as a result of thermally-driven processes. All of the aforementioned characteristics are crucial in the construction of this study's cost model; the reasons for which are explored in detail throughout Section 3.4 and Section 4.1.

A particularly unfortunate informational deficiency as it relates to alkanolamine properties in carbon capture is the proprietary nature of *Econamine FG*'s MEA-based solvent. Chapel, Mariz, and Ernest (1999) indicate that the formulation of the solvent includes some kind of corrosion inhibitor, which alters the performance characteristics of the solvent, reducing solvent regeneration requirements from that of the two-part water-MEA solvent included in this analysis. Access to this information would likely yield a reduced cost assessment of the coal required to heat the reboilers of the alkanolamine models included in this thesis.

3. Simulation Methodology

3.1 Methodological Overview

The principal objective of this thesis was to simulate a carbon capture process that resembles *Fluor's Econamine FG* technology and the *Girbotol Process*, using several different solvents, to establish multiple rigorous cost models for comparison, with consideration given to the physical, chemical, and engineering nuances that contribute to cost determinations. With this objective in mind, a flue gas carbon capture system employing MEA was designed based on available literature, and all relevant parameters defining the operating conditions were established by citation or calculation. Subsequently, prices, either fixed or variable, for the necessary components were determined. The internal benefit of the cost avoided from not purchasing carbon credits (which is considered a transfer payment to the firm here), and the external benefit of not emitting (quantified by the social cost of carbon) were also determined. Following chemical literature, changes to the operating parameters based on the necessities of other alkanolamines were quantified. All values were then tabulated in a spreadsheet, to obtain an output in terms of days of carbon dioxide capture required to, in a sense, break even, from a net internal, external, or social (a combination of net internal and net external benefits) perspective.

3.2 Flue Gas Carbon Capture Process

The methodological approach to the cost model of the simulations necessitated the development of a conceptual layout for a flue gas carbon capture plant. To this end, a capture system very similar to the model of Abu-Zahra et al (2006) was planned. A process flow diagram of the planned carbon capture plant is shown in Figure 3.2. While this process excludes some components found in a real *Econamine FG* plant, all of the most critical components to the plant's operation are included. Section 3.3 outlines the basis for neglection of the excluded components.

Figure 3.2: Process Flow Diagram of Simulation Carbon Capture System

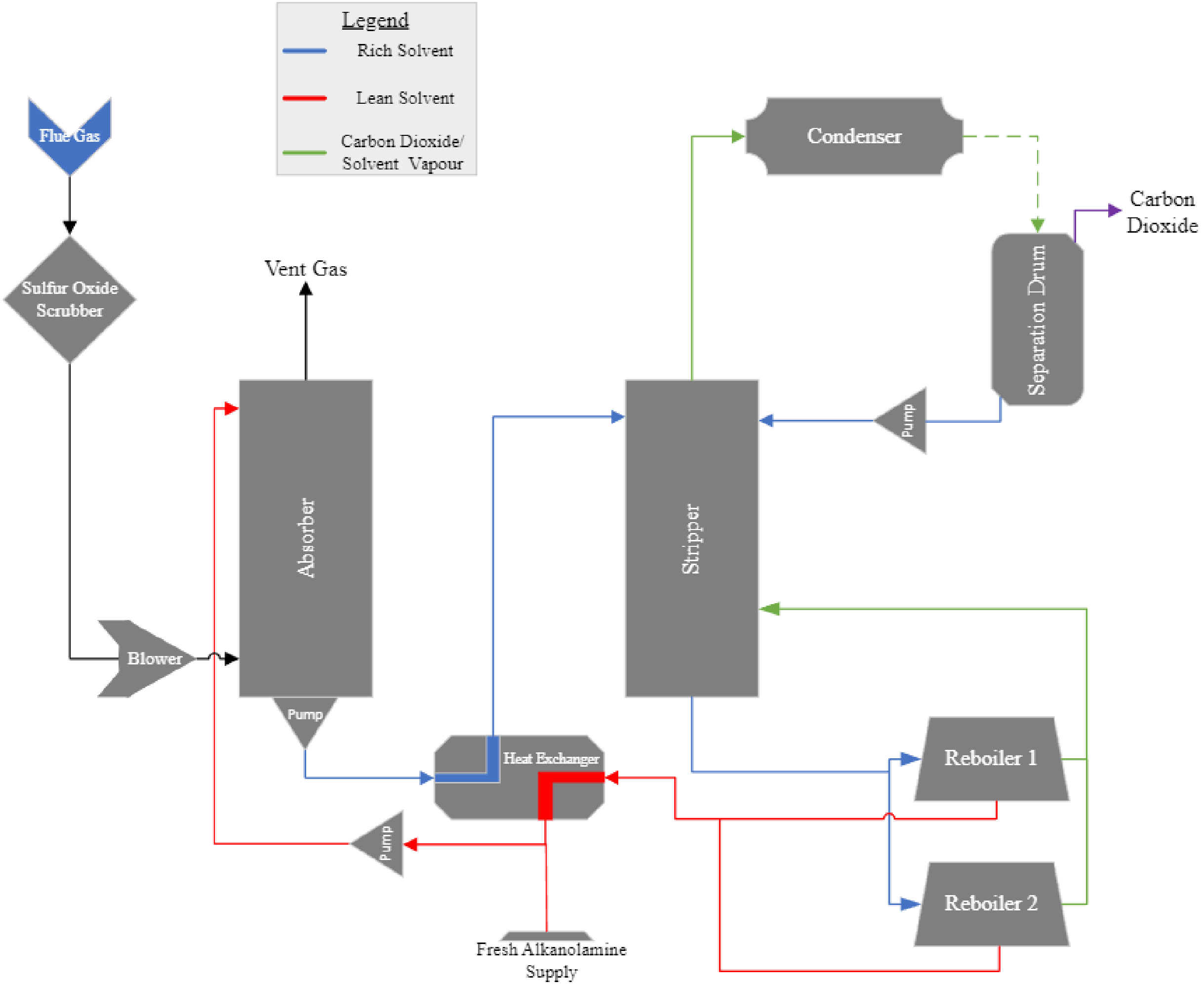

Figure 3.2: This presents the process flow of the flue gas carbon capture plant used in the simulations. It incorporates all conceptual assumptions discussed in section 3.3.

The process begins by introducing flue gas from the power plant into the system. The flue gas first passes through sulfur oxide scrubbing, which reduces the concentration of SO_2 to 10 ppmv, while the concentration of SO_3 is assumed to be unchanged by the scrubbing and remains at 50 ppmv. The scrubbed flue gas then passes through the blower to overcome the pressure difference in the absorber. The flue gas flows upwards, against the “current” of the lean solvent being sprayed downwards through the absorber. The carbon dioxide and sulfur oxide contamination are entirely absorbed in the countercurrent flow of the absorber, and the now rich, aqueous solvent pools at the bottom. It is worth noting that the terms rich and lean refer to the quantity of carbon dioxide captured and still contained by the alkanolamine in the solvent. Rich solvent contains more CO_2 than the lean solvent. The decarbonized, desulfurized gas then exits the absorber at the top and is vented to the atmosphere, now containing only nitrogen, oxygen, and water. The rich solvent in the absorber is pumped through the heat exchanger, which heats the rich solution, and cools the lean solution making its way back to the absorber for reuse. The rich solution then enters the stripper. Here, a countercurrent flow is seen again, where rich solution is further heated by rising solvent and carbon dioxide vapours. Each heating step will facilitate the liberation of carbon dioxide, but the majority of the carbon dioxide will be liberated by the reboilers. The aqueous rich solution then exits the stripper at the bottom and flows to the reboilers. In the reboilers, the concentration of unliberated carbon dioxide is lower than what is found in previous steps due to the active liberation occurring. Thus, here, some of the aqueous solution exits the reboilers, passes through the heat exchanger, and is pumped back to the absorber, along with some addition of fresh alkanolamine, for further use in carbon capture. The reboilers also deliver solvent vapours and liberated carbon dioxide gas to the stripper. These gases exit the stripper at the top, and proceed to the condenser. The condenser cools the vapours, returning the solvent to a liquid state, while leaving the carbon dioxide as a gas. This gas-liquid mixture then flows to the separation drum where the carbon dioxide gas exits the system, and the lean solvent is reintroduced to the stripper for further use in the capture process.

3.2.1 Alkanolamines

As previously described, the simulations of this study employ four alkanolamines independently in their own carbon capture process: MEA, DEA, MDEA, and AMP. Each solvent was formulated to have 30 percent of total solvent weight (30 wt%) be a given alkanolamine, and the remaining 70 percent be water. For all solvent methodologies included in this study, the same conceptual layout was used, with variations to the necessary operation parameters to ensure complete carbon capture was achieved.

Each alkanolamine presents certain advantages and disadvantages in its use as a carbon capture agent as a result of the molecules' differing chemical properties. Many existing analyses of flue gas carbon capture seek to reduce the costs of the process by various means, be it a reduction in power consumption, minimizing solvent loss, or otherwise. Each of the alkanolamines presented in this study assist in that respect by virtue of their property differences, and this makes a cost analysis of their use under similar physical conditions worthwhile. Table 3.2.1 presents a general relative (to MEA) overview of the differences in relevant chemical properties. The methods by which they were quantified, their cost implications, and their relevance to the models are explored in subsequent sections.

Table 3.2.1: Relevant Chemical Properties Compared Relative to MEA (Qualitative)

Property	MEA	DEA	MDEA	AMP
Regeneration Energy Requirement	High	Moderate	Low	Moderate
CO_2 Absorption Efficiency	High	Moderate	Very Low	Moderate
Degradation Rate	High	High	Very High	Very Low
Contamination Susceptibility	High	Moderate	Very Low	High

3.3 Conceptual Assumptions

There are a number of assumptions in terms of the capture plant's operation which are intended to facilitate cost determinations and minimize uncertainty arising from costs that lacked sufficient data, wholesale listings, or parameter requirements. Many of these assumptions are simply component omissions from the capture processes described by Mariz (1998) and Chapel, Mariz, and Ernest (1999). In general, these components require no power and were assumed to require no specialized manufacturing. Thus they were assumed to have a negligible cost and were omitted from the cost models, a prime example being the heat exchanger.

Firstly, most solvent cooling steps were omitted from a cost and process flow standpoint. These components use water as the cooling agent, which is assumed to be freely available. Additionally, the pumps included in the cost models are the components which mechanically move the solvent through the process, and thus the coolers contribute nothing in terms of power usage. Furthermore, the water pressure at the facility was assumed to be sufficiently high to maintain an acceptable water flow rate in the coolers. By similar logic, the cost of the heat exchanger was also omitted. In a slightly different sense, the cost of the solvent reclaimer was omitted, as Chapel, Mariz, and Ernest (1999) indicate it is not used consistently during the capture process. It was thus assumed that its task is performed by the reboilers in these simulations.

Potentially a more contentious cost omission was that of any filtration steps. Filters tend to use consumable resources like activated carbon, and would thus have a cost associated with their implementation. However, due to a lack of data pertaining to the precise requirements of the filters at various scales of operation, these costs could not be determined and were thus omitted. For similar reasons, labour costs were not included. Waste management costs prove even more troublesome in this regard, as each alkanolamine is liable to form different waste products in their decomposition. The type of waste products and the rate they are formed have too little data in the literature, and thus to mitigate uncertainty, this cost was excluded. It is worth noting that in the operation of a real capture plant such as this, filtration is a crucial step in the removal of precipitated solids in the solvent arising from contamination and decomposition. Gilmartin et al (2014) indicates that without a filtration/solvent reclamation system, the entire volume of solvent would have to be periodically drained and replaced, though they do not specify how often.

A potential cost that cropped up in the more recent literature was the maintenance requirement resulting from corrosion. Unfortunately, there is almost no literature describing the rates at which the corrosion of components occurs, and thus this cost could not be included with any degree of accuracy. There is an area of active research that is seeking to optimize the composition of the metal that the components are made of. Reddy et al (2017) offers some insight in this regard.

The focus of this thesis was directed towards the chemical and engineering nuances of the carbon capture process, and less so towards the logistical aspect of the plant's operation. It was in this spirit that many of the aforementioned costs were omitted, and additionally, the transportation and any property costs/taxes were excluded as well.

An assumption unrelated to capital costs was that of power consumption and the source of said power. It was assumed that power would be supplied from the associated power plant at no direct cost. This leaves the cost incurred from power consumption as an opportunity cost. In the development of the simulations, it was decided that the data pertaining to the power consumption of the selected components was insufficient to provide a base for calculations. Thus, no direct analysis of the plant's power consumption was incorporated in the simulations. That being said, power requirements can still be inferred about a component, relatively speaking, based on its capacity. Still, however, power consumption was omitted entirely from all cost analyses.

Other conceptual assumptions unrelated to omissions were these: any carbon dioxide produced (namely by the reboilers) in the capture process is subsequently redirected into the capture system and included in the total quantity of carbon dioxide captured. Furthermore, despite the fact the lean solvent still contains some absorbed quantity of carbon dioxide, it is assumed to still be able to capture the flue gas carbon dioxide at a 1:1 molar ratio. There is a well-developed body of literature pertaining to the mechanics of CO_2 loading, and the implications of CO_2 loading are somewhat captured in the absorption efficiency coefficient (given these coefficients were measured at 0.25 mol CO_2/mol loading), however, for simplicity's sake, the aforementioned assumption was made. Finally, it must be highlighted that this carbon capture system processes gaseous components. Much of the literature indicates that the pressures these gasses are under can vary significantly between the stages of the capture process (Chang and Shih, 2007), (Schach et al, 2010). Additionally, literature shows that the capture process can be optimized for a specific solvent by optimizing the pressure in the stripper, leading to significantly lower (on the order of 20 % or more) regeneration energy requirements (Abu-Zahra et al, 2006). Unfortunately, these data are reported for solvents whose compositions are incongruent with those used in this study and they do not report data for MDEA or AMP, thus making the inclusion of their findings in the simulations difficult to justify from an uncertainty mitigation standpoint. Further uncertainty mitigation challenges are found in the fact that many of the price data for components used in the simulations of this thesis did not specify the pressure capacities/requirements in the listings. Mariz (1998) reports that many stages of the *Econamine FG* capture process (the engineering basis for the capture process described in this thesis), including the stripper, operate at lower pressures when compared to other similar processes. Furthermore, many of the chemical data used in subsequent cost determinations were experimentally determined at standard atmospheric pressure (Aroonwilas and Veawab, 2004). It was therefore assumed that the entire capture process operates at atmospheric pressure.

While all of these conceptual assumptions/omissions serve to simplify the simulation process and somewhat mitigate uncertainty, it must be noted that in the hypothetical scenario where they could be accurately included, the results of the simulations would most likely differ. The magnitude of the difference is extremely difficult to assess. The assumptions that are likely to be the most impactful in this regard are the filtration omission, the disregard for CO_2 loading, and the atmospheric pressure assumption. For filtration, each alkanolamine, as stated, will degrade at a different rate, into different products which require filtration. This would introduce an additional upkeep cost, whose magnitude would largely depend on the rate of decomposition product formation. The degree to which this would impact the results is too uncertain to speculate on, however. In terms of CO_2 loading, Aroonwilas and Veawab (2004) shows that at higher levels of CO_2 loading, the absorption efficiencies of each alkanolamine studied here all decrease significantly. In a real-world application of alkanolamine flue gas carbon capture, the level of CO_2 loading can vary depending on the precise concentration of CO_2 in the flue gas. This will necessitate the variation of some operational parameters (such as solvent circulation rate, solvent volume, etc.) if the objective of the capture process is to extract 100 % of the carbon dioxide in the flue gas. Incorporating this aspect in these simulations would likely yield different results, due to impacts on both capital and upkeep costs which arise from the operational parameter changes. Finally, including gas pressures in the simulated capture process and incorporating the potential operational requirements dictated by them would most likely significantly influence the results of the simulations. Firstly, as the literature reports, a reduction in the regeneration energy requirement for the reboilers would significantly impact the coal consumption rate in each simulation. Secondly, some components included in this simulation may be entirely incompatible, thus necessitating their replacement. Incorporating the aspect of gas pressure, data availability permitting, would be valuable. It would offer the ability to optimize the process for a given alkanolamine without significantly changing the capture process, assuming all components remained compatible. Unfortunately, this was not possible due to a lack of necessary data in terms of component specifications and experimental results pertaining to all four alkanolamines being studied under the same conditions and at the correct concentrations.

3.4 Numerical Assumptions

Many of the foundational assumptions of this model were taken from Chapel, Mariz, and Ernest, (1999), the principal of which was the quantity of carbon dioxide to be captured per day. This can be said to be the most important assumption of the model, as it is the driving factor of many subsequent calculations. Chapel, Mariz, and Ernest (1999) indicates that typical *Econamine FG* plants capture between 90 and 1000 tonnes of carbon dioxide per day. It was discovered during the research process that selecting a daily capture rate towards the higher end of this range severely limited the set of components with reasonably close processing rates to what would theoretically be needed. Thus, for simplicity of calculations, and to maximize the set of acceptable components to construct the model, a daily capture value of 100 metric tonnes of carbon dioxide per day was selected. Additionally, a carbon dioxide concentration in the flue gas of 13 % was selected. Though arbitrary, this figure is consistent with carbon dioxide concentrations used in similar studies, and is crucial in determining the minimum initial solvent volume requirement.

Chapel, Mariz, and Ernest (1999) outlines typical sulfur oxide concentrations found in the flue gas of coal combustion. This is an important parameter for two reasons: it dictates the cost of scrubbing sulfur oxides from flue gas, and it approximates the rate of solvent loss to sulfur contamination. The removal of sulfur oxides is a critical step in the carbon capture process, because the alkanolamines used in this model are all susceptible to an irreversible reaction with SO_x molecules to varying degrees. This is a reaction which renders the alkanolamine molecule incapable of further carbon capture, and necessitates the lost alkanolamine's replacement. The concentration of sulfur oxides in the flue gas are directly dependent on the chemical composition of the coal being burned. It is worth noting that of all combustible fossil fuels that are used in energy production, coal contains some of the highest concentrations of sulfur oxides, subject to the specific variety of coal in question. Chapel, Mariz, and Ernest (1999) asserts that typical flue gas concentrations of sulfur oxides range from 300 ppm to 5000 ppm. This includes all relevant forms of sulfur oxides that carry solvent loss implications. For the base case of these models, a value of 500 ppm was selected. Additionally, it was assumed that the sulfur content was 90 % SO_2 and 10% SO_3. This is an important assumption as scrubbing efforts are mostly limited to the removal of most SO_2 in the flue gas, while the majority of SO_3 will escape scrubbing and proceed to degrade the solvent. In terms of SO_3, this model takes a 'worst case' approach, and assumes that no SO_3 is removed whatsoever and 10 ppm SO_2 escapes scrubbing. In addition, all sulfur contamination entering the capture system is assumed to react with the alkanolamine in a 1:1 molar ratio.

The chemical properties of each alkanolamine used are crucial in determining their necessary replacement rate, regeneration energy requirement, and the necessary circulation rate to capture a sufficient quantity of carbon dioxide. All of these factors play a crucial role in cost determinations. The relevant chemical properties or alkanolamine characteristics defined in the simulations are: the carbon dioxide absorption efficiency, the heat of reaction with carbon dioxide, the thermal degradation rate, and the sulfur oxide contamination susceptibility.

- The carbon dioxide absorption efficiency impacts the necessary solvent circulation rate.
- The heat of reaction with carbon dioxide implies the necessary energy required to reverse the reaction and liberate the captured carbon dioxide, thus regenerating the solvent for continued use.
- The thermal degradation rate and sulfur oxide contamination susceptibility determine the loss rate of solvent, and thus, the necessary replacement rate.

The regeneration energy requirement, absorption efficiency, and to a lesser extent, the thermal degradation rate, can all be reasonably estimated based on existing literature. The data that would describe the contamination susceptibility of the alkanolamines, however, is severely lacking in relevant literature. The method by which this parameter was determined is explored in Section 4.1.2. Given the abundant availability of literature for carbon capture employing MEA, and literature reporting relevant properties of the other alkanolamines, it was decided to quantify each of the aforementioned properties/characteristics relative to MEA in the form of coefficients, which are used for various calculations or cost determinations in a specific alkanolamine's simulation. The literature-available parameters are given in Table 3.4.

Table 3.4: Relevant Chemical Properties (Quantified)

Coefficient or Parameter	MEA	DEA	MDEA	AMP
Relative Regeneration Energy Requirement (Heat of Reaction with CO_2 (kJ/kg))	1 (1689)	0.941 (1590)	0.734 (1240)	0.924 (1560)
Relative CO_2 Absorption Efficiency at 0.25 mol CO_2/mol Loading	1	0.93	0.15	0.89
Thermal Degradation Rate (percent of alkanolamine volume per day)	0.5	0.5	0.57	0.143

Another important numerical assumption is the precise cost selected for the social cost of carbon. In the base case, the principal value proposed by Nordhaus, adjusted for inflation, was used. More specifically, the social cost of carbon was said to be 45.52 USD/tonne of carbon dioxide for the simulations of this thesis. The results section includes an analysis of the net external and net social benefits for each alkanolamine over the entire range of values Nordhaus proposes for the social cost of carbon.

3.5 Simulation Overview and Output Interpretation

It is important to provide an explicit overview of the simulations' approach in order to better understand where and how the parameters of the simulations play their role in cost and incentive analyses. Additionally, detailing the methods by which results are obtained and incentive analyses are conducted further facilitates their interpretation. The mechanisms through which the simulations here make use of the input data to output the results are relatively simple in comparison to other simulations that appear in the literature. That being said, the data themselves had methods of determination that were much more involved than simple sample collection—the specific details of which have been or will be discussed in other sections. It is in these methods, however, where the cost-impacting chemical and engineering nuances of the process are incorporated into the simulations.

Figure 3.5 details a general overview of how each simulation functions. All simulations in this thesis follow this approach, and each alkanolamine-specific simulation makes use of the same types of data. The values of these data are subject to change, however, dependant on the specific operational requirements dictated by the chemical properties of each alkanolamine.

Figure 3.5: Simulation Process Overview

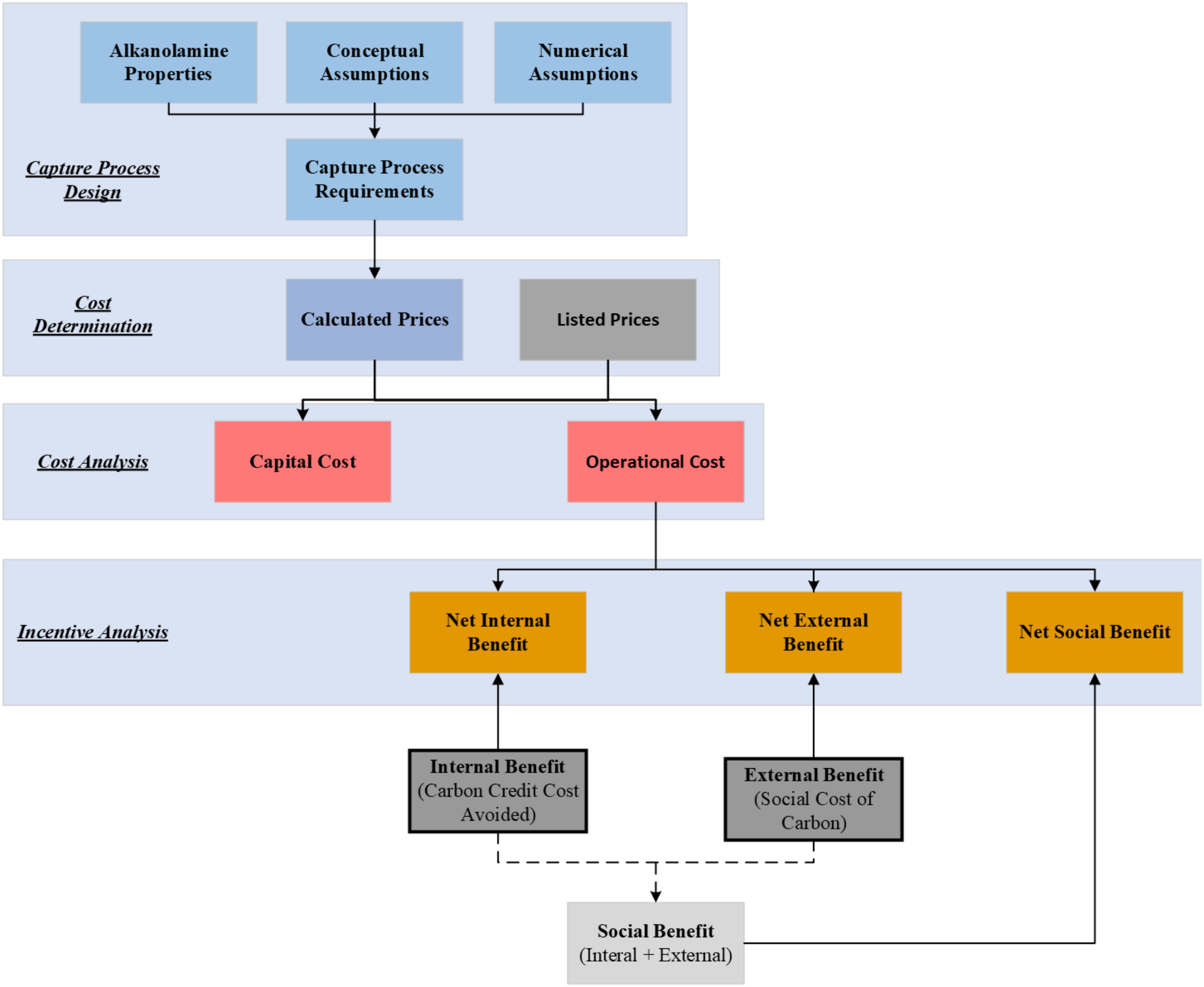

Figure 3.5: This figure describes a general outline of how each simulation is conducted in this thesis. The simulations begin by defining the alkanolamine-specific operational requirements, they then derive the costs associated with these requirements. Capital and operational costs are defined, then the degree of a firm's incentivization is quantified.

Each simulation firstly necessitates the establishment of alkanolamine-specific capture process requirements, in order to form a quantitative base from which costs can be derived. This quantitative base is built by considering the conceptual and numerical assumptions about the capture process, as well as the relevant chemical properties of the alkanolamine in question. With this information, capture process requirements such as solvent circulation rate, component capacity, reboiler fuel requirements, and many others are determined. Once all the necessary alkanolamine-specific capture process requirements are quantified, the costs associated with these specific requirements are determined. Additionally, listed costs (this notion is discussed at greater length in Section 4.2, but in essence, refers to any cost that could be taken as given in an online listing—requiring no manipulation) are considered, and these two factors allow the total capital and operational costs of an alkanolamine-specific capture process to be determined, yielding the first set of outputs from the simulations.

With operational costs of a given alkanolamine's capture process established, the incentive quantification and analysis can be conducted. Incentives are divided into three categories: internal, external, and social. The internal incentive is quantified by the cost of carbon credit purchases avoided, and is considered a transfer payment to the firm, thereby justifying its nature as an internal (private) benefit. Its value is directly proportional to the quantity of carbon dioxide captured (i.e., not emitted), and is determined by multiplying the total quantity of carbon dioxide captured by the price per unit of a carbon credit. The external benefit is quantified by the social cost of carbon described by Nordhaus (2017). It is representative of what could be considered either a regulatory cost avoided (not considered to be a transfer payment), or an ethical benefit. In either case, it is also directly proportional to the total quantity of carbon dioxide captured, and is determined by multiplying the total quantity of carbon dioxide captured by the social cost of carbon per unit. The social benefit is quantified as the sum of the internal and external benefit.

Incentive analysis is conducted by determining net benefits. These are distinctly different from the previously described benefits. A net benefit (be it internal, external, or social) is determined by subtracting the operational costs from the benefit. The net benefits describe the degree of incentivization in a similar manner to a profit calculation, where, as many are familiar with, profit is the difference of revenue and costs. Here, revenue is the benefit, costs are the operational costs, and profit is the net benefit. This comprises the final set of outputs.

The total capital and operational/upkeep costs can subsequently be directly compared across alkanolamine carbon capture process simulations, by virtue of the fact each simulation makes use of the same conceptual capture process layout: a chemical ceteris paribus. Additionally, the net benefits can compared in a similar manner. Finally, it is worth noting that a firm is considered to be incentivized to engage with/adopt this carbon capture technology if a given net benefit is positive.

4. Data

4.0 Limitations

Due to the somewhat ad hoc nature of the costs and parameters of the components in the models, there are several areas in which uncertainty inherent to the data, assumptions, or calculations can influence the results. Firstly, many components do not have a sufficiently large market to determine a “true” market price. This is problematic because with a limited quantity of price data, assessing the accuracy of price estimates is difficult, which may introduce uncertainty. The alkanolamines themselves fall victim to this. Furthermore, firms that engage in flue gas carbon capture may have access to supply chains that would be able to produce and deliver these chemicals more efficiently than simply making a purchase from a wholesaler, and the prices they would see in this case are unlikely to be publicly available. This notion goes beyond pure speculation. Much of the preliminary flue gas carbon capture literature was written by engineers at firms such as *Fluor* (Mariz, 1998), about plants which were built by the firm itself, which also has the infrastructure and/or business relationships (such as with *Dow*) established to manufacture or acquire the required chemicals. This notion also extends to the physical machinery involved in the process, introducing uncertainty into all price determinations.

Assumptions about the chemical properties or their behaviour in the capture process also add uncertainty. It is rare for a physical (or chemical) process to behave identically to its theoretically projected behaviour. Take, for example, calculating the velocity of a ball thrown across a field while accounting for air resistance. While this may be feasible on paper with predefined values, how, in practice, can one account for unpredictable shifts in wind direction and velocity perfectly in every experiment? It is in this sense that another degree of uncertainty is inherent to these models, made worse by a foundation of several assumptions–not physical constants or centuries old, well-established physical relationships. A notable example of this is the sulfur oxide concentration in the flue gas. Given the incredibly low probability of two naturally-occurring samples being identical (in the same way no two snowflakes are identical), the sulfur concentration in any two samples of coal is highly unlikely to be identical, introducing uncertainty in the sulfur oxide scrubbing cost

Additionally, in scaling the capacity and costs of components where it was required, the scaling equation described by Kölbel and Schulze (1960) was used. While this piece of literature is valuable and insightful, it is unclear how accurate this method of cost determination truly is. That being said, the cost determination of the stripper and absorber seem to support the equation to some degree, however, the uncertainty here is highlighted by the difference in the exponent found in the equation described by Kölbel and Schulze (1960) and the exponent of the power series fit of the stripper's and absorber's brief empirical cost-scale analysis in Section 4.2.2.

4.1 Calculated Parameters

The total power output of the power plant, while not directly used in any cost analysis, is still a relevant figure to note for the purposes of scale comparison between this thesis, other literature, and real-world examples. According to the *U.S. Energy Information Administration*, in 2019 coal-fired electricity production produced 253 892 liters of carbon dioxide gas per MWh of electricity. With the total quantity of carbon dioxide captured per day already known, the total power generation of the simulation's power plant was calculated to be 214.969 MWh or 8.957 MW per day (McGrath, 2021). Which is extremely small when compared to the power output of real coal-fired power plants in use today.

Chapel, Mariz, and Ernest (1999) indicates that a typical Econamine FG employing MEA in the capture process requires a rich solvent circulation rate which can be approximately calculated by Equation 4.1:

$$\textit{Circulation Rate } (m^3/hr) = 0.71 \cdot (\textit{tonnes } CO_2 \textit{ captured per day}) \tag{4.1}$$

The circulation rate of the solvent must be sufficiently high enough that the stoichiometric amount of alkanolamine passing through the absorber is roughly equal to the stoichiometric amount of carbon dioxide passing through the absorber over the same period of time. If it is less, then there will be an insufficient amount of alkanolamine present to absorb the carbon dioxide, and thus carbon dioxide will be vented with the vent gas, which is unacceptable for the purposes of this model. The reaction between the alkanolamine and carbon dioxide is not of zeroth order. While there is an extensive body of well-established literature on reaction kinetics, the important takeaway from this is that the reaction occurs quickly at first, but as the concentration of the reactants decreases, the rate of reaction slows. Therefore, it is especially important to maintain as high a concentration of fresh alkanolamine as possible, especially in the case of alkanolamines with low absorption efficiency, to ensure that absorption is occurring as efficiently as possible. While the equation described by Chapel, Mariz, and Ernest (1999) is intended for plants employing MEA (given the fact it approximates the molar mass ratio of MEA and CO_2), it is scaled here based on the ratio of the molar mass of a different alkanolamine and that of MEA, to ensure the minimum stoichiometric quantity requirement is met. Thus, the necessary circulation rate requirement used in this model was calculated according to a similar equation, shown in Equation 4.1.2.

$$\text{Circulation Rate } (m^3/hr) = \left(\frac{\text{molar mass alkanolamine}}{\text{molar mass MEA}}\right)\cdot\left(\frac{1}{A}\right)\cdot(\text{tonnes } CO_2 \text{ captured per day}) \qquad (4.1.2)$$

where A is the absorption efficiency coefficient of the relevant alkanolamine.

The process of regenerating the solvents requires that they be heated so that the captured CO_2 is liberated. This requires the use of industrial boilers. The layout of these models necessitates two boilers. Powering these boilers electrically would not be feasible, given their size and the quantity of liquid that must be vapourized in each case implies the power requirement would exceed the total output of the power plant. Thus, these boilers must be heated by other means, the simplest of which being coal combustion. There are several methods by which coal combustion can be utilized to heat industrial boilers. The following calculations are for the least efficient heating method, a fixed bed system, in which coal is added to the system and burned directly, with no modification of any kind. The total fuel requirement for the boilers operating with a fixed bed in terms of tonnes of coal per day is used to calculate a baseline fuel requirement. It is then converted to the fuel requirements of the much more energy efficient fluidized bed system. The fuel requirement for a one boiler fixed bed system is calculated by Equation 4.1.3:

$$\textit{Fuel Requirement (kg coal/hr)} = \textit{Heat Input / Calorific Value of Fuel} \qquad \textbf{(4.1.3)}$$

where the calorific value of coal[3] was estimated to be 30 MJ/kg and the heat input is calculated by Equation 4.1.4.

$$\textit{Heat Input (kJ/hr)} = 4.184 \cdot [R \cdot C \cdot (H_S - H_L)] / E \qquad (4.1.4)$$

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[3] The calorific value of coal typically ranges from 25 MJ/kg to 35 MJ/kg , and is considered by the *European Commission* to never fall below 24 MJ/kg. The exact middle ground was selected here.

where:

- R = Regeneration Energy Requirement of Alkanolamine
- C = Boiler Capacity
- H_S and H_L = enthalpy of steam and feed liquid, respectively
- E = Boiler Efficiency (assumed to be 75%)

The fixed bed system assumes all fuel added is consumed every hour. For a fluidized bed system, all fuel is consumed approximately every twenty minutes, however the total mass of fuel required to maintain the system is approximately one percent by weight. The other 99 % of the fuel mixture is composed of non-combustible materials. Thus, these components are not consumed in the combustion process and are neglected in the cost model. While this cost-determining approach may appear brash at first glance, the neglected components consist of sand, ash, and/or limestone, which may well be freely available or already produced by the power plant in a real world setting. The conversion of fuel requirements for a fluidized bed system are shown in Equation 4.1.5.

$$\text{Fluidized Bed Requirement (tonnes/hr)} = \text{Fixed Bed Requirement} \cdot 0.01 \cdot 3 \qquad (4.1.5)$$

where the 0.01 factor adjusts for the fuel requirement and the 3 factor adjusts for combustion rate. Fluidized beds operate by passing an air stream through the fluid mixture so as to keep it suspended. The principal efficiency advantage of a fluidized bed is twofold; on one hand, the fluidlike behaviour of the fuel allows for significantly more efficient energy transfer, and on the other, the coal matter of the fuel is of markedly smaller size than the lumps used in a fixed bed system (Morley, Pisupati, Scaroni, 2017). This smaller size drastically increases the surface area to volume ratio of the coal, decreasing its combustion time while also decreasing the quantity of uncombusted solid to which heat can be wastefully absorbed (Lappas and Heracleous, 2016).

As previously discussed, an alkanolamine's susceptibility to contamination is an important factor to consider as it will determine the necessary replacement rate of the solvent to maintain a consistent processing capacity. The relative rate at which an alkanolamine will irreversibly react with sulfur oxide contaminants is a function of the degree of the molecule's steric bulk compared to the steric bulk of MEA. Steric bulk is the notion of how "crowded" a bonding site is by the rest of the structure of a molecule for a given reaction. The greater the steric bulk, the more difficult it will be for an individual molecule to proceed with a given reaction. In the case of the reactions with either carbon dioxide or a sulfur oxide, the more sterically hindered alkanolamines will proceed with both reactions more slowly. In other words, their carbon dioxide absorption efficiency will be lower, but they will also react with sulfur oxides less frequently. This is because the electrons of an atom tend to repel each other, as a result of their like charges, requiring more energy to bring them in close proximity. A greater energy requirement to close the distance between atoms implies a greater energy requirement to initiate a reaction. Thus, the more electrons there are occupying a given area in space, the more energy will be required to have other atoms approach that space. Alkanolamines proceed through both aforementioned reactions with CO_2 and SO_x by use of their nitrogen atom. There are three varieties of nitrogen atoms (amine groups) in the four alkanolamines studied in this model: primary, secondary, and tertiary. MEA and AMP are primary amines, meaning their nitrogen atoms are bound to only one other non-hydrogen substituent. DEA is a secondary amine, meaning its nitrogen atom is bound to two other non-hydrogen substituents. MDEA is a tertiary amine, meaning its nitrogen atom is bound to three other non-hydrogen substituents. In general, the magnitude of steric bulk hindering a reaction (steric hindrance) of this nature is primary < secondary < tertiary, where primary amines are the least hindered. AMP, however, is a special case. Despite the fact it is a primary amine, the geometry of its molecular structure places two methyl groups in close proximity to its nitrogen atom. This introduces more steric bulk around the relevant functional group than MEA, the other primary amine. The relative steric bulk of the alkanolamines in this model is as follows: MEA < DEA < AMP < MDEA where MEA is the least sterically hindered. This notion is further supported by the rate constants for the reaction of these alkanolamines with CO_2 in the literature. Rate constants indicate the speed at which a given reaction proceeds, and are determined experimentally. Additionally, as stated, a slower rate of reaction with CO_2 implies a slower rate of reaction with SO_x on the basis of steric hindrance. The general trend of these rate constants in the literature agree that MEA reacts the fastest with CO_2 and MDEA reacts the slowest, however, the specific order of AMP and DEA does not have a consensus, and varies with each experiment. For the purposes of this model, the data presented by Aroonwilas and Veawab (2004) are used to determine the absorption efficiency of each alkanolamine as it directly presents experimental data of this parameter, and the rate constants presented by Sema et al (2013) were used to determine implied steric bulk and thus infer the contamination susceptibilities relative to MEA via a Taft-esque equation. These parameters are presented in Table 4.1. The Taft equation quantifies the effects of various molecular forces, including steric bulk, on the rate of a reaction. The approach here deviates from Taft's methods somewhat, as his equation relates the rate constants of a substituent reaction with that of a methyl group. If one is to conceptualize the methyl group as a reference reaction, then this approach is justified insofar as MEA's reaction with CO_2 is the reference reaction, and the other alkanolamines' reactions are the reactions of other substituents. Ideally, the rate constants of the alkanolamines' reaction with both sulfur oxide species would be used here, however the literature does not exist.

Table 4.1: Determination and Presentation of Contamination Susceptibility Coefficients

	MEA	DEA	AMP	MDEA
$\left\|\log\left(\frac{k}{kMEA}\right)\right\|$*	0	1.159	1.099	2.983
Relative Contamination Susceptibility Coefficient	1	0.863	0.91	0.335

*Here, k is the rate constant of a given alkanolamine's reaction with CO_2. The inverse of this value is used as the relative contamination susceptibility coefficient. MEA is the reference reaction, and thus has coefficient 1.

4.2 Cost Determination

4.2.1 Alkanolamines

The methods by which a price for each alkanolamine was determined were roughly consistent across all four studied in this model. Listings for an alkanolamine on *Alibaba.com, Madeinchina.com,* and other similar websites were collected, and the average cost per liter across all selected listings was used. In the case of DEA and AMP, ten listings were selected. In the case of MEA, a large enough market exists to offer what could be considered a market price. However, this price differs substantially from those of wholesale listings, thus it was included as one of ten prices when calculating the average. Due to a lack of data for MDEA, only six prices were able to be collected. Appendix A contains all listings and sources used in the price determination of the alkanolamines in the model, as well as all mechanical component listings.

4.2.2 Absorber and Stripper

On the basis of the assumption that both the absorber and stripper required identical dimensions, the same method was used to determine the price for both. These two components are incredibly versatile in terms of their use cases, and thus, have a fairly sizable wholesale market. The approach taken to determine their costs was as follows. First, ten listings for compatible components with varying processing capacities were selected. The cost of each component was plotted against its corresponding processing capacity, which is shown in Figure 4.2.2. In this case, processing capacity is in terms of the flow rate of gas volume per hour (m^3/hr). A power series fit was then applied in the spirit of illustrating to what degree returns to scale impact the proportion of cost increase with scale. The equation of the power series fit was then used to calculate the cost of each component by determining the precise gas flow rate based on the initial assumption of 100 tonnes of CO_2 captured per day and 13 % flue gas carbon dioxide concentration. These assumptions yield a total flue gas processing rate of 17 493.25 m^3 / hr, and thus an absorber or stripper cost of 5033.17 USD each.

It is worth noting that the sample of prices used in the cost determination here is far from random. Each price was handpicked from the wholesaler websites, with mixing between the materials used to construct the components, and the purposes for which they were intended. Listings that appeared to show some degree of price gouging, or those that were suspiciously inexpensive were not included. It appears that the primary function of these wholesaler websites is simply to advertise products and attract potential customers, with little intent to convey which price is the “true” price. This is demonstrated by many instances of a single company having more than a dozen listings for the same product, at widely variable prices.

Figure 4.2.2: Power Series Fit of Absorber/Stripper Price-Capacity Pairs

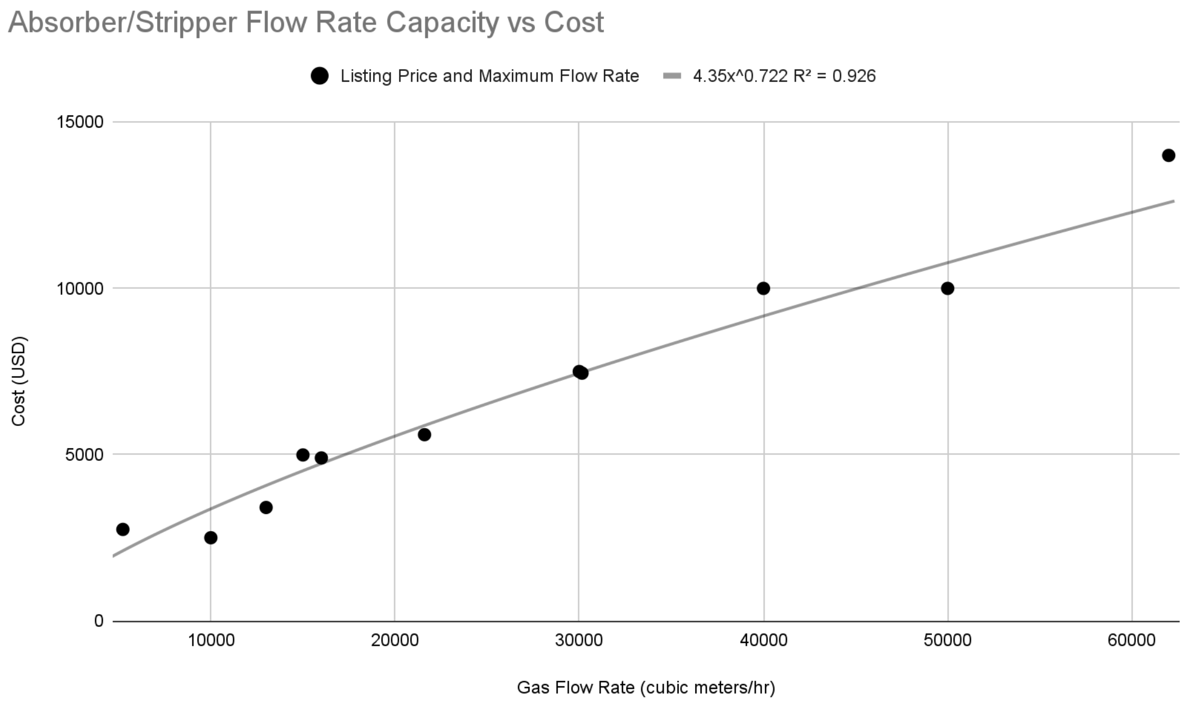

Figure 4.2.2: This figure presents all price-capacity pairs of the listings selected for absorber and stripper price determination. It is worth noting the exponent is indicative of increasing returns to scale.

4.2.3 Reboilers

The cost of the boilers used for solvent regeneration and CO_2 liberation was determined by first selecting a compatible model listed by an online wholesaler, then the cost scaling equation described by Kölbel and Schulze (1960) was used to scale the boiler's cost with the correct capacity. The scaling equation is presented in Equation 4.2.3, and (as Dr. Andrew Davis, an expert in macroeconomics, highlighted) coincidentally closely resembles a production function in which total factor productivity is eliminated by dividing the equation by itself, and the second output value is brought from the left hand side of the equation to the right.

$$\text{Cost of Scaled Component} = \text{Cost of Reference Component} \cdot \left(\frac{\text{Scaled Capacity}}{\text{Reference Capacity}}\right)^{0.6} \qquad (4.2.3)$$

The capacity of the boiler is dependent on each solvent's required circulation rate. Due to a lack of available listings for boilers whose capacities approximate what would be necessary, the boiler selected for the MEA simulation was used as the reference component price for all subsequent alkanolamine simulations. It is worth noting that the value of the exponent in equation 4.2.3 proposed by Kölbel and Schulze (1960) is also supported by Chapel, Mariz, and Ernest (1999). An exponent less than one implies decreasing marginal cost with increasing scale, and therefore, increasing returns to scale in the context of flue gas carbon capture machinery. This is well-illustrated if one conceptualizes this equation as a cost function of scaling the component's capacity. Ceteris paribus, as the scaled component capacity increases, the second order derivative of the cost function with respect to scaled capacity is negative, indicative of decreasing marginal costs. Figure 4.2.3 depicts this relationship graphically. From an engineering standpoint, this relationship is sound. In terms of a component like a boiler, whose capacity is in units of volume, to increase the capacity, one must increase the surface area of the vessel. The relationship between surface area and volume is that of a squared unit to a cubed one, in other words, volume increases at a greater rate than surface area when scaling up size. Therefore, in theory, less raw material is required in the construction of a component of greater capacity, and thus, cost would not increase proportionally with capacity.

Figure 4.2.3: Graphical Depiction of the Marginal Cost Relationship with Scale

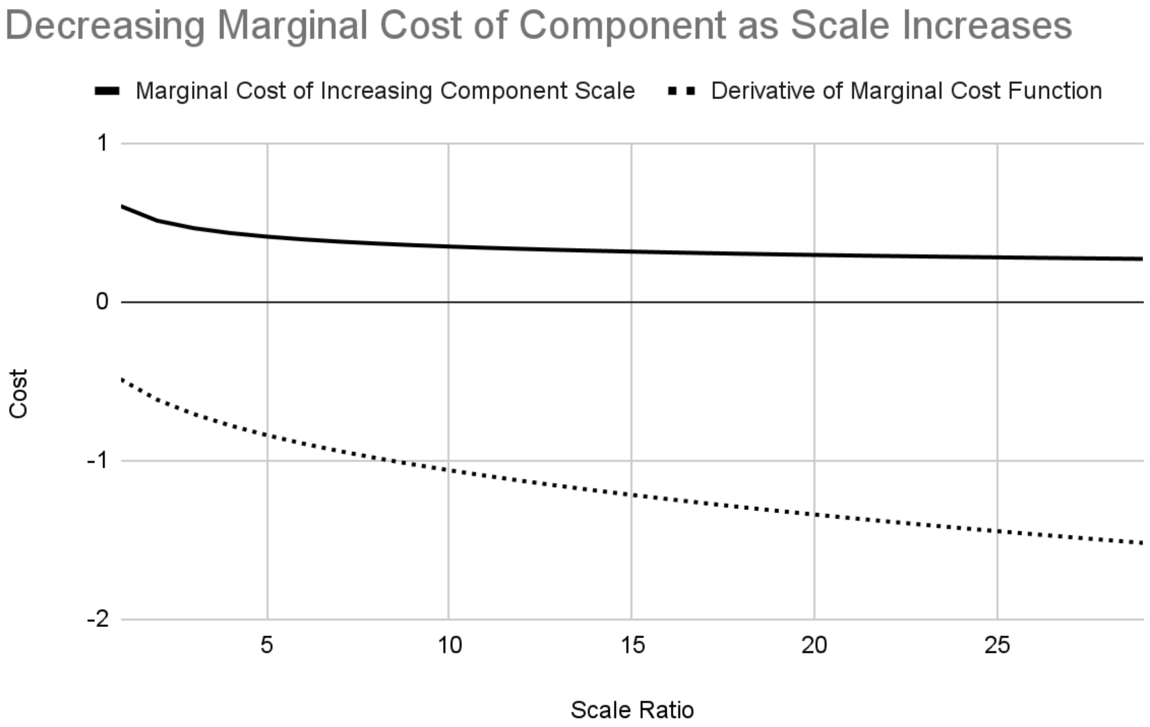

Figure 4.2.3. This figure depicts the relationship between the marginal cost function (derived from the scaling equation Kölbel and Schulze (1960) proposes) and its derivative as the scale ratio increases, indicating increasing returns to scale. For the purposes of clarifying the relationship, the cost of the reference component is 1.

4.2.4 Blower

The blower is responsible for moving the flue gas from the power plant into the capture process at a sufficient pressure. Similarly to the reboilers, a compatible component was found in an online listing, and was scaled using the same equation as the reboiler. For all solvent methods used however, the cost of the blower remains the same, given the necessary scale is equal to the total volume of flue gas entering the system per day. The cost of the scaled blower is 169.25 USD.

4.2.5 Pumps

The plant layout used for this model necessitates three pumps of sufficient capacity to move the liquid solvent through the capture process. The same method of component selection as the blower and reboilers was used. Fortunately, a model with sufficient capacity to be used in all simulations was available, thus no cost scaling was necessary. The ISW Horizontal Pipeline Centrifugal Pump was selected at a cost of 800.00 USD per unit.

4.2.6 Condenser

The condenser is responsible for condensing gaseous solvent back into a liquid in order to fully separate the solvent vapours from the liberated CO_2. Again, the same selection method was employed. In this case the necessary scale could be no more than the total flue gas processing volume per day, thus a fixed cost could be established for all solvent techniques. Fortunately, a component of compatible size exists and thus required no cost scaling. The KEN520 Evaporative Condenser model was selected from an online wholesaler listing, at a price of 12 000 USD.

4.2.7 Sulfur Oxide Scrubbing

Sulfur oxide scrubbing tends to be a proprietary process, where any given scrubbing apparatus is constructed to fit the unique needs of an individual operation. Fortunately, studies have been conducted such as Baasel (1988) which provides a cost estimate in terms of USD/lb of sulfur removed from a flue gas stream. This study was published in 1988, thus adjusting for inflation, and converting metric units of sulfur volume to imperial units of mass, sulfur oxide removal was determined to cost 555.24 USD per day. In all simulations conducted here, the numerical assumptions of the flue gas constituents and the capture process operation are such that the sulfur oxide scrubbing requirements, and thus cost, do not vary in the base case.

4.2.8 Startup Alkanolamine

To begin the carbon capture process, a bulk quantity of the relevant alkanolamine must be purchased. The exact quantity necessary was determined by first converting the assumption of a solvent concentration of 30 wt% alkanolamine to a value in volume %, then to a concentration value in moles per liter. Given the total moles of CO_2 being processed per day is given by the model's assumptions, the quantity of solvent necessary to begin the process was determined by dividing the moles of CO_2 processed per hour by the alkanolamine concentration. This gives a solvent volume in liters that ensures there is a sufficient stoichiometric quantity of alkanolamine available in the system to capture all the carbon dioxide, whose units are congruent with those of the circulation rate.

4.2.9 Coal

The operation of this capture process necessitates some quantity of coal for each alkanolamine model to heat the reboilers. The exact price of coal used was determined by taking the spot price of coal originating from Central Appalachia, Northern Appalachia, and The Illinois Basin, according to the *U.S Energy Information Administration,* and using the average of the three prices as listed on April 7th, 2023. This yielded a price of 94.93 USD / tonne (U.S. Energy Information Administration, 2023).

4.3 Summary Tabulation of Simulation Parameters

All costs and prices that varied between each simulation are listed in Table 4.3 and all costs and prices that remained constant across each simulation are listed in Table 4.3.1. These two tables account for all final[4] and the most relevant and contextually insightful preliminary[5] calculated or literature-sourced simulation parameters. The parameters that are not included in these tables were those that contribute little to the general understanding of the simulation. These include parameters such as molar quantities of either sulfur oxide species entering the capture process or the enthalpy of steam in the reboilers. Most simulation parameters are included in these tables, and few are excluded.

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[4] A parameter directly used in a cost determination.

[5] A parameter not directly used in a cost determination but one which contributed to the determination of a final parameter's value. The preliminary parameters are italicized in Table 4.3 and 4.3.1.

Table 4.3: Varying Parameter Values Across Simulations

	Alkanolamine			
Price	MEA	DEA	MDEA	AMP
Alkanolamine (USD/L)	1.52	1.93	5.03	3.05
Reboiler (USD)	13 990.16	20 414.71	65 767.25	18 983.81
Alkanolamine Properties				
SO_x Contamination Susceptibility Coefficient	*1*	*0.863*	*0.335*	*0.91*
Absorption Efficiency Coefficient	*1*	*0.93*	*0.15*	*0.890*
Relative Regeneration Energy Requirement	*1*	*0.941*	*0.734*	*0.924*
Thermal Degradation Rate (% Volume/day)	*0.5*	*0.5*	*0.57*	*0.143*
Alkanolamine Losses				
SO_x Contamination (L/day)	*225.264*	*285.643*	*125.633*	*255.294*
Thermal Degradation (L/day)	*33.545*	*45.667*	*61.823*	*11.602*
Net Loss* (L/day)	258.809	331.310	187.455	268.370
Capture Operation Parameters				
Solvent Circulation Rate (L/hr)	72 053	131 411	943 422	116 421
Startup Solvent Volume (L, 30 %w/w)	22 586.86	33 184.903	37 599.89	28 127.311
Implied Solvent Density (g/cm^3)	*1.00297*	*1.02477*	*1.01154*	*0.97880*
Reboiler Parameters (Single Boiler)				
Required Processing Capacity (kg/hr)	*36 133.52*	*67 333.10*	*467 048.40*	*56 976.60*
Heat Input Required (MJ/hr)	*436 097.45*	*764 700.75*	*4 137 435.29*	*635 392.05*
Fuel Requirement - Fluidized Bed (tonnes coal/day)	10.47	18.35	99.30	15.25

*Net alkanolamine loss implies the quantity of alkanolamine that must be added over a given timeframe to satisfy the operational requirements defined in Sections 3 and 4.

Table 4.3.1: Constant Parameter Values Across All Simulations

Parameter	Value
CO_2 Captured (Tonnes/Day)	100
CO_2 Concentration in Flue Gas (%)	*13*
Flue Gas Volume Processed (L/hr)	54 579 000
Net SO_x Concentration of Flue Gas (ppmv)	500
SO_2 Composition (%) | SO_3 Composition (%)	90 | 10
SO_2 Escaping Scrubbing (ppmv)	10
Component	Price
Carbon Credit Futures Price (USD/Tonne)	87.38
Coal Average Spot Price (USD/Tonne)	94.93
Social Cost of Carbon (USD/Tonne)	45.52
Condenser (USD)	12 000
Absorber (USD)	5033.17
Stripper (USD)	5033.17
Blower (USD)	169.25
Pump (USD)	800.00
SO_x Scrubbing (USD)	555.24

5. Simulation Results and Incentive Analyses

5.1 Comparative Cost Results

The two major factors that influenced capital costs were the reboilers and the price of the alkanolamines themselves. The reboiler capacity, and implicitly its cost, was dictated by the necessary solvent circulation rate. Thus, MDEA suffered the most in this respect, with total capital costs made worse by the alkanolamine's high price. DEA and AMP had similar capital cost requirements, with trade-offs being made between reboiler costs and alkanolamine costs. Ultimately, by virtue of AMP's cost, it proved slightly more expensive from a capital cost perspective. MEA was the clear winner in this context, with capital costs far lower than the other three. A breakdown of capital cost by component for each model is shown in Figure 5.1.

Figure 5.1: Capital Cost by Component

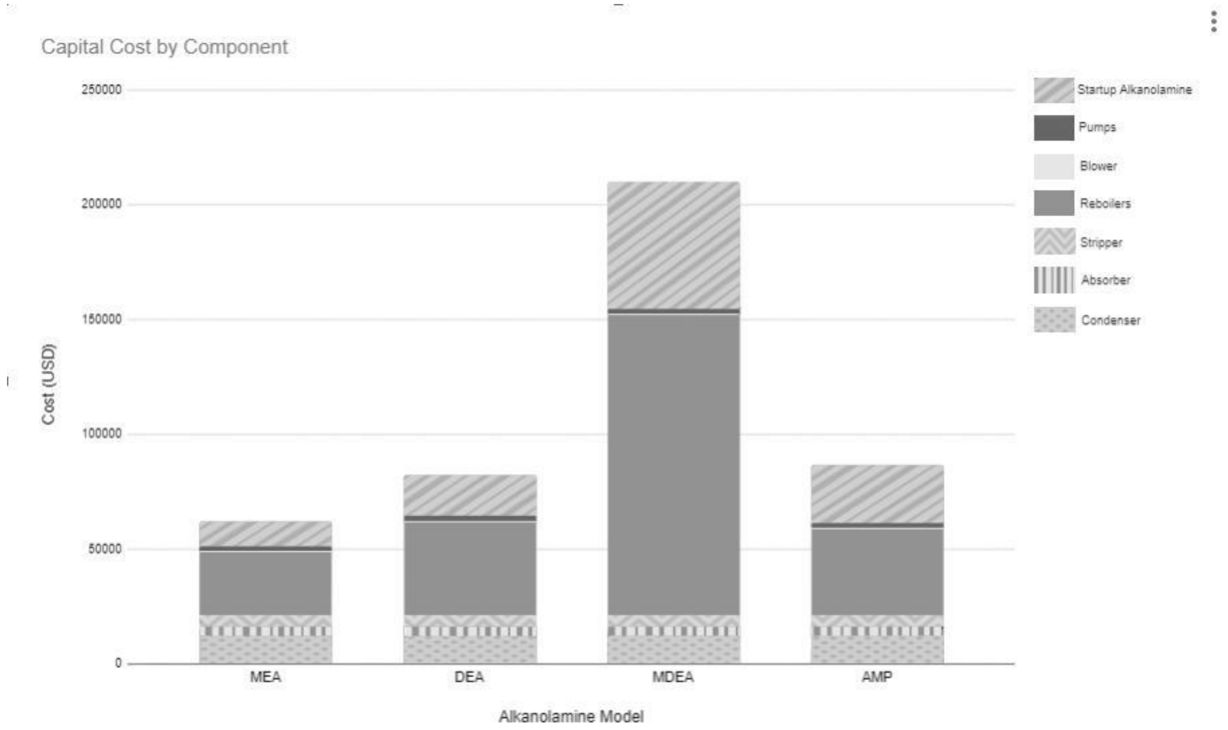

Figure 5.1: This figure presents a breakdown by component of the total capital costs in all simulations.

Upkeep costs were used in the determination of net internal, external, and social benefits. MDEA, again, suffered as a result of its high circulation rate requirement. This necessitated an extremely high rate of consumption of coal for the reboilers. In conjunction with a significantly higher price of alkanolamine, MDEA proved to be the most expensive alkanolamine carbon capture process to sustain. DEA and AMP had comparable upkeep costs. In this context, AMP proved less expensive by virtue of its lower solvent circulation rate, despite its higher alkanolamine price and lower loss rate. Again, however, MEA proved to be the most affordable capture process by upkeep costs given the lowest circulation rate, lowest alkanolamine price, and highest absorption efficiency, in spite of its high relative loss rate. Figure 5.1.1 presents upkeep costs broken down by component for all alkanolamines in this study.

Figure 5.1.1: Upkeep Costs by Component

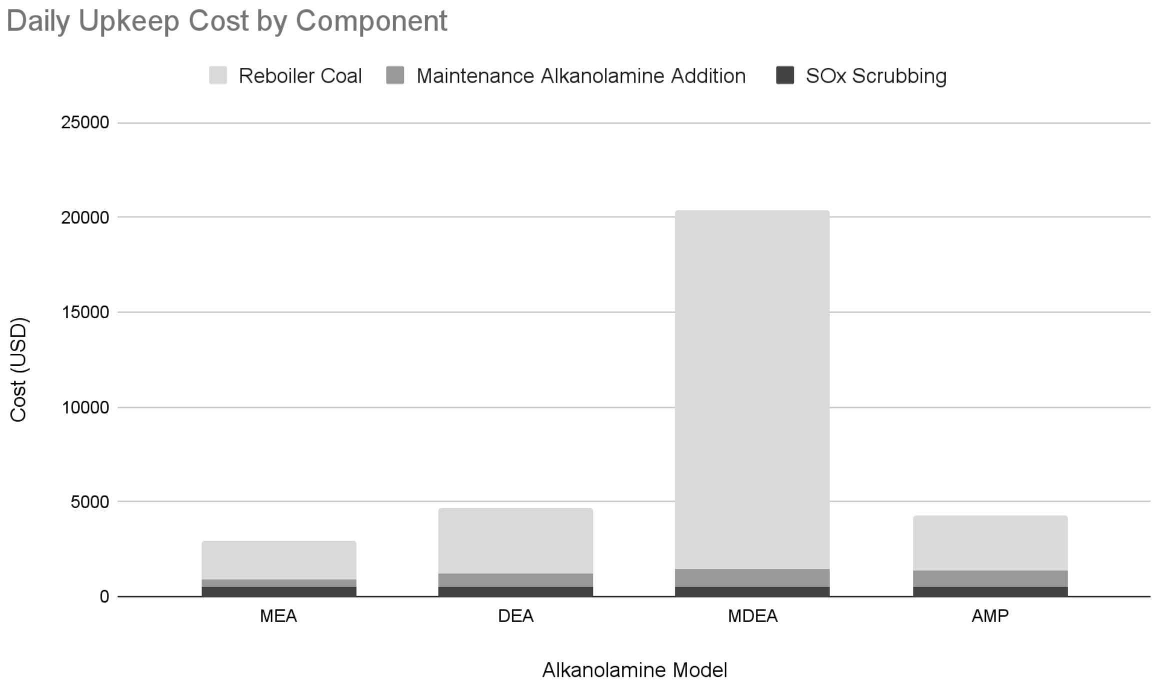

Figure 5.1.1: This figure presents the upkeep costs of each simulation broken down by component.

An interesting result was seen in the comparison of costs resulting from sulfur oxide contamination loss at different concentrations of sulfur oxides in the flue gas. In this case, AMP proved to be the most expensive loss to replace. Given its relatively high contamination susceptibility, and high price, this is logical. Subsequently, it is here where MDEA proves its merit, despite the poor performance shown in previous sections. Its extremely low contamination susceptibility outweighs its high price, and it outperforms AMP in this context. DEA slightly outperforms MDEA here, by virtue of its lower price, in spite of its higher contamination susceptibility. Somewhat unsurprisingly, MEA proved to be the winner again. Its extremely low price relative to the others was shown to be the determining factor in contamination loss costs, despite the highest contamination susceptibility. Figure 5.1.2 illustrates the costs of alkanolamine loss over a range of sulfur oxide flue gas concentrations. This data would prove useful in a setting where the sulfur oxide component of coal is subject to a high degree of variability.

Figure 5.1.2: Quantified Cost of Alkanolamine Loss at Different Sulfur Oxide Concentrations

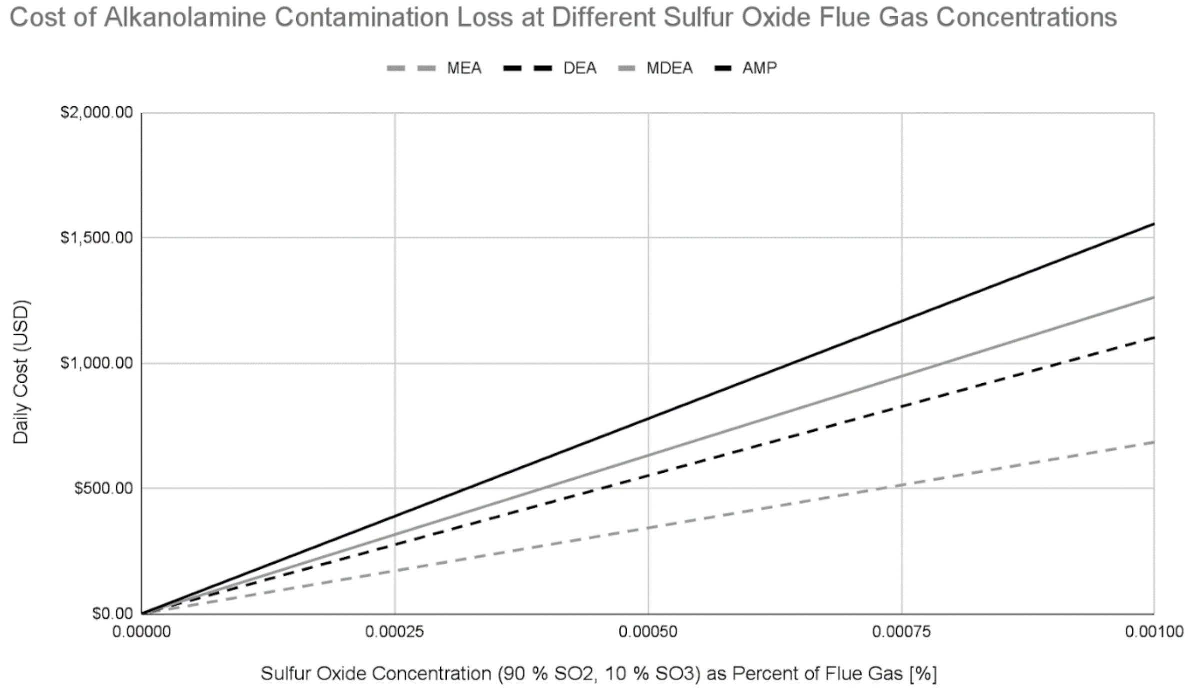

Figure 5.6.2: This figure presents the theoretical cost arising from the quantity of alkanolamine lost at a given concentration of sulfur oxides in the flue gas.

Finally, the days of operation necessary for the total net benefits accrued to outweigh total capital expenditures, from each net benefit standpoint, are listed in Table 5.1. While this is a useful comparison of capital costs and net benefits, it also shows which net benefits are positive or negative with the parameter values used in each simulation. Implicitly, a positive net benefit will eventually outweigh capital expenditures whereas a negative net benefit will never do so. This table also provides a context in which the magnitudes of the net benefits can be compared in and across each simulation.

Table 5.1: Days of Operation Required for Accrued Net Benefits to Outweigh Total Capital Expenditures

Net Benefit Standpoint	MEA	DEA	MDEA	AMP
Internal	10.826	20.471	Not Possible	19.526
External	38.863	Not Possible	Not Possible	303.769
Social	6.066	9.650	Not Possible	9.678

This concludes the comparative cost results, and the subsequent results subsections will outline the individual simulation results of each alkanolamine in greater detail and undertake individual alkanolamine incentive analyses.

5.2 MEA Results and Incentive Analysis

For MEA, from any net benefit standpoint be it internal, external, or social, capital costs will be outweighed by total accrued net benefits after at most approximately seven weeks of operation (in the case of net external benefits). The results demonstrably show MEA to be the most cost efficient alkanolamine for this flue gas carbon capture process, which is not surprising. For one, it is the least expensive of the four, benefiting from the economies of scale arising from its pervasive use in other industries. The lower relative cost necessitates lower capital expenditures for startup and reduced upkeep costs relative to the other alkanolamines, despite its high contamination susceptibility and moderate thermal degradation rate. Additionally, the high absorption efficiency and low relative molar mass imply a lower solvent circulation rate, reducing the capacity requirement and thus cost of the boilers, and requiring less coal for said boilers. Furthermore, the capture process was designed based on capture process literature that primarily employed MEA, thus, the argument that MEA is the most optimal alkanolamine for this specific process is not without merit. In a similar sense, a process more optimized for the characteristics of the other alkanolamines could see MEA outperformed.

Figure 5.2 presents the net internal, external, and social benefits arising from some non-zero resale value of the captured carbon dioxide. These values are determined by taking the benefit of not emitting carbon dioxide (either the internal or external benefit), subtracting the upkeep costs, and adding the revenue of the sale of carbon dioxide at a given price. A negative net benefit indicates the firm, or the firm and society, incur a cost during operation from a given benefit standpoint. In all benefit perspectives for this model however, any revenue from the sale of carbon dioxide can be viewed as an added bonus. This is because all net benefits were positive (for these simulation parameter values), thus carbon dioxide resale revenue is not necessary to yield a positive net benefit from one that would otherwise have been initially negative.

Figure 5.2: Net Daily Internal, External, and Social Benefits for the MEA Process Incorporating Carbon Dioxide Resale Revenue into the Determination

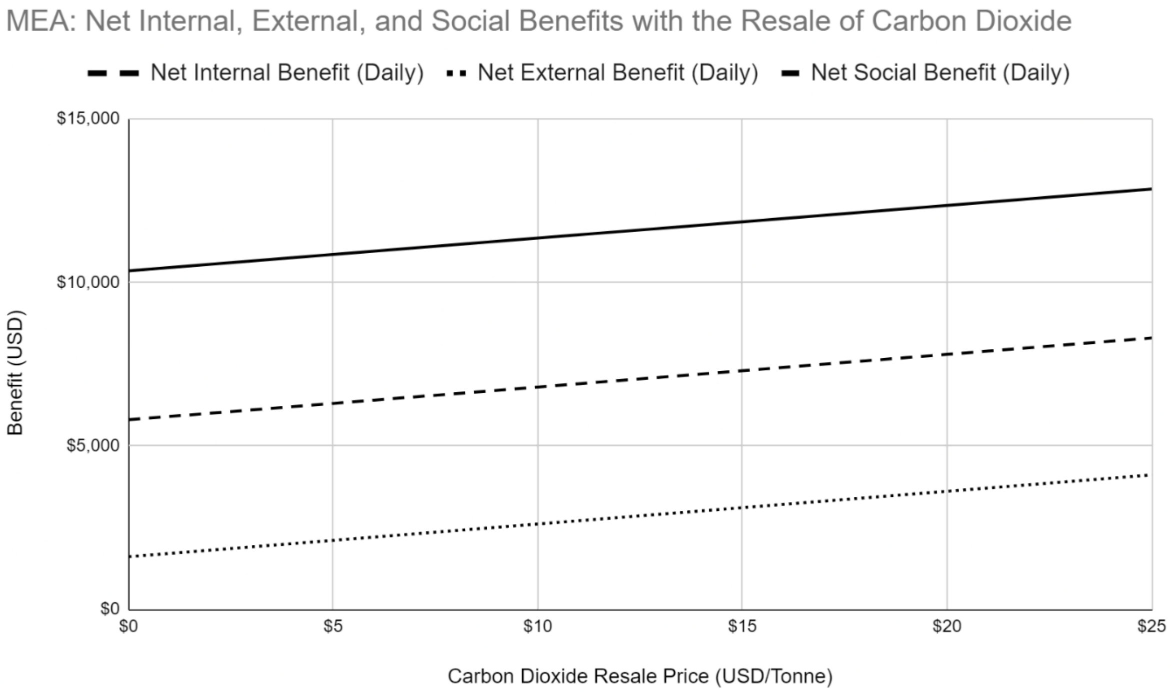

Figure 5.2: This figure incorporates the revenue generated from the resale of captured carbon dioxide over a range of potential sale prices into the net daily internal, external, or social benefit quantification for the MEA process.

Figure 5.2.1 presents the net internal, external, or social benefits over a range of coal prices. The net benefits were determined in a similar way to those of the scenario with carbon dioxide resale, though the price of coal was factored into the upkeep cost instead. Despite the fact the net benefit is not negative with the selected market price of coal in the MEA simulation, Figure 5.2.1 provides an indication of where net benefits would become negative from a given benefit perspective if the price of coal were to reach that level. In theory, all else being held equal, the MEA capture process could see the total accrued net benefits outweigh the total capital expenditure (after a sufficient amount of time) from a net social benefit standpoint up to a coal price of 589.47 USD / tonne. That is to say, the net social benefit remains positive up to this price.

Figure 5.2.1: Net Daily Internal, External, and Social Benefits for the MEA Process over a Range of Coal Prices

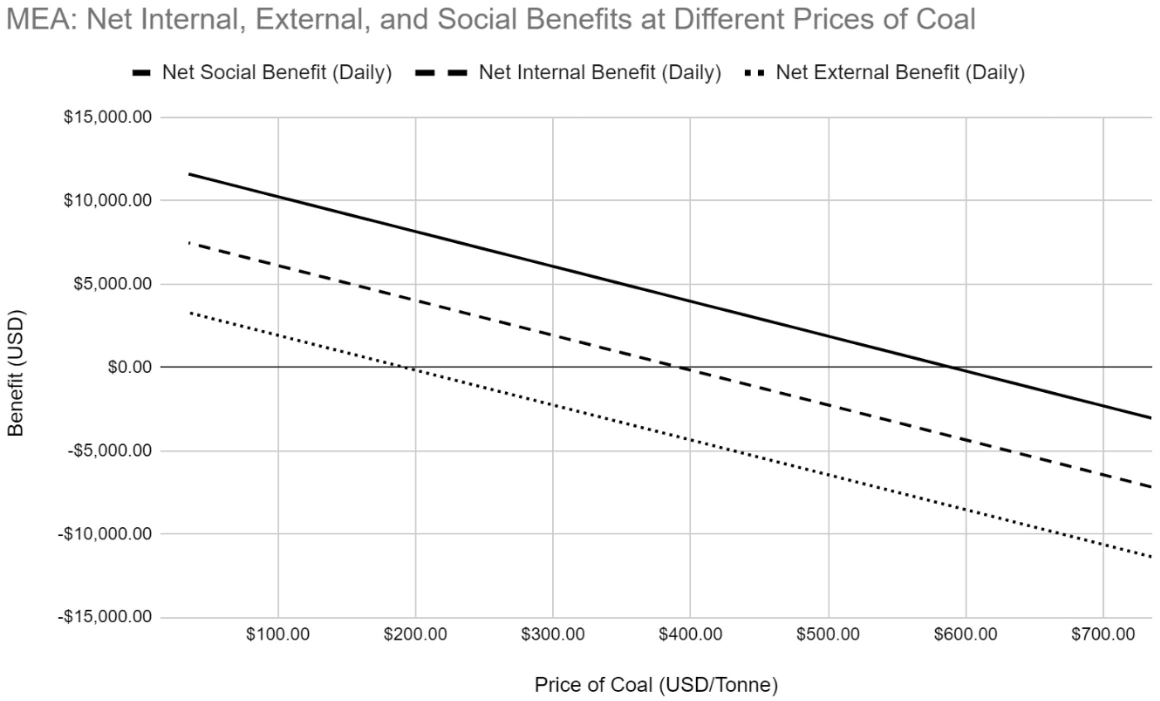

Figure 5.2.1: This figure depicts the net daily internal, external, and social benefits over a range of coal prices for the MEA process, and illustrates up to which price the process can maintain a net benefit from a given standpoint.

Figure 5.2.2 presents the range of values for the social cost of carbon that Nordhaus proposes under different assumptions, and the net external or net social benefit arising from all values in that range. From a net social benefit standpoint, the capture process always yields a positive net benefit to the firm and society, regardless of the social cost of carbon. From a net external benefit standpoint, however, the net benefit is negative below a social cost of carbon less than 29.38 USD / tonne.

Figure 5.2.2: Net Daily External and Net Social Benefits for the MEA Process over the Range of Social Cost of Carbon Values Proposed by Nordhaus

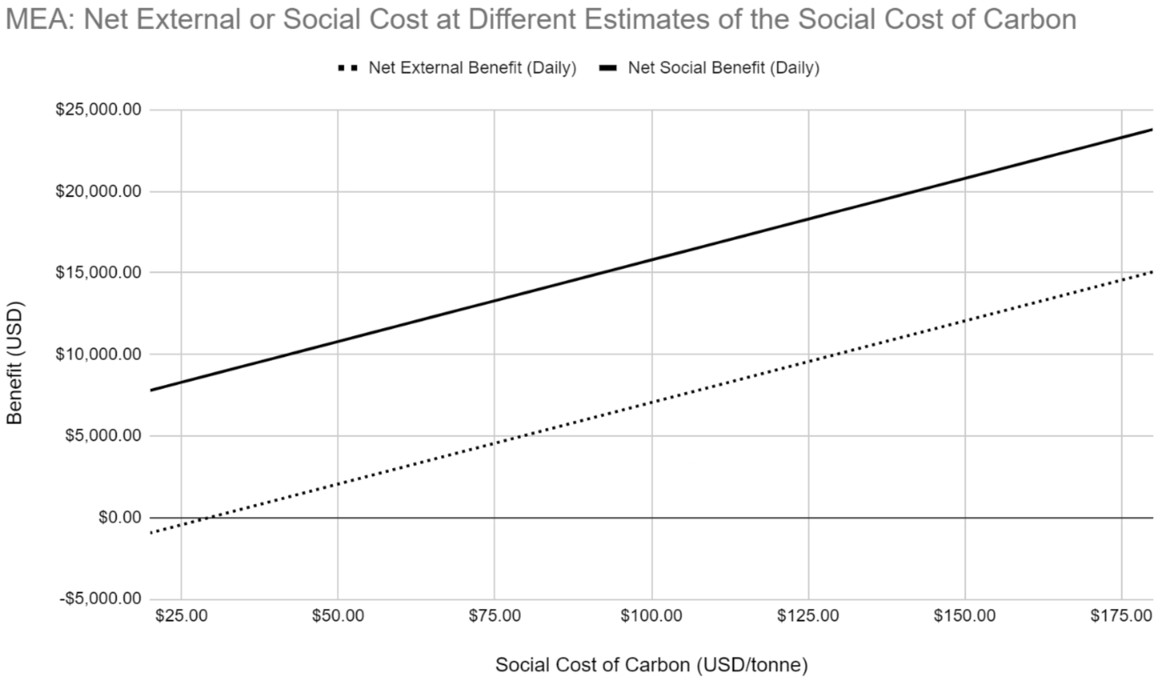

Figure 5.2.2: This figure depicts the daily net external and net social benefits for the MEA process over the range of social cost of carbon estimates according to Nordhaus, and illustrates up to which price of the estimate the process can maintain a positive net benefit from either standpoint.

5.3 DEA Results and Incentive Analysis

For DEA, from a net internal or social benefit standpoint, capital costs will be outweighed by total accrued benefits within, at most, approximately twenty days of operation. From an external benefit standpoint however, the net benefit is negative (for the simulation parameter values used) and thus capital expenditures can never be outweighed by total accrued net benefits from this perspective. This is due to an upkeep cost that outweighs the external benefit garnered from not emitting the carbon dioxide by just over 120 USD per day. The higher upkeep cost is primarily a result of higher circulation rate resulting from a lower (relative to MEA) absorption efficiency, necessitating notably higher coal consumption for the reboilers, despite the relatively smaller regeneration energy requirement. DEA is also approximately 30 % more expensive than MEA, resulting in more expensive daily alkanolamine loss to contamination in spite of its slightly lower relative contamination susceptibility. That being said, DEA remains a viable alternative to MEA from the net social and net internal benefit perspectives. Figure 5.3 shows that net external benefits will yield a positive net benefit above a price of 1.20 USD / tonne with the resale of the captured carbon dioxide. Alternatively, Figure 5.3.1 and Figure 5.3.2 show that a price of coal reduced below 91.37 USD / tonne or a social cost of carbon greater than 46.82 USD / tonne will also accomplish this.

Figure 5.3: Net Daily Internal, External, and Social Benefits for the DEA Process Incorporating Carbon Dioxide Resale Revenue into the Determination

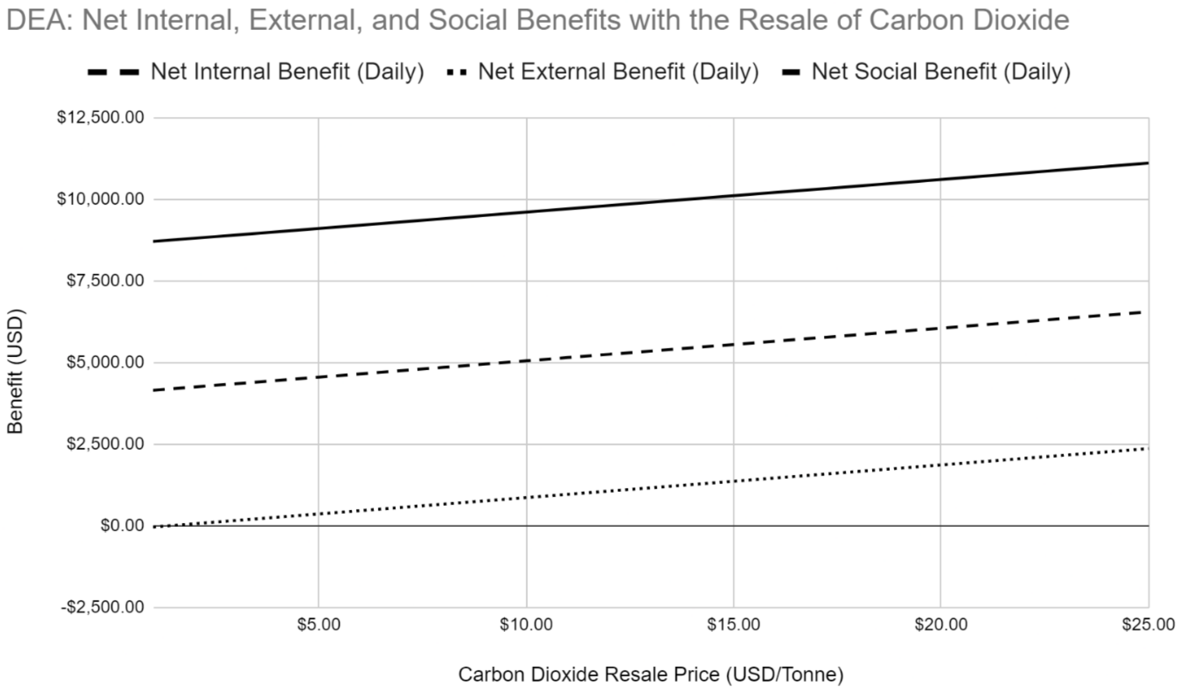

Figure 5.3: This figure incorporates the revenue generated from the resale of captured carbon dioxide over a range of potential sale prices into the net daily internal, external, or social benefit quantification for the DEA process.

Figure 5.3.1: Net Daily Internal, External, and Social Benefits for the DEA Process over a Range of Coal Prices

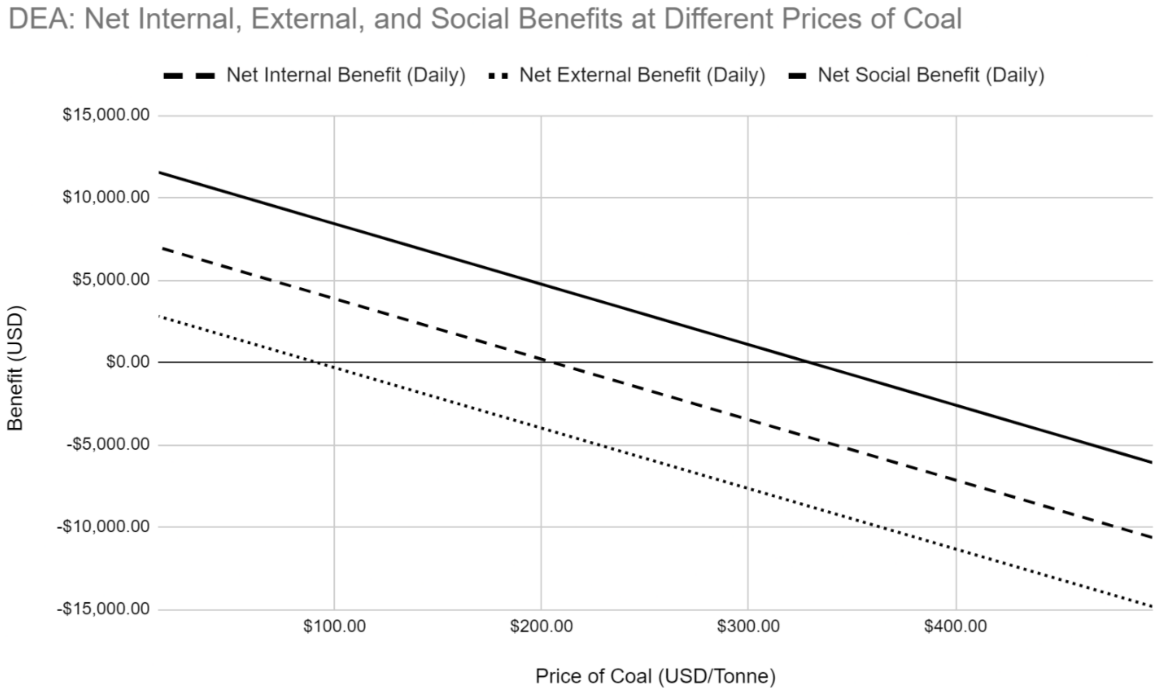

Figure 5.3.1: This figure depicts the net internal, external, and social benefits over a range of coal prices for the DEA process, and illustrates up to which price the process can maintain a positive net benefit from a given standpoint.

Figure 5.3.2: Net Daily External and Net Social Benefits for the DEA Process over the Range of Social Cost of Carbon Values Proposed by Nordhaus

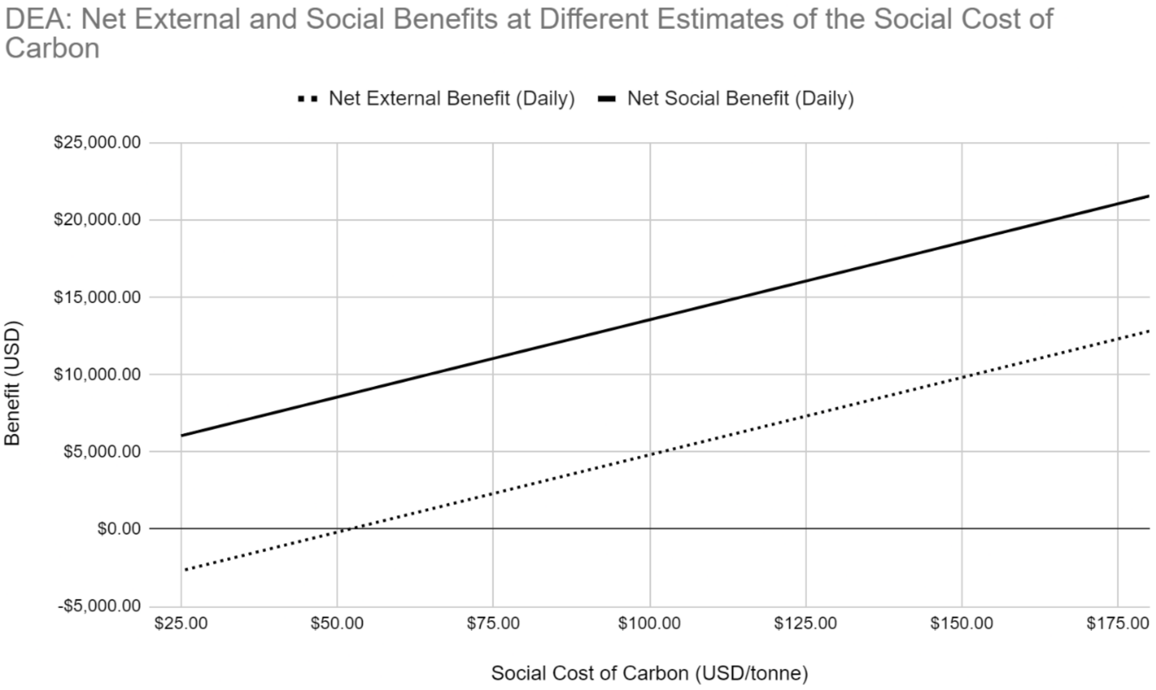

Figure 5.3.2: This figure depicts the daily net external and net social benefits for the DEA process over the range of social cost of carbon estimates according to Nordhaus, and illustrates up to which price of the estimate the process can maintain a positive net benefit from either standpoint.

5.4 MDEA Results and Incentive Analysis

For MDEA from any net benefit perspective, this process always yields a negative net benefit for the parameter values used in this simulation. MDEA suffers significantly from its extremely low relative absorption efficiency and high price, which outweigh its unique and potentially cost-reducing chemical properties: relatively low contamination susceptibility and regeneration energy requirement. The low relative absorption efficiency necessitates a monstrously high solvent circulation rate, resulting in equally elevated coal consumption costs. It can be argued that this capture process is poorly optimized for MDEA. A process which manages to capture the same quantity of carbon dioxide at a lower circulation rate will almost certainly yield better results, as the reboilers would have a lower individual capacity requirement. Literature has also shown that blended solvents incorporating MDEA tend to capture carbon more efficiently (in terms of energy efficiency) than what these results indicate (Chang and Shih, 2007).

Figure 5.4 illustrates that, with the resale of the captured carbon dioxide, a positive net social benefit can be achieved above a price of 70.64 USD / tonne. A positive net internal benefit can be achieved at a resale price above 116.16 USD / tonne, and a positive net external benefit can be achieved above a price of 158.02 USD / tonne. That being said, without market data for the bulk sale of carbon dioxide, it is difficult to assess if demand exists at these prices.

Figure 5.4.1 demonstrates perhaps the most feasible method of achieving a positive net benefit for the process involving MDEA. As depicted, a price of coal below 59.24 USD / tonne will yield a positive net social benefit from the process, while a price below 36.36 USD / tonne or 15.33 USD / tonne will yield a positive net benefit from the internal or external standpoints respectively.

Within the range of values proposed by Nordhaus for the social cost of carbon, a positive net benefit is achievable only from the social standpoint for this process at a social cost of carbon above 116.16 USD / tonne. The net external and social benefits are shown in Figure 5.4.2.

Figure 5.4: Net Daily Internal, External, and Social Benefits for the MDEA Process Incorporating Carbon Dioxide Resale Revenue into the Determination

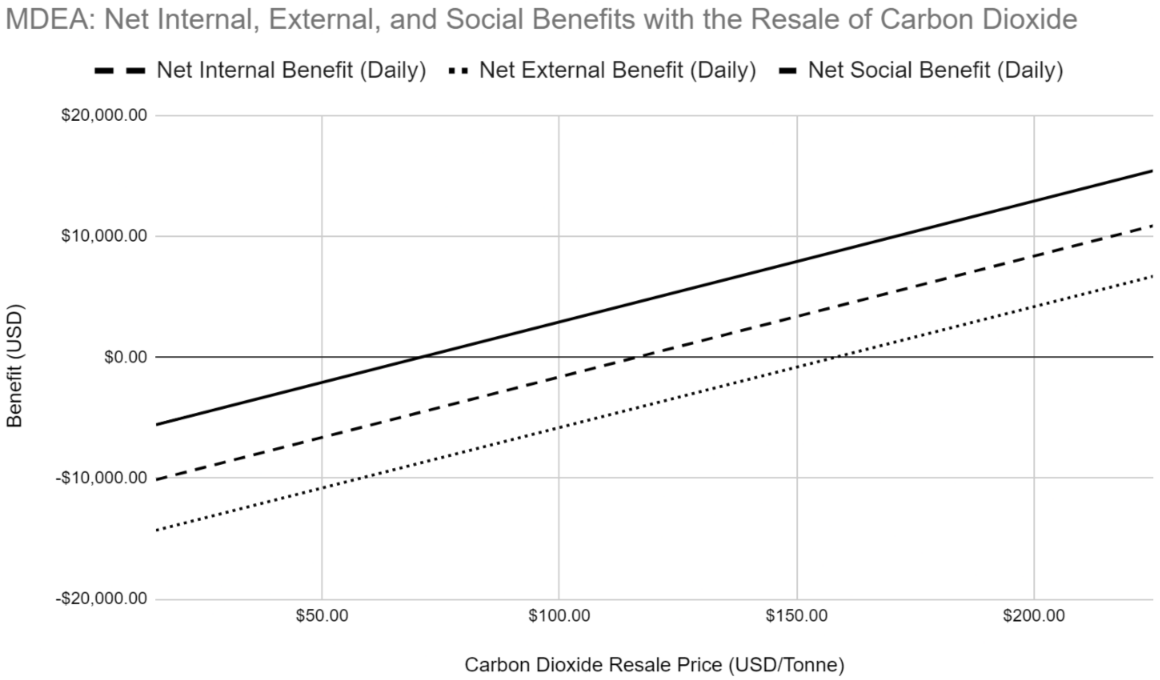

Figure 5.4: This figure incorporates the revenue generated from the resale of captured carbon dioxide over a range of potential sale prices into the net daily internal, external, or social benefit quantification for the MDEA process. It also depicts at which price a positive net benefit could be yielded from any standpoint.

Figure 5.4.1: Net Daily Internal, External, and Social Benefits for the MDEA Process over a Range of Coal Prices

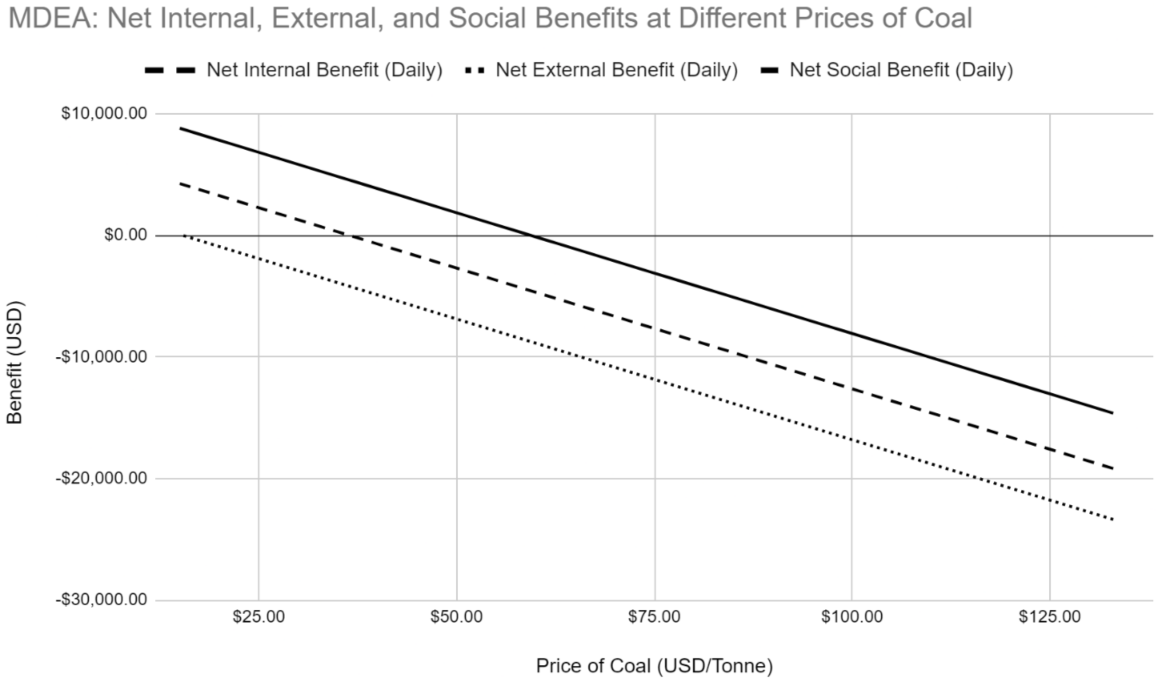

Figure 5.4.1: This figure depicts the net internal, external, and social benefits over a range of coal prices for the MDEA process, and illustrates below which price the process can yield a positive net benefit from a given standpoint.

Figure 5.4.2: Net Daily External and Net Social Benefits for the MDEA Process over the Range of Social Cost of Carbon Values Proposed by Nordhaus

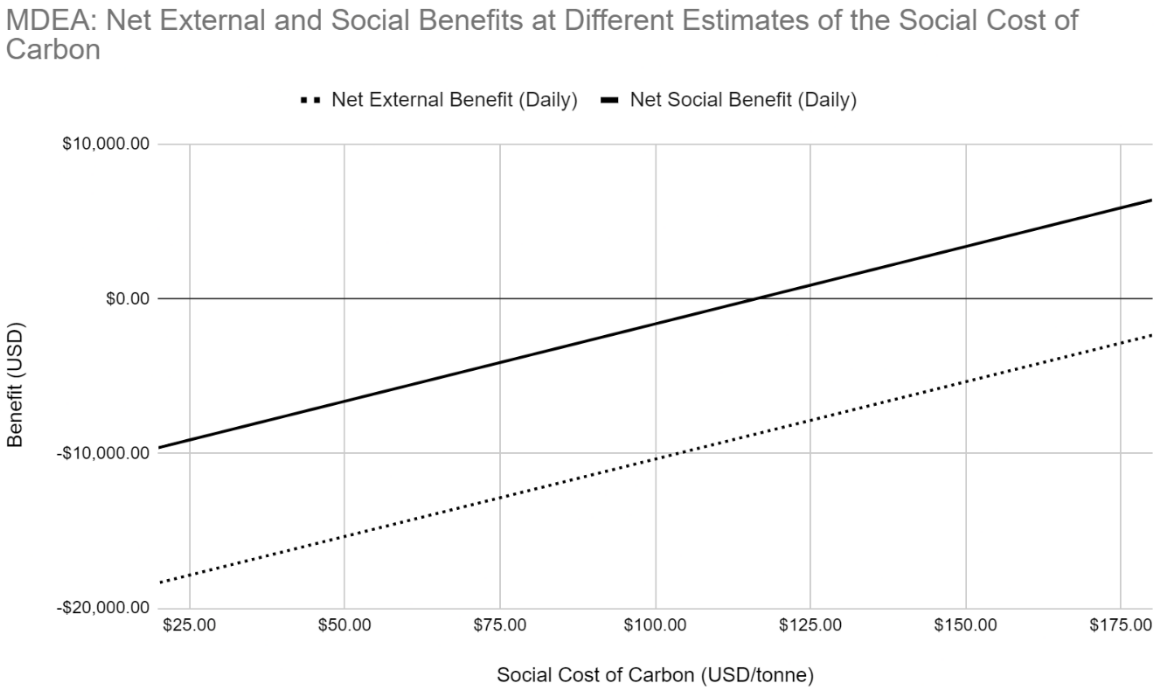

Figure 5.4.2: This figure depicts the daily net external and net social benefits for the MDEA process over the range of social cost of carbon estimates according to Nordhaus, and illustrates at which price of the estimate the process can yield a positive net social benefit.

5.5 AMP Results and Incentive Analysis

The simulation results of this capture process using AMP proved particularly interesting. While its relative contamination susceptibility and capture efficiency are both comparable to DEA, it benefits from a significantly lower molar mass relative to the other alkanolamines in this study. This results in the second highest alkanolamine solvent concentration (3.366 mol / L) of the four being studied here. The literature sources used to define the solvent composition describe the alkanolamine concentration in units of weight percent, not molar concentration (Mariz, Chapel, Ernest, 1999). Thus, subject to a solvent's density, the alkanolamines with lower molar masses, generally speaking, yield solvents in which a higher quantity of alkanolamine molecules are present in a given volume, thus necessitating lower solvent circulation rates. The lower circulation rate, as stated previously, lowers the coal consumption of the reboilers, and processing capacity requirements of several components. In addition, its extremely low thermal degradation rate serves to reduce the daily alkanolamine loss, which is of particular benefit for AMP as it is the second most expensive alkanolamine presented in this study.

AMP is the only other solvent in which capital costs are eventually outweighed by total accrued net benefits from all standpoints, though, it will take nearly ten months of operation from the net external benefit perspective to achieve this. The implication of this being that all net benefit perspectives yield a positive net benefit, thus in Figure 5.5

where the carbon dioxide is resold, the revenue is an added bonus from any benefit point of view.

Figure 5.5.1 shows that the AMP process yields a positive net social benefit up to a coal price of 390.69 USD / tonne, a positive net internal benefit up to 241.44 USD / tonne, and a positive net external benefit up to 104.20 USD / tonne.

Figure 5.5.2 indicates a minimum social cost of carbon of 39.69 USD / tonne is required to yield a positive net external benefit, whereas a positive net social benefit is always incurred regardless of the social costs of carbon.

Figure 5.5: Net Daily Internal, External, and Social Benefits for the AMP Process Incorporating Carbon Dioxide Resale Revenue into the Determination

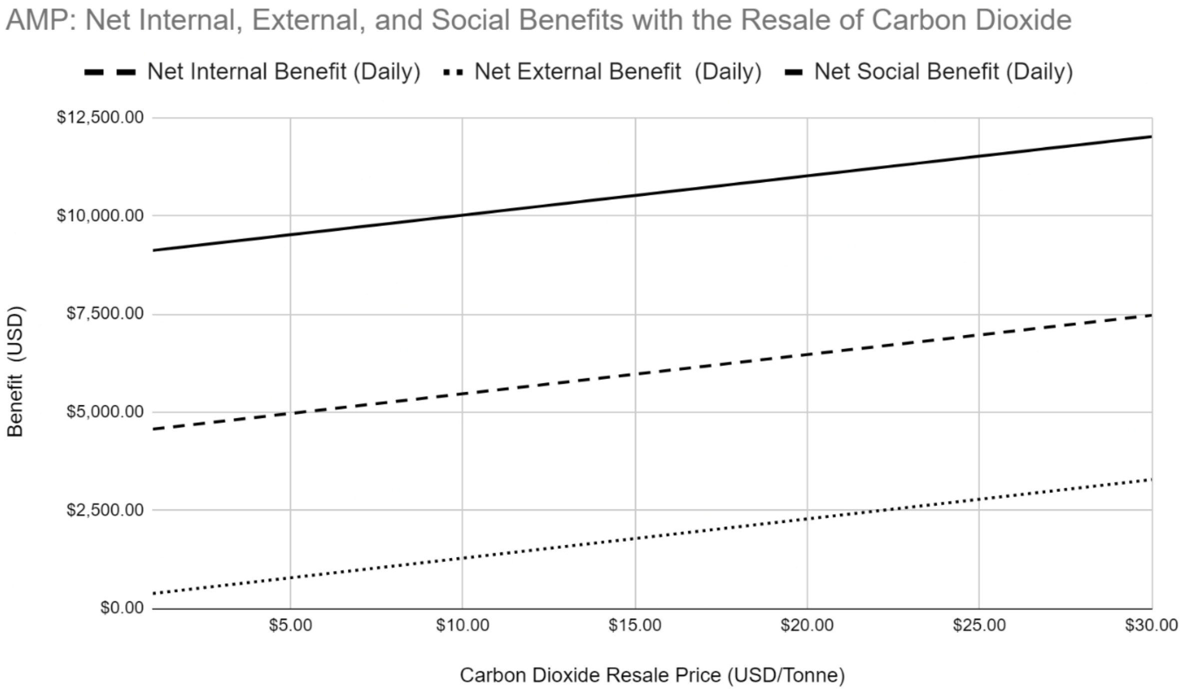

Figure 5.5: This figure incorporates the revenue generated from the resale of captured carbon dioxide over a range of potential sale prices into the net daily internal, external, or social benefit quantification for the AMP process.

Figure 5.5.1: Net Daily Internal, External, and Social Benefit for the AMP Process over a Range of Coal Prices

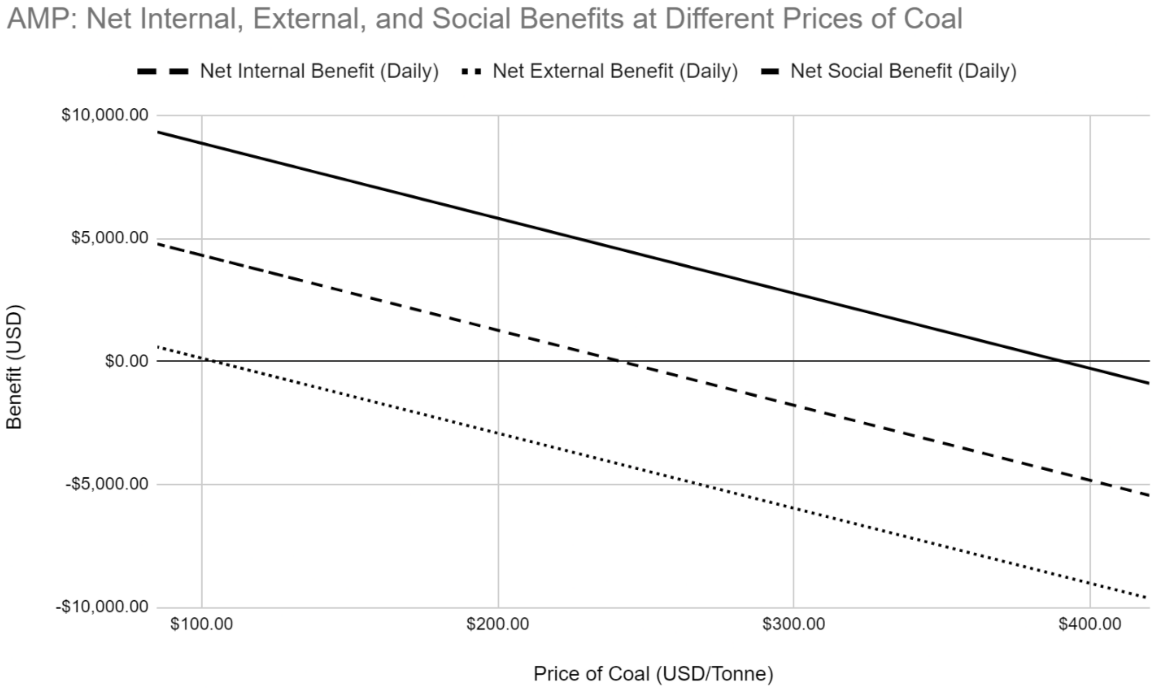

Figure 5.5.1: This figure depicts the net internal, external, and social benefits over a range of coal prices for the AMP process, and illustrates up to which price the process can maintain a positive net benefit from a given standpoint.

Figure 5.5.2: Net Daily External and Net Social Benefits for the AMP Process over the Range of Social Cost of Carbon Values Proposed by Nordhaus

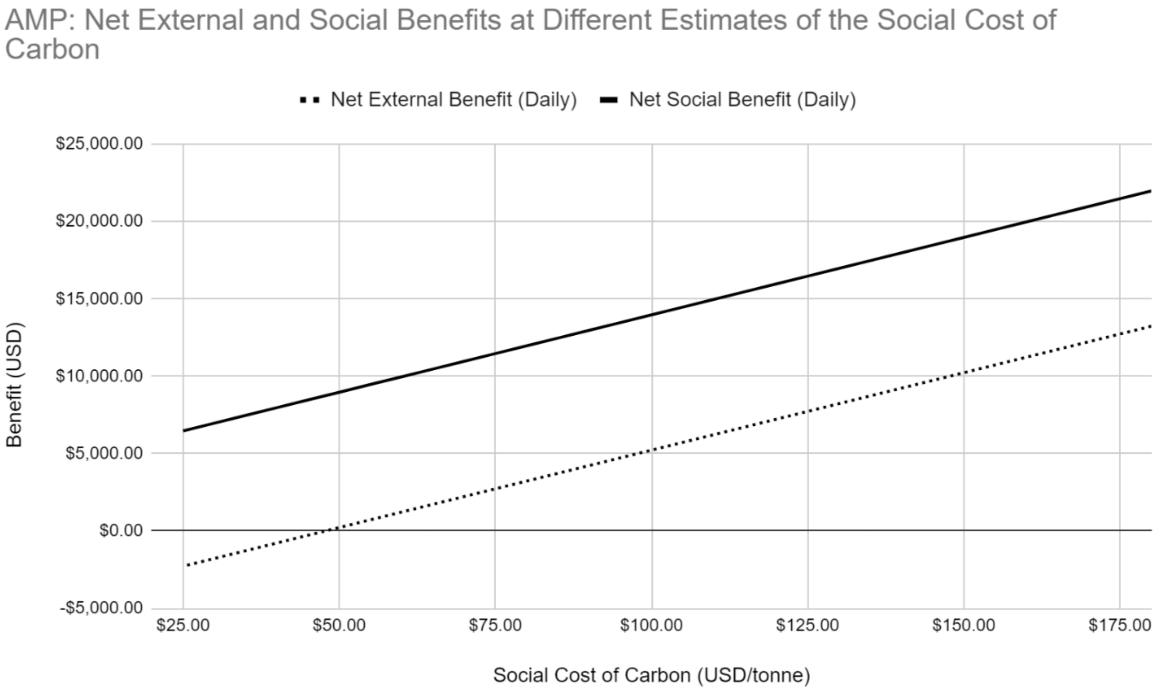

Figure 5.5.2: This figure depicts the daily net external, and net social benefits for the AMP process over the range of social cost of carbon estimates according to Nordhaus, and illustrates up to which price of the estimate the process can maintain a positive net benefit from either standpoint.

6. Conclusion

6.1 Conclusive Overview

This thesis presents four simulations of the capital and operating costs of a 100 tonne per day flue gas carbon capture plant employing four different alkanolamines in the same conceptual carbon capture process. The principal focus was to give careful consideration to the cost impact of the varying chemical properties between the alkanolamines. Results presented in terms of net capital costs indicate the MEA capture process is the least expensive to construct as a result of the alkanolamine's low price and low necessary circulation rate. DEA and AMP were somewhat similar in terms of capture process construction costs, with DEA being slightly less expensive overall. The primary differences between the two were the reboiler cost and the price of the alkanolamine itself. A theoretical capture process different from the one presented here should take into account the specific solvent volume requirement, and reboiler capacity to determine which alkanolamine between DEA and AMP would be more advantageous. The most expensive capture process was that of MDEA, which suffered heavily from its high solvent circulation rate requirement, and high price of alkanolamine. In terms of upkeep costs MEA was again the least expensive for the same reasons as the capital costs. AMP was the second least expensive, beating DEA by a slim margin as a result of its lower overall solvent losses and reboiler fuel requirements. MDEA was the most expensive from an operating cost standpoint, resulting again from its high solvent circulation rate requirement.

Making a comparison between these results and those of the literature is difficult. For one, the process described in these simulations is on a much smaller scale than those found in the literature. Additionally, some costs included in literature models such as utilities, labour, maintenance, or property were omitted in these models, and also suffer from the scaling issue. Furthermore, data is severely lacking for models that incorporate DEA, MDEA, and AMP for capital or operations cost analyses. Therefore, it cannot be asserted with any degree of certainty whether these results are consistent with those of the literature or not. Additionally, cost data pertaining to capture plants in operation is restricted by corporate confidentiality constraints, which makes it difficult to compare between these simulations and this variety of data. Even if this data was available, the conceptual assumptions/omissions of these simulations make such a comparison unreasonable, given the impacts they may have on the results.

The most impactful limitation of these simulations was the method, or methods, of component cost determination. While the semi-empirical method used to determine the price of the absorber and stripper could be considered the most exhaustive, it was impossible to employ this method for every component either due to a lack of online listings altogether, or a lack of listings for a capacity/scale that was reasonably similar. Component cost determinations would benefit greatly from a more extensive body of price data. Another factor that is likely to create a disparity between these theoretical results and those that would be observed in practice is the numerous assumptions of consistent or ideal chemical behaviour. As described in Section 4.0, these assumptions holding true in practice would be a rare occurrence. There is likely to be variation in practical results that stem from this factor.

This thesis does highlight several areas for improvement, subsequent simulation development, and further research. Firstly, a more grounded cost determination method for all components would be useful in creating consistency, and allow for a robust sensitivity analysis on capital costs. Secondly, it may be worthwhile to conduct experiments to determine the rate constants of a given set of alkanolamines' reactions with sulfur oxides. This would allow for a more accurate determination of alkanolamine loss to sulfur oxide contamination, and thus a more accurate cost impact. It would also give merit to the introduction of a somewhat variable flue gas sulfur oxide concentration in the simulations, creating a more representative alkanolamine loss cost assessment of what would be seen in practice. Thirdly, conducting experiments or empirical analysis to enable the incorporation of the omitted components/costs described in Section 3.3 with a reasonable degree of accuracy would be immensely constructive. This would allow for a comparison to empirical data from capture plants in operation that approximate the same conditions of these simulations, that is, assuming this data would be publicly accessible.

6.2 Capture Process and Policy Implications

Coal consumption by the reboilers proved to be the most expensive component of operational costs in each simulation, primarily as a result of the conceptual assumptions, which omit several other potential operating costs. There are numerous ways this cost could theoretically be reduced. In the case of MDEA, finding an alternative carbon capture process that is capable of capturing the same amount of carbon dioxide at a significantly lowered solvent circulation rate would be an approach worth investigating from an engineering perspective.

Ironically, another approach to cost reduction, from a policy perspective, would be to provide a coal subsidy for firms operating carbon capture plants, perhaps stipulating that all carbon dioxide from the subsidized coal must also be captured. In a different scenario where the conceptual assumptions do not restrict the diversity of upkeep costs, other subsidies may prove more effective. However, as shown here, a coal subsidy would increase the incentive to engage in carbon capture operations, as the results of Section 5 show the possibility for a net benefit to the firm in all simulations where the price of coal is lower. This approach may be favourable as it not only creates incentives for fossil fuel power generation firms, but it can also impact the incentives of other sectors responsible for a sizable share of global carbon dioxide emissions. At the very least, it incentivizes a more efficient means of carbon dioxide mitigation than would otherwise be seen by subsidizing direct capture from the atmosphere.

Finally, a different avenue for positive incentivization by means of policy would be that of an equipment subsidy. Targeted equipment subsidies would lower the barriers to entry for smaller firms from a capital cost standpoint and enable engagement from CO_2 emitters who would otherwise not be able to afford the implementation of alkanolamine carbon capture technology. Figure 5.1 shows that the reboilers and the startup alkanolamine components incur the largest combined share of capital costs, thus subsidizing these components specifically would be the most effective method of lowering the barriers to entry. Furthermore, subsidizing the alkanolamine would also contribute to reduced operational costs, but this would not be as effective as a coal subsidy based on the results of these simulations.

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Appendix A

Links to Listings Used in Price Determination

Highlighted links indicate the listing has changed or no longer exists as of April 23, 2023.

Type	Name	Link
Alkanolamine		
	MEA	
		https://businessanalytiq.com/procurementanalytics/index/monoethanolamine-price-index/
		https://www.alibaba.com/product-detail/Factory-Supply-Industrial-Grade-99-5_1600729859354.html?spm=a2700.galleryofferlist.0.0.4e037b57lpZmrh
		https://www.alibaba.com/product-detail/High-Quality-MonoethanolAmine-MEA-Mono-Ethanol_1600412322420.html?spm=a2700.galleryofferlist.normal_offer.d_title.4e037b57lpZmrh
		https://www.alibaba.com/product-detail/Hot-sales-Product-Best-Price-99_1600703863778.html?spm=a2700.galleryofferlist.normal_offer.d_title.4e037b57lpZmrh
		https://www.alibaba.com/product-detail/Factory-directly-sell-Monoethanolamine-Ethanolamine-CAS_1600740284993.html?spm=a2700.galleryofferlist.normal_offer.d_title.4e037b57lpZmrh

	https://www.alibaba.com/product-detail/Monoethanolamine-MEA-cas-141-43-5_1182475139.html?spm=a2700.galleryofferlist.normal_offer.d_title.4e037b57lpZmrh
	https://www.alibaba.com/product-detail/JINGBANG-High-Quality-99-Ethanolamine-Monoethanolamine_1600547727006.html?spm=a2700.galleryofferlist.normal_offer.d_title.4e037b57lpZmrh
	https://www.alibaba.com/product-detail/Mono-Ethanol-Amine-99-Cheap-Price_10000010792071.html?spm=a2700.galleryofferlist.normal_offer.d_title.4e037b57lpZmrh
	https://www.alibaba.com/product-detail/Bravo-Top-quality-high-purity-141_1600754281003.html?spm=a2700.galleryofferlist.normal_offer.d_title.4e037b57lpZmrh
	https://www.alibaba.com/product-detail/High-quality-active-agent-diethanolamine-absorbent_1600452699025.html?spm=a2700.galleryofferlist.normal_offer.d_title.6a021af9xvlyyU
DEA	
	https://www.echemi.com/productsInformation/pd20160329201536890-diethanolamine.html
	https://www.chemicalbook.com/ProductDetail_EN_1204618.htm
	https://www.chemicalbook.com/ProductDetail_EN_1417712.htm

	https://www.alibaba.com/product-detail/CAS-111-42-2-Industrial-Grade_1600606502629.html?spm=a2700.galleryofferlist.normal_offer.d_title.6a021af9xvlyyU
	https://www.alibaba.com/product-detail/Diethanolamine-DEA-Cas-No111-42-2_1600296547288.html?spm=a2700.galleryofferlist.normal_offer.d_title.6a021af9xvlyyU
	https://www.alibaba.com/product-detail/Diethanolamine-DEA-Cas-111-42-2_1600599904488.html?spm=a2700.galleryofferlist.normal_offer.d_title.6a021af9xvlyyU
	https://www.alibaba.com/product-detail/Factory-wholesale-CAS-111-42-2_1600342308227.html?spm=a2700.galleryofferlist.normal_offer.d_title.6a021af9xvlyyU
	https://www.alibaba.com/product-detail/Diethanolamine-DEA-CAS-111-42-2_1600743258683.html?spm=a2700.galleryofferlist.normal_offer.d_title.6a021af9xvlyyU
	https://www.alibaba.com/product-detail/Factory-price-Diethanolamine-DEA-99-Cas_62014377603.html?spm=a2700.galleryofferlist.normal_offer.d_title.6a021af9xvlyyU
	https://www.alibaba.com/product-detail/High-quality-active-agent-diethanolamine-absorbent_1600452699025.html?spm=a2700.galleryofferlist.normal_offer.d_title.6a021af9xvlyyU

MDEA	
	https://www.guidechem.com/trade/n-methyldiethanolamine-id3655996.html
	https://www.alibaba.com/product-detail/Manufacturer-cas-105-59-9-N_1600688474937.html?spm=a2700.galleryofferlist.normal_offer.d_title.108c2155mE0TUE
	https://www.alibaba.com/product-detail/Factory-supply-cas-105-59-9_1600674542288.html?spm=a2700.galleryofferlist.normal_offer.d_title.108c2155mE0TUE
	https://cemotech1.en.made-in-china.com/product/bxkUVpATqihW/China-Reliable-Supplier-N-Methyldiethanolamine-CAS-No-105-59-9-with-Wholesale-Price.html
	https://www.chemicalbook.com/ProductDetail_EN_768566.htm
	https://www.chemicalbook.com/ProductDetail_EN_1312738.htm
AMP	
	https://www.indiamart.com/proddetail/2-amino-2-methyl-1-propanol-19415918191.html
	https://xtdktech.en.made-in-china.com/product/sZhaMvSoPepy/China-AMP95-Aminomethyl-Propanol-2-Amino-2-Methyl-1-Propanol-CAS-124-68-5-AMP-Buffer.html

https://guange-chemapi.en.made-in-china.com/product/LOjteHaAYlUP/China-Factory-Supplier-in-Stock-2-Amino-2-Methyl-1-Propanol-CAS-124-68-5-Aminomethyl-Propanol.html
https://hebeiaifosen.en.made-in-china.com/product/hZtaLfvMJzYU/China-Factory-2-Amino-2-Methyl-1-Propanol-CAS-124-68-5.html
https://www.alibaba.com/product-detail/Aminomethyl-Propanol-2-Amino-2-Methyl_1600088385688.html
https://www.alibaba.com/product-detail/95-2-Amino-2-methyl-1_1600432887386.html?spm=a2700.galleryofferlist.normal_offer.d_title.317d52d1ezmvVm
https://www.alibaba.com/product-detail/Aminomethylpropanol-AMP-PH-Regulator-2-amino_1600254573913.html?spm=a2700.galleryofferlist.normal_offer.d_title.317d52d1ezmvVm
https://www.alibaba.com/product-detail/2-Amino-2-Methyl-1-Propanol_10000004418610.html?spm=a2700.galleryofferlist.normal_offer.d_title.317d52d1ezmvVm
https://www.alibaba.com/product-detail/High-quality-2-Amino-2-methyl_1600587445784.html?spm=a2700.galleryofferlist.normal_offer.d_title.317d52d1ezmvVm

		https://www.alibaba.com/product-detail/2-Amino-2-methyl-1-propanol_62452131089.html?spm=a2700.galleryofferlist.normal_offer.d_title.317d52d1ezmvVm
Mechanical Component		
	Absorber/Stripper	
		https://www.alibaba.com/product-detail/Quality-Gas-Biogas-Scrubbers-Wet-Desulphurization_60817222819.html?spm=a2700.galleryofferlist.normal_offer.d_title.65473b3buRGvYP
		https://www.alibaba.com/product-detail/High-Efficiency-Exhaust-Gas-Fertilizer-Industry_1600430880670.html?spm=a2700.galleryofferlist.normal_offer.d_title.4cac4075GcVPyz
		https://www.alibaba.com/product-detail/Fiberglass-Reinforced-Plastics-Packed-Tower-Cyclone_1600293066003.html?spm=a2700.galleryofferlist.normal_offer.d_title.4cac4075GcVPyz
		https://www.alibaba.com/product-detail/Stainless-Steel-Spray-Granulation-Washing-Spray_1600317284082.html?spm=a2700.shop_plgr.41413.115.7af16057nNY4PZ
		https://www.alibaba.com/product-detail/Spray-Tower-for-Waste-Gas-Treatment_1600292542821.html?spm=a2700.details.0.0.35b22ffdaaQJoc

	https://www.alibaba.com/product-detail/Factory-direct-sale-High-efficiency-stainless_1600229153267.html?spm=a2700.galleryofferlist.normal_offer.d_title.4c804bbfFXZKWH
	https://www.alibaba.com/product-detail/Gas-Absorption-Tower-CO2-SO2-exhaust_1600700581963.html?spm=a2700.shop_plgr.41413.11.7af16057nIfsJz
	https://www.alibaba.com/product-detail/10000m3-h-Wet-Scrubber-For-The_1600545996362.html?spm=a2700.shop_plgr.41413.21.7af16057nIfsJz
	https://www.alibaba.com/product-detail/Industrial-absorption-column-absorption-tower-Wet_60819107398.html?spm=a2700.shop_plgr.41413.49.7af16057nIfsJz
	https://www.alibaba.com/product-detail/Industrial-wet-dust-collector-systems-gas_60839774919.html?spm=a2700.shop_plgr.41413.81.7af16057nIfsJz
Condenser	
	https://china-coolingtower.en.made-in-china.com/product/tBpQOKiVbvrY/China-China-Industrial-Nh3-R717-R507-Evaporative-Condenser-Price.html

Blower	https://www.alibaba.com/product-detail/4-72-centrifugal-blower-fan-industrial_60744801193.html?spm=a2700.galleryofferlist.normal_offer.d_title.59e01802oE2krh
Reboiler	https://www.alibaba.com/product-detail/Industry-Exhaust-waste-gas-heat-recovery_62037893078.html?spm=a2700.galleryofferlist.normal_offer.d_title.79b37e44BuD26p
Pump	https://www.alibaba.com/product-detail/Factory-price-liquid-pump-industrial-heavy_1600760469815.html?spm=a2700.galleryofferlist.normal_offer.d_title.6ea0286atplYbS