Activated Carbon-based Carbon Dioxide Adsorption Process

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Abstract
This process uses activated carbon to adsorb 65 tonnes of CO₂ from a coal-fired power plant per day using activated carbon sorbents at 93% purity using a two-stage adsorption process that uses vacuum-swing adsorption. The flue gas first is pressurized and dehydrated using cooling and chilled water. The stream is then sent into a packed activated carbon column at 1.11 bar until CO₂ saturation, upon which the column is depressurized to 0.5 bar and the CO₂ is desorbed. The gas is then sent into a second adsorption stage at 1 bar until CO₂ saturation, and desorbed at 0.52 bar. The resulting CO₂-rich stream is then sold and transported by pipeline for enhanced oil recovery at $20/tonne CO₂. The total cost of the process, per tonne CO₂ captured, is $28.16, beating out previously done economic analyses of activated carbon-based CO₂ capture processes.

Disciplines
Biochemical and Biomolecular Engineering | Chemical Engineering | Engineering
Dear Dr. Vrana, Dr. Seider, Dr. Sinno, and Dr. Targett,

Enclosed is a process designed to fit the specifications of the problem statement presented by Dr. Matthew Targett (LP Amina) in “Sorbent based CO$_2$ Capture Method.” A Vacuum Pressure Swing Adsorption (VPSA) process utilizing two sets of adsorption columns packed with activated carbon adsorbent is able to adsorb 100-ton CO$_2$/day at 65% from the flue gas stream of a coal-fired power plant. The captured CO$_2$ is then sold to an oil company for enhanced oil recovery.

The process was designed according to a model implemented in MATLAB which ran an optimization process using existing isotherm data to find ideal operating conditions. This optimization ran thousands of combinations of input variables in order to find the ones that best met the process goals.

An in-depth economic and profitability analysis was done on the process, giving a net cost per tonne of CO$_2$ captured of $28.16. This is a promising cost, as it is lower than existing figures such as the one given in the problem statement ($37/tonne). We believe activated carbon based CO$_2$ capture is a promising method to reduce CO$_2$ emissions from coal-fired power plants at a relatively low cost.

Sincerely,

___________________________
Eric Chen

___________________________
Katie Rolin

___________________________
Zachary Stillman
April 18, 2017

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Section 1: Introduction

1.1 Project Motivation

Increasing global greenhouse gas emissions strongly correlate with many harmful environmental changes, including ocean acidification and anomalous temperature rises\(^1\). Carbon dioxide makes up the overwhelming majority of greenhouse gas emissions (Figure 1.1), and the amount of carbon dioxide emitted, as well as atmospheric carbon dioxide levels, will continue to rise if rapid changes are not made to emission schedules (Figure 1.2). Approximately 84% of greenhouse gas emissions from all IPCC sectors comes from the production of electricity, most of which comes in the form of carbon dioxide. Consequently, reducing carbon dioxide emissions from energy production has the potential to make palpable changes in global atmospheric carbon dioxide concentrations (Figure 1.3).

![Gross U.S. Greenhouse Gas Emissions by Gas (MMT CO₂ Eq.)](image)

Figure 1.1. Carbon dioxide, methane, nitrous oxide, and various fluorinated gas emissions in the US and US territories from 1990 to 2014.\(^2\)

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\(^1\) Steffen, Will and Grinevald, Jacques, “The Anthropocene: Conceptual and Historical Perspectives,”

A short-term solution to energy production-related carbon dioxide emissions is needed to mitigate the harmful effects of climate change including ocean acidification and rising global temperatures. The stabilization triangle, shown in Figure 5.4 a, depicts the amount of carbon dioxide that must be eliminated to stabilize greenhouse gas emissions at 2004 levels over the course of the next 50 years. This triangle is split into 7 wedges, each representing 1 billion tons of carbon dioxide to be saved from 2004 to 2054 (Figure 5.4 b). One strategy to accomplish a wedge’s carbon dioxide removal goal requires 1 million tons of carbon dioxide to be captured per year, which is equivalent to capturing all of the emitted carbon dioxide from 800 large coal-fire electricity plants. To make this carbon dioxide removal strategy more feasible, it is necessary to implement the most effective and economically viable carbon capture practices for these power plants.

---


Figure 1.3. Sources of carbon dioxide emission equivalents and sinks (negative values) in the US from 1990 to 2014. Data source: U.S. EPA

Figure 1.4 a (left), b (right). To conceptualize carbon capture strategy efficacy, each strategy takes off CO₂ visualized by a wedge. Seven different strategies, each avoiding 1 billion tons of CO₂ by 2054, are required to avoid doubling CO₂ emissions. ⁵

⁵ Carbon Mitigation Initiative, “The Stabilization Triangle: Toackling the Carbon and Climate Problem with Today’s Technologies” (Princeton Environmental Institute, 2005).
### 1.2. Carbon Capture and Storage

In the context of short-term solutions to the ever-increasing concentrations of carbon dioxide worldwide, carbon capture and storage (CCS) is being explored in an attempt to slow the release of carbon dioxide into the atmosphere (for warming) and oceans (for acidification). On a basic level, carbon capture broadly refers to use of technologies to either remove carbon dioxide from the atmosphere directly or during the carbon dioxide generation process, either pre-combustion or post combustion⁶. The storage aspect of CCS typically involves pumping the carbon dioxide underground, either to large depths so that it will liquefy and remain underground or for enhanced oil recovery, in which the carbon dioxide is pumped into the ground to force the oil into production wells⁷.

### 1.3. Project Goals

The problem statement for this project is to use activated carbon sorbent-based carbon dioxide capture with vacuum-swing pressure adsorption (VPSA) to capture 65% of a coal-fired power plant’s carbon dioxide emissions at a purity of 92% or greater, while minimizing the costs of the removal process. The 92% purity requirement is based on the purity expected of carbon dioxide to be used for enhanced oil recovery⁸, which is an option for selling carbon dioxide to improve the economics of the removal process. Furthermore, 65% removal is a requirement.

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⁶ [http://www.ccsassociation.org/what-is-ccs/capture/](http://www.ccsassociation.org/what-is-ccs/capture/)
⁷ [http://www.ccsassociation.org/what-is-ccs/storage/](http://www.ccsassociation.org/what-is-ccs/storage/)
arbitrarily chosen as a benchmark of efficacy of the removal process for activated carbon sorbent-based carbon dioxide capture.
Section 2: Market and Competitive Analysis

2.1. Carbon-Saving Incentives

The current US political climate makes it difficult to predict exactly what kinds of incentives companies will have for reducing their carbon footprint by the time the process will be ready. Therefore, a conservative assumption was made to omit any potential carbon credits or tax benefits, but to assume there would be no income tax as a result of the sale of the captured carbon dioxide.

Figure 2.1. Projected Carbon Dioxide Market 2020-2050 in USD

---

High (square), low (circle), and mid (triangle)-case scenarios are shown in Figure 2.1 and are primarily based upon the future of the political standing of carbon dioxide in US policy. The high cost estimate assumes that strict regulations of the Clean Power Plan are implemented, which may mandate that electricity-sector emissions are reduced to 90% or more (below 2005 levels) by 2050. Accordingly, the high-cost estimate scenario would certainly seek lower-cost emission reduction measures; however, this scenario is extremely unlikely. The low-cost estimate assumes lenient (or nonexistent) carbon dioxide emission regulations. For the sake of costing carbon dioxide sold for enhanced oil recovery, prices were taken from the middle-case scenario, assuming the current market price will remain nearly steady until 2020, yielding a selling price of $20 per ton of carbon dioxide.

2.2. Enhanced Oil Recovery Using Carbon Dioxide

Enhanced oil recovery (EOR), or tertiary oil recovery, is the process of injecting chemicals into otherwise spent oil wells to mix with the oil, recovering approximately 10 to 20% more oil than if only primary and secondary recovery were performed.\textsuperscript{10} Carbon dioxide is often used for this process, as it is relatively inexpensive and readily dissolves oil at high carbon dioxide densities, so the carbon dioxide used for EOR must be above 92% purity.\textsuperscript{11} Many large oil companies use EOR to get the maximum revenue from a single oil well, and as such have constructed an extensive pipe network for supercritical CO\textsubscript{2} transportation (Figure 2.2); plans exist to expand this network by 2040 (Figure 2.3). As noted above, this process design will use a

\textsuperscript{10} Mott Macdonald, “Enhanced Oil Recovery.”
\textsuperscript{11} James P Meyer, “Summary of Carbon Dioxide Enhanced Oil Recovery (CO2EOR) Injection Well Technology.”
cost of $20 per ton of carbon dioxide, as is projected until 2020 and is the price currently used for EOR.  

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12 Radosz et al., “Flue-Gas Carbon Capture on Carbonaceous Sorbents.”
13 National Energy Technology Laboratory, “A Review of the CO2 Pipeline Infrastructure in the U.S.”
Section 3: Customer Requirements

3.1. CO₂ Emission Reduction Incentives

While carbon taxes in the US are not widespread (nine counties in the San Francisco Bay Area tax emissions at 4.4 cents per tonne of carbon dioxide emitted) with many bills for carbon taxes in the works.¹⁴,¹⁵ Furthermore, the Clean Power Plan requires that power plants cut down carbon emissions 32% by 2030.¹⁶ While the future of this plan is uncertain, fossil fuel plants must still comply and seek ways to lower their greenhouse gas emissions.

3.2. Enhanced Oil Recovery Carbon Dioxide

As previously mentioned, oil dissolution for tertiary oil recovery only occurs at high carbon dioxide densities. This is because carbon dioxide can only act as a good solvent for the oil at high densities. Otherwise, light hydrocarbons in the oil will not be able to dissolve in the carbon dioxide. The minimum purity for carbon dioxide that allows the oil to readily dissolve is 92%, so the recovered carbon dioxide from the capture process must meet this requirement.

¹⁴ Kelly Zito, “Air Quality Board to Fine Bay Area Polluters.”
¹⁵ Carbon Tax Center, “Carbon Tax Center: Progress in States.”
¹⁶ EPA, “Components of the Clean Power Plan.”
Section 4: Process Overview

4.1. Vacuum Pressure Swing Adsorption Using Activated Carbon Adsorption Processes

Adsorption is one of the leading methods used for carbon capture because of the technology’s potential to be a low energy, relatively simple, and easily maintained method of carbon dioxide removal. In the context of carbon capture, adsorption involves the contacting of a carbon dioxide-containing phase with a solid adsorbent to which the carbon dioxide (and potentially other components of the gas phase) is adhered, either via chemical adsorption (chemisorption) or physical adsorption (physisorption). Chemisorption involves chemical bond formation between the adsorbate (molecule being adsorbed) and adsorbent (solid to which the molecules adsorb), causing it to be energetically favorable to bond to the surface of the adsorbate. Physisorption, on the other hand, involves sorption via weak molecular interactions, namely van der Waals forces.

Adsorption processes involve the use of “swings,” in which the system cycles between states of high amount adsorbed (adsorption) and low amount adsorbed (desorption) to selectively separate components in a fluid stream (typically gas), where certain components of the stream preferentially adsorb over others. During the adsorption phase, the fluid phase flows over the adsorbent until the solid’s capacity for holding the adsorbate is reached, as determined from a thermodynamic equilibrium at the processing conditions (temperature and pressure). At equilibrium, the rate of adsorption is equal to the rate of desorption, yielding a constant amount of adsorbate loaded per mass of adsorbent. The equilibrium condition is defined by the

---

temperature and adsorbate partial pressure during adsorption, the latter of which can be found using Dalton’s Law of Partial Pressures. Once the equilibrium condition is known, adsorption isotherms are used to determine the loading for the prescribed conditions. Figure 4.1, an example adsorption isotherm, shows the loading (moles of adsorbate adhered per mass of adsorbent) for different temperatures and across a range of partial pressures for carbon dioxide and nitrogen on Acticarb G1200 activated carbon. For example, for a gas stream composed of 20% by mole carbon dioxide and 80% by mole nitrogen at 20 °C, 100 kPa total pressure, Figure 4.1 shows that, at equilibrium, the loading of carbon dioxide is 1.3 moles of carbon dioxide per kg of activated carbon (20 kPa partial pressure) and the loading of nitrogen is 0.25 moles of nitrogen per kg of activated carbon (80 kPa partial pressure).

Figure 4.1 Adsorption isotherms of nitrogen and carbon dioxide on Acticarb G1200 activated carbon. As seen from the data, the loading of adsorbate is dependent on both temperature and the partial pressure of adsorbate.

---


4.2. Vacuum Pressure Swing Adsorption

One category of adsorption technology, which is commonly used for carbon capture because of its shorter cycle times, relatively low power requirements, and smaller adsorption vessels, is pressure swing adsorption (PSA). As its name implies, pressure swing adsorption involves cycling between two pressures, a high pressure at which there are high amounts of adsorbent adhered at equilibrium (adsorption), and a low pressure at which a lower amount is adsorbed (desorption). The difference between the amount adsorbed per mass of adsorbent during adsorption and that during desorption, known as the working capacity \( WC \), is a key factor in determining the effectiveness of a PSA process. The working capacity can be found by subtracting the amount of adsorbate remaining on the adsorbent during the desorption step \( q_{des} \) from the amount adhered during the adsorption step \( q_{ads} \) (per mass of the adsorbent) shown in in Equation (4.1) below.

\[
WC = q_{ads} - q_{des}
\]  

(4.1)

One variation of PSA that involves desorption at sub-atmospheric pressures, referred to as vacuum pressure swing adsorption (VPSA), is often utilized for carbon capture, as the selective removal of carbon dioxide over nitrogen (the other major component in the flue gas stream) improves when desorbing at lower pressures (which increases the working capacity of carbon dioxide relative to that of nitrogen). Moreover, VPSA also reduces the amount of adsorbent required per cycle since the working capacity increases with lower adsorption pressures. However, costs associated with lowering pressure also increase as the desorption pressure is reduced.\(^{22}\)


4.3. Adsorbent: Activated Carbon

One of the key components in the adsorption design process is the selection of a suitable adsorbent for the system being designed. Activated carbon is selected as the adsorbent for this VPSA process because of a few crucial characteristics that it possesses: activated carbon preferentially adsorbs carbon dioxide over nitrogen, is mildly water resistant, and is relatively inexpensive. The combination of these factors make it a prime candidate for removal and purification of carbon dioxide from the flue gas of a coal-fired power plant. Furthermore, activated carbon is a good selection for the adsorbent because, although it preferentially adsorbs water over carbon dioxide, adsorbed water can be removed at moderate vacuum. Zeolites, on the other hand, would not be as effective as the adsorbent since water binds strongly, causing a reduction in the capacity for carbon dioxide adsorption, which will be the case given a typical water content of 8% water by volume in the flue gas stream.

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Section 5: Preliminary Process Synthesis

5.1. Process Concept

As seen in Figure 5.1, the design of the VPSA process for removal of carbon dioxide from flue gas for coal-fired power plants involves a water removal step, an adsorption step, and a desorption step. The inlet flue gas stream enters the process at 55°C and 1 bar with a water content of around 8% by volume. As mentioned in Section 4, although activated carbon is mildly water resistant, it preferentially adsorbs water over carbon dioxide. Accordingly, a water removal step is necessary to maximize the amount of carbon dioxide adsorbed per mass of activated carbon. Following this step is the adsorption step of carbon dioxide on activated carbon at some optimized temperature and pressure to minimize the cost of carbon dioxide removal. Similarly, the desorption step involves determining the temperature and pressure to minimize cost while achieving the desired specification of 92% or greater purity of carbon dioxide. Within this general framework, there are three main process configuration options of primary concern; water removal, number of adsorption columns, and number of adsorption/desorption phases.

Figure 5.1. Block Flow Diagram of General Process Overview.
5.2. Process Configuration Options: Water Removal

The first step of the VPSA process, water removal (dehumidification), can be performed through two main methods; use of a condenser or use of a desiccant. These two methods can also potentially be used in tandem, although the capital costs associated with adding a second method cannot be justified, given that adding additional size/cooling/desiccant to the primary process (to achieve further water removal) would be cheaper than construction and operation of an additional vessel.

The first method of water removal, condensation, typically involves a combination of temperature change and pressure change to a gas stream, although a single state-changing operation can be used as well. These changes cause certain components of the stream to condense as a function of volatility. In the case of the flue gas, water will effectively be the only component to condense during cooling/pressurization since carbon dioxide and nitrogen have very high volatilities (boiling points of -78.5 and -210 °C, respectively, at atmospheric pressure). Thus, they remain in the gas phase even at elevated pressures and depressed temperatures (above 0°C).

To accomplish these changes in temperature, heat exchange with cooling/chilled water is performed, while increases in pressure can be accomplished using a compressor or blower. The primary costs associated with this method of water removal will stem from the capital costs of the heat exchanger and the compressor/blower, as well as from the operating costs stemming from use of cooling water and electricity use accompanying pressure increases.

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26 See Appendix A for ASPEN Stream Results after water removal
The second option for water removal, the use of desiccants, has been explored both commercially and industrially, including for dehumidification of the flue gas stream leaving power plants.\textsuperscript{27} Desiccants range from liquid solutions to solid adsorbents, the latter of which is more commonly used. Typical desiccant operation requires cycling between saturated and non-saturated states, typically using heating (similar to TSA processes), or may require replacement or treatment of the desiccant/solution in some other way to regenerate it for further use.\textsuperscript{28}

While desiccants were considered for water removal, the cost advantages of operating the process at lower temperatures (higher working capacity of carbon dioxide and greater purity) outweigh the cost advantages of using a desiccant at higher temperatures (since cooling would not be necessary). Since purity goes down at higher temperatures, if a desiccant were to be used, not only would more VPSA stages be needed to achieve the 92% purity goal, but more activated carbon, and therefore larger columns, would also be necessary to capture equivalent amounts of carbon dioxide. Both factors greatly increase costs, as more sets of adsorption columns (that are also larger in size), as well as accompanying blowers/compressors/vacuum pumps for the pressure swing increase both capital and operating costs. A quick analysis shows that even if the costs associated with water removal are ignored, the cost per tonne of carbon dioxide removed is greater than the initial estimates found in the literature because of the aforementioned capital and operating costs increases at higher process temperatures.

Furthermore, typical desiccants function more effectively at lower temperatures\textsuperscript{29}, so cooling the gas stream prior to desiccation may be advantageous. However, at these temperatures, water condenses even without the use of a desiccant. Using a desiccant may be

\textsuperscript{29} https://www.sorbentsystems.com/desiccants_charts.html
prudent for zeolite applications; however, since activated carbon is able to remove water during the desorption step, the addition of a desiccant is unnecessary for this process.

5.3. Process Configuration Options: Number of Adsorption Columns

The use of multiple columns in each stage of VPSA increases efficiency through smaller adsorption columns and pressure equalization between columns. This configuration has huge advantages over single-column stages, which necessitate cyclic operation of the entire VPSA process to prevent flue gas accumulation (i.e., the gas would have to be added cyclically at much greater molar flow rates). In the single-column configuration, the processing equipment for pressurization and water removal must undergo startup through each (relatively short) VPSA cycle, which greatly reduces process efficiency. In addition, because only one phase of the VPSA cycle (adsorption or desorption) can be performed at a time, the gas volumetric flow rate must be double that used in continuous operation, necessitating larger and more expensive equipment. Although capital costs increase with multiple adsorption columns because of the additional activated carbon and columns, the size of the pressurization units and water removal units decrease and efficiency increases, as these units will have continual operation at lower flow rates.

Furthermore, VPSA’s cyclical nature opens the possibility of introducing a more complex flow cycle configuration known as the Skarstrom cycle. Skarstrom cycles refer to cases in which there is a cyclic shift between different steps in the VPSA cycle for different adsorbers. As shown in the example in Fig. 5.1, as the top adsorber undergoes step 1 (pressurization), the bottom adsorber is undergoes step 6 (depressurization/desorption). The top column enters into

---

stage 2, the feed/adsorption step, while the bottom adsorber undergoes a purge step, using a portion of the product stream (or input stream, in some cases) to aid in the removal of residual gas remaining in the column. Then, adsorption in the top column is completed and pressure equalization begins, in which gas flows between the two columns with no gas leaving either. This step allows for demand reduction on the respective pieces of equipment used to reduce and increase pressure in the column.

Figure 5.2: (a) General representation of the steps of the Skarstrom cycle for a two-column system. Step 1 is pressurization, step 2 is adsorption, step 3 is pressure equalization (high to low), step 4 is depressurization and desorption, step 5 is the purge step, and step 6 is pressure equalization (low to high). (b) General representation of the pressure in both columns during different steps of the Skarstrom cycle.

5.4. Process Configuration Options: Number of Adsorption/Desorption Stages

As mentioned during the discussion of water removal, another variable to consider is the number of VPSA stages for the capture of carbon dioxide. Each stage requires the use of at least two columns for continuous operation, as well as the equipment associated with the pressurization and depressurization of the two columns. Thus, minimizing the number of stages

---

will also theoretically minimize cost. This may not be the case if the cost of compressing the gas and/or reducing pressure with a vacuum pump is greater than that of another stage of adsorption using positive displacement blowers instead\textsuperscript{32}.

Since carbon dioxide can be sold for enhanced oil recovery for around $20 per tonne, the designed adsorption process must hit the goal of 92% (or greater) purity to aid in offsetting the cost of capture. It is theoretically possible that the cost of a second stage of VPSA may be more expensive than the $20 per tonne of carbon dioxide, but, as shown in the economic analysis of our processes,\textsuperscript{33} the second stage of adsorbers is only $6.32, making a second stage of VPSA economically advantageous.\textsuperscript{34}

\textbf{5.5. Economic Analysis for Optimization of Vacuum-Pressure Swing Adsorption Process}

Optimal conditions for the CO\textsubscript{2} capture process were determined by costing the blowers, adsorption columns, and heat exchangers over a range of five variables: process temperatures, adsorption pressures for both the first and second columns, and desorption temperatures for the first and second columns (Table 1). When these five variables are input into the MATLAB code (found in Appendix B), the scripts yield values for volumetric flow rates between unit processes, column sizes, volumes of activated carbon for each column, and required cooling utilities. These 13 process variables were used to cost the equipment using methods from Product and Process Design Principles, 4\textsuperscript{th} Ed. To determine the lowest cost of the process, a VBA script (found in Appendix C) was used in conjunction with the MATLAB sizing functions and costing

spreadsheets across a wide range of input variable combinations (shown in Table 5.1). The conditions that yielded the lowest cost while also meeting purity requirements are shown in Table 5.2, with example optimization curves shown in Figure 5.3 for sweeps across the desorption pressure of column 1.

Table 5.1. Variable Ranges used in Optimization Scan

<table>
<thead>
<tr>
<th>Process Temperature (°C)</th>
<th>Adsorption Pressure of Column 1 (bar)</th>
<th>Desorption Pressure of Column 1 (bar)</th>
<th>Adsorption Pressure of Column 2 (bar)</th>
<th>Desorption Pressure of Column 2 (bar)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15-54.5</td>
<td>1-2</td>
<td>0.5-1</td>
<td>0.9-2</td>
<td>0.5-1</td>
</tr>
</tbody>
</table>

Table 5.2: Optimal Process Conditions

<table>
<thead>
<tr>
<th></th>
<th>Column 1</th>
<th>Column 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adsorption Pressure (bar)</td>
<td>1.11</td>
<td>1.0</td>
</tr>
<tr>
<td>Desorption Pressure (bar)</td>
<td>0.50</td>
<td>0.52</td>
</tr>
<tr>
<td>Inlet Flow Rate (ft³/min)</td>
<td>9080</td>
<td>1818</td>
</tr>
<tr>
<td>Outlet Flow Rate (ft³/min)</td>
<td>1818</td>
<td>1467</td>
</tr>
<tr>
<td>Height (ft)</td>
<td>19.3</td>
<td>5.55</td>
</tr>
<tr>
<td>Diameter (ft)</td>
<td>9.65</td>
<td>2.78</td>
</tr>
<tr>
<td>Volume of Activated Carbon (ft³)</td>
<td>733</td>
<td>23.3</td>
</tr>
<tr>
<td>Process Temperature (°C)</td>
<td>20.0</td>
<td></td>
</tr>
</tbody>
</table>

The process temperature was scanned from 15 °C to 54.5 °C, the temperature of the flue gas stream leaving the desulfurization step. Accordingly, this would be the process temperature should no cooling occur. The scan revealed that at temperatures below 18 °C, though purity increased, the increase in cooling costs and decrease in working capacity caused the cost per tonne of carbon dioxide to increase and thus, operating in that temperature range could not be justified. The adsorption and desorption pressure ranges were selected by investigating the full pressure range within blowers’ 1 bar pressure differential limitation for positive displacement and 0.5 bar pressure differential limitation when reducing pressure.

Fig. 5.3 provides an example of the process of optimization over a small range for two of the input variables. The MATLAB script used, however, swept over a wide range of five input
variables, using a MATLAB script to run sizing scripts in five nested loops (Appendix B). These results were then imported into an Excel sheet for costing with VBA assistance. The results of costing were then imported back to MATLAB for organization. After determining the variable combination that yielded the lowest cost per tonne of carbon dioxide (while still meeting the project goal requirements), the sweep was further focused for future scans until the absolute minimum was found.

The process temperature is the most sensitive variable, as it affects every piece of equipment. As temperature decreases, activated carbon’s working capacity increases, so the column sizes can decrease while still meeting the goal of 100 tonnes of carbon dioxide captured per day. Simultaneously, the heat exchangers must flow more cooling water through to cool the flue gas stream, and the blowers pressurize different volumetric flow rates of gas, increasing the cost of the process. The optimum cost occurs where these competing factors yield a minimum cost per tonne of carbon dioxide captured while also maintaining the purity goal of 92%.

A decrease in adsorption pressure leads to an increase in purity while decreasing working capacity. Decreases in desorption pressure increases purity while also increasing working capacity, but causes an increase in utility costs when stronger vacuum is pulled. It is therefore advantageous for the first column to remove the bulk of nitrogen from the stream at a higher adsorption pressure and lower desorption pressure in a smaller column and allow the second column to, at a lower adsorption pressure, purify the flue gas to meet the project goal requirement.
Section 6: Assembly of Database

Table 6.1 (shown below) displays the relevant thermophysical properties of the components of the system. Properties such as viscosity, heat capacity, and heat of adsorption were determined from several sources\textsuperscript{36,37,38,39,40} with the viscosity of the constituent molecules modeled using the Sutherland approximation with the associated code found in appendix B. Furthermore, the cost of activated carbon was determined from a price quote from the Acticarb company. Since the properties of gases change with temperature and pressure, Table 6.1 includes values tabulated at 20 °C and 1 bar although sources used (NIST, Sutherland formula) allow for determination of new properties with changes in with temperature and pressure.

Table 6.1: Compilation of thermophysical properties of relevant chemical components of the VPSA adsorption system including both the gas phase components and solid sorbent.

<table>
<thead>
<tr>
<th>Chemical Component</th>
<th>Molecular Weight (g/mol)</th>
<th>Viscosity (kg/m*s)</th>
<th>Heat Capacity (kJ/kg*K)</th>
<th>Heat of Adsorption (kJ/mol)</th>
<th>Cost ($/tonne)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>18</td>
<td>0.000010</td>
<td>1.86</td>
<td>43.5</td>
<td>N/A</td>
</tr>
<tr>
<td>Carbon Dioxide</td>
<td>44</td>
<td>0.0000148</td>
<td>0.83</td>
<td>23.17</td>
<td>20</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>28</td>
<td>0.0000175</td>
<td>1.04</td>
<td>18.11</td>
<td>N/A</td>
</tr>
<tr>
<td>Activated Carbon</td>
<td>12</td>
<td>N/A</td>
<td>0.85</td>
<td>N/A</td>
<td>2800</td>
</tr>
</tbody>
</table>

Another key set of data utilized for modelling the adsorption process was the adsorption isotherms for carbon dioxide and nitrogen on activated carbon. As mentioned in Section 5, the

isotherms accompany the type of activated carbon used, which, in this case, is Acticarb GC1200. The isotherms for this activated carbon are showed in Fig. 6.141, as are the extrapolated isotherms in Fig. 6.2 a and 6.2 b. Literature sources only had data for pressures up to 100 kPa and using MATLAB, a fit of the form \( y = ax^{0.5} + bx \) was used to extrapolate the data to slightly higher pressures (200 kPa). The MATLAB code used to fit the carbon dioxide and nitrogen curves can be found in appendix B.

Figure 6.1 Adsorption isotherms for carbon dioxide and nitrogen on Acticarb GC1200 activated carbon over a range of temperatures and pressures.42

Figure 6.2 Extrapolated isotherms based on the data for carbon dioxide (a) and nitrogen (b) shown in Fig. 6.1 using a fit of the form \( ax^{0.5} + bx \).

**Section 7: Adsorption Modeling**

Central to the entire optimization process is adsorption and breakthrough modeling. This aspect of the design is central to sizing the adsorption columns, determining cycle times, purity of the product gas stream, temperature of operation, pressure of adsorption, and pressure of desorption when utilized in conjunction with costing optimization scripts (for both sets of columns).

In the context of this process design, adsorption modeling involves prediction of the loading of carbon dioxide and nitrogen on activated carbon throughout the pressurization, adsorption, depressurization, and desorption steps. The adsorption model uses a mass balance, shown in Equation 2,\(^{43}\) which is a balance on a component, \( i \) (either carbon dioxide or nitrogen), with axially dispersed plug flow. The concentration of the component is given by \( c_i \), the interstitial velocity by \( u \), bed porosity by \( e \), the density of the particle by \( \rho_P \), the axial dispersion

---

coefficient by $D_l$, and the loading per unit mass by $\bar{q}_i$. This mass balance on component $i$ shows that the change in axial dispersion plus changes in convective flow plus accumulation in the fluid with time plus adsorption changes with time equal zero because of conservation of mass.

$$-D_l \frac{\partial^2 c_i}{\partial z^2} + \frac{\partial (uc_i)}{\partial z} + \frac{\partial c_i}{\partial t} + \rho_p \frac{(1-e)}{e} \frac{\partial \bar{q}_i}{\partial t} = 0$$  (2)

While this model is accurate for the system described, solving it is computationally expensive and thus a simpler model was implemented to allow for more rapid calculation to determine the cost minimum as described in Section 5. With that in mind, a few simplifying assumptions are implemented to describe the system in simpler terms. These assumptions include constant interstitial velocity, negligible axial dispersion, and instant equilibrium.

Constant interstitial velocity is a simplifying assumption often implemented in simplified literature models, as it approximates the bed behavior without large amounts of radial dispersion.\textsuperscript{44,45} Negligible axial dispersion is implemented in the context of bulk fluid flow dominating mass transfer in the system, which also is reasonable given the high throughput of gases. The instant equilibrium assumption, while not entirely accurate, gives a reasonable estimation of system behavior since adsorption for carbon dioxide and nitrogen on activated carbon occurs rapidly.\textsuperscript{46} With instant equilibrium, the gas phase above the adsorbent immediately changes its number of moles to reach a state in which the partial pressure of each component of the gas phase matches the corresponding molar adsorption as shown by the adsorption isotherms. This approximation does not hold well under short cycle times since the gas phase over the adsorbent changes rapidly during short times and may not reach a state in


which the gas in the bed is of the same pressure and composition as that entering the bed. However, with longer cycle times, these “short time” effects become less apparent, and the gas phase in the bed approximates that of the incoming stream, increasing the accuracy of the model. However, instant equilibrium implies that there will be a 100% carbon dioxide capture rate since the carbon dioxide in the gas stream will be instantly adsorbed onto the adsorbent, even as the bed approaches saturation.

The bed model is completed utilizing MATLAB by performing a finite element in both time and space dimensions using instant equilibrium to determine loading in space slices of the bed, given the aforementioned assumptions of no axial dispersion and constant interstitial velocity. Even in this case, however, calculation time is high (on the order of one minute) and thus a further simplified version of the model is implemented to determine approximate pressurization times, breakthrough times, and purities. The pressurization time is determined by assuming that during the initial stages of gas admittance, little adsorption occurs and thus the pressure can be determined using the ideal gas law for the free volume of the packed bed since the number of moles is known. Following pressurization, the saturation time is determined by dividing the saturation capacity of the bed at the adsorption partial pressure by the molar flow rate of carbon dioxide into the bed. While these approximations do not reflect the true times for the bed, the total time for adsorption and pressurization is accurate, as is the final state of the bed (amount of carbon dioxide and nitrogen adsorbed). A similar process is also performed for the pressure equalization, depressurization, and desorption steps to determine their times and the associated flow rates. This simplified model is used for the process cost optimization, as the overall behavior is pertinent in the sizing and costing of equipment, and calculation times were on the order of 0.1 seconds.
The MATLAB code utilized for both the finite-element model and the simplified bed model (used in the process optimization) can be found in Appendix A.
Section 8: Process Flow Sheet and Material Balances

Figure 8.1. Flow Diagram for Activated Carbon-Based VPSA carbon dioxide Capture Process
**Initial Water Removal**

<table>
<thead>
<tr>
<th>Stream Number</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5, 6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (°C)</td>
<td>120</td>
<td>35</td>
<td>35</td>
<td>20</td>
<td>20</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1.11</td>
<td>1.11</td>
<td>1.11</td>
</tr>
<tr>
<td>Vapor Fraction</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Mass Flow (kg/hr)</td>
<td>20140</td>
<td>19690</td>
<td>450</td>
<td>19388</td>
<td>302</td>
<td>78</td>
<td>19294</td>
</tr>
<tr>
<td>Molar Flow (kmol/hr)</td>
<td>683.9796</td>
<td>659</td>
<td>25</td>
<td>642</td>
<td>17</td>
<td>4</td>
<td>638</td>
</tr>
</tbody>
</table>

Stream Components (mol fractions)

<table>
<thead>
<tr>
<th>Component</th>
<th>Stream 1</th>
<th>Stream 2</th>
<th>Stream 3</th>
<th>Stream 4</th>
<th>Stream 5, 6</th>
<th>Stream 7</th>
<th>Stream 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂</td>
<td>0.138</td>
<td>0.144</td>
<td>0.000</td>
<td>0.147</td>
<td>0.000</td>
<td>0.000</td>
<td>0.148</td>
</tr>
<tr>
<td>N₂</td>
<td>0.785</td>
<td>0.814</td>
<td>0.000</td>
<td>0.836</td>
<td>0.000</td>
<td>0.000</td>
<td>0.839</td>
</tr>
<tr>
<td>H₂O</td>
<td>0.077</td>
<td>0.042</td>
<td>1.000</td>
<td>0.017</td>
<td>1.000</td>
<td>1.000</td>
<td>0.013</td>
</tr>
</tbody>
</table>
Section 8: Process Flow Sheet and Material Balances

Figure 8.1. Flow Diagram for Activated Carbon-Based VPSA carbon dioxide Capture Process

CO₂-Lean Stream to Atmosphere

CO₂-Rich Stream to PIPELINE
The process from here on out is considered isothermal (20 °C) and always in the gas phase.

### Material Balances for Column Set 1, Phase 1

<table>
<thead>
<tr>
<th>Stream Number</th>
<th>A-1</th>
<th>A-2</th>
<th>8</th>
<th>9-11</th>
<th>12, 14</th>
<th>15, 19</th>
<th>16</th>
<th>17</th>
<th>20, 21, 22</th>
<th>23</th>
<th>24</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure (bar)</td>
<td>1.11</td>
<td>0.5</td>
<td>1.11</td>
<td>1.11</td>
<td>1.11</td>
<td>0.5</td>
<td>1</td>
<td>1.00</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mass Flow (kg/hr)</td>
<td>-</td>
<td>19294</td>
<td>19294</td>
<td>13935</td>
<td>5358</td>
<td>109</td>
<td>5243</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Molar Flow (kmol/hr)</td>
<td>638</td>
<td>638</td>
<td>498</td>
<td>140</td>
<td>16.016</td>
<td>134.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Stream Components (mol fractions)</td>
<td>CO2</td>
<td>0.148</td>
<td>0.148</td>
<td>0</td>
<td>0.675</td>
<td>0</td>
<td>0.706</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>N2</td>
<td>0.839</td>
<td>0.839</td>
<td>1</td>
<td>0.265</td>
<td>0.000</td>
<td>0.277</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>H2O</td>
<td>0.013</td>
<td>0.013</td>
<td>0</td>
<td>0.059</td>
<td>1.000</td>
<td>0.017</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Section 8: Process Flow Sheet and Material Balances

Figure 8.1 Flow Diagram for Activated Carbon-Based VPSA carbon dioxide Capture Process
### Material Balances for Column Set 1, Phase 2

<table>
<thead>
<tr>
<th>Stream Number</th>
<th>A-1</th>
<th>A-2</th>
<th>8</th>
<th>9-11, 13</th>
<th>12, 14</th>
<th>15</th>
<th>16, 21, 22</th>
<th>17-19</th>
<th>20</th>
<th>23</th>
<th>24</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure (bar)</td>
<td>0.50</td>
<td>1.11</td>
<td>1.11</td>
<td>1.11</td>
<td>0.5</td>
<td>1.11</td>
<td>1</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mass Flow (kg/hr)</td>
<td>-</td>
<td>19294</td>
<td>19294</td>
<td>5358</td>
<td>13935</td>
<td>109</td>
<td>5243</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Molar Flow (kmol/hr)</td>
<td>-</td>
<td>638</td>
<td>638</td>
<td>140</td>
<td>498</td>
<td>16.016</td>
<td>134.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Stream Components (mol fractions)

- CO2: 0.14845, 0.14845, 0.675, 0, 0, 0.706
- N2: 0.83855, 0.83855, 0.265, 1, 0.000, 0.277
- H2O: 0.013, 0.013, 0.059, 1.000, 0.017

### Material Balances for Column Set 2, Phase 1

<table>
<thead>
<tr>
<th>Stream Number</th>
<th>A-3</th>
<th>A-4</th>
<th>24</th>
<th>25, 27, 30</th>
<th>26, 28, 29</th>
<th>31</th>
<th>32, 35</th>
<th>33, 36</th>
<th>35, 36</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure (bar)</td>
<td>1.00</td>
<td>1.00</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1</td>
<td>0.52</td>
<td></td>
</tr>
<tr>
<td>Mass Flow (kg/hr)</td>
<td>5423</td>
<td>5423</td>
<td></td>
<td>1074</td>
<td>4348</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Molar Flow (kmol/hr)</td>
<td>140.2</td>
<td>140.2</td>
<td></td>
<td>38.2</td>
<td>102.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Stream Components (mol fractions)

- CO2: 0.706, 0.706, 0, 0.929
- N2: 0.277, 0.277, 1, 0.049
- H2O: 0.017, 0.017, 0, 0.022
Section 8: Process Flow Sheet and Material Balances

Figure 8.1. Flow Diagram for Activated Carbon-Based VPSA carbon dioxide Capture Process
<table>
<thead>
<tr>
<th>Stream Number</th>
<th>Pressure (bar)</th>
<th>Mass Flow (kg/hr)</th>
<th>Molar Flow (kmol/hr)</th>
<th>CO2</th>
<th>N2</th>
<th>H2O</th>
</tr>
</thead>
<tbody>
<tr>
<td>42</td>
<td>1.00</td>
<td>5423</td>
<td>140</td>
<td>0.706</td>
<td>0.277</td>
<td>0.017</td>
</tr>
<tr>
<td>44</td>
<td>1.00</td>
<td>5423</td>
<td>140</td>
<td>0.929</td>
<td>0.049</td>
<td>0.022</td>
</tr>
<tr>
<td>43, 36</td>
<td>0.52</td>
<td>4348</td>
<td>102.0</td>
<td>0.706</td>
<td>0.277</td>
<td>0.017</td>
</tr>
<tr>
<td>34, 35</td>
<td>CLOSED</td>
<td>38.21952</td>
<td></td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>31, 36</td>
<td>CLOSED</td>
<td>1074</td>
<td></td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>
Section 9: Process Description

9.1. Flue Gas Dehydration

The flue gas enters the system from the desulfurization process of the power plant at 54.5 °C and atmospheric pressure with 7.7% water content by volume. Since the adsorption process requires cooler and more pressurized flue stream with negligible water content, the flue gas goes through two heat exchangers, one using cooling water and the second using chilled water and a positive-displacement blower. The first heat exchanger drops the flue gas stream to 35 °C and 4.2% H₂O by volume. The second heat exchanger drops the flue gas stream to 20 °C and 1.7% H₂O by volume. Finally, the blower pressurizes the stream to 1.11 bar, dropping the flue gas water content to 1.3% H₂O by volume. The rest of the flue gas content is 14.8% carbon dioxide and 84% N₂.

9.2. Adsorption/Desorption Process

After the flue gas stream is pressurized to 1.11 bar, it enters one of the two adsorption columns, which will be determined from the timed valve configuration. The column to be used will be whichever column has been evacuated and is ready for pressurization and adsorption. During the pressurization stage, no gas will leave this column; however, after pressurization is complete, a carbon dioxide-lean stream will exit the adsorber column and be vented into the atmosphere.

After the adsorption step of the Skarstrom cycle, pressure equalization will be performed, so that gas will flow from the high-pressure column to the low-pressure column, which will have just finished undergoing the desorption and depressurization steps. During the desorption/depressurization steps, a second blower will be used to generate moderate vacuum
and pull a 140 kmol/hr carbon dioxide rich stream from the column at 0.5 bar and 67.5% carbon dioxide. This stream is then pressurized up to 1 bar by a third blower before entering the second set of columns to allow for enhanced adsorption in the second set of columns. This blower condenses out another 16 kmol/hr of water, bringing the carbon dioxide content up to 70.6%. The second blower could have been replaced by a vacuum pump and the third by a compressor, but, as described previously, the equipment and operating cost of using compressors/vacuum pumps instead of blowers make their use prohibitively expensive.

As with the first set of columns, the flow entering the second set of columns will enter the adsorption column that has completed desorption and needs to be pressurized for adsorption. The remaining steps of gas flows in the second set of adsorbers are qualitatively the same as for the first set of columns, with a carbon dioxide-lean stream leaving during adsorption and a carbon dioxide-rich stream removed by a blower during the depressurization/desorption steps. This fourth and final blower will remove the carbon dioxide at 0.52 bar and will send this final stream, composed of 92.85% carbon dioxide by volume, into a pipeline for use by customers for enhanced oil recovery.
Section 10: Energy Balance

The energy balance for the adsorption and desorption steps can be found in Equation (3) below, where \( \dot{q} \) is the rate of heat release/absorption from adsorption/desorption, \( \dot{m}_i \) is the mass flow rate of component \( i \), which is either carbon dioxide or nitrogen, \( m_{AC} \) is the mass of activated carbon, \( C_{p,i} \) is the heat capacity of component \( i \), and \( \Delta T_i \) is the temperature change of component \( i \).

\[
\dot{q} = \dot{m}_{\text{CO}_2} C_{p,\text{CO}_2} \Delta T_{\text{CO}_2} + \dot{m}_{\text{N}_2} C_{p,\text{N}_2} \Delta T_{\text{N}_2} + m_{\text{AC}} C_{p,\text{AC}} \Delta T_{\text{AC}}
\]  

(3)

The transfer of heat for this process occurs as the adsorption and desorption processes occurs, which greatly complicates the analysis of the system without simplifying assumptions. As has been the case in some processes explored in literature, some adsorption processes are designed under the assumption that the system functions isothermally. To test whether the isothermal assumption may be valid in the case of this process design, a pseudo-steady state calculation was used to determine the temperature increase of the system. For this calculation, the entire system was treated as a large, well-mixed tank containing all of the gas adsorbed over the course of a single adsorption cycle as well as the activated carbon. The model system then absorbs all of the heat released by adsorption of carbon dioxide (21 kJ/mol) and nitrogen (18 kJ/mol) through a single adsorption cycle. Through this calculation, it was determined that the temperature increase of the system would be 7 °C, and, since this calculation is a high-end temperature estimate for the flue gas since the gas would only experience high temperatures over a short timescale, the isothermal assumption was used since temperature increases are minimal.
This approximation is further supported by the transfer of heat to the external (lower temperature) environment, as well as by the longer cycle time (ten minutes), since the temperature front will move through the bed as the adsorption process proceeds, with a large portion of the bed returning to thermal equilibrium with the input gas stream. The longer cycle time also means that the bed will be greater in length, which may increase capital costs, but also means a smaller fraction of the bed will be affected by the temperature front moving through the bed.
Section 11: Equipment List and Unit Descriptions

Adsorption Columns

Adsorption Column 1:
Length: 13.3 ft
Diameter: 6.7 ft
Material: Carbon Steel
Pressure: 10.5 psig
Activated Carbon Volume: 232 ft³

Adsorption Column 2:
Length: 5.5 ft
Diameter: 2.8 ft
Material: Carbon Steel
Pressure: 7 psig
Activated Carbon Volume: 23 ft

The adsorption columns used were designed using heuristics provided by industrial consultant Adam Brostow (Air Products and Chemicals, Inc.) regarding the sizing rules for packed beds/columns used in industry. Mr. Brostow explained that industrially, packed beds typically utilize a two to one height to diameter ratio when sizing columns with a maximum diameter set by transportation ability (smaller than the lane width of roads: approximately 10 feet)⁴⁷. This heuristic allowed for column sizing when used in conjunction with literature studies of VPSA processes, which typically utilize bed porosities of around 0.33, which corresponds to the void fraction of a packed bed of spheres, meaning that the entire column height is utilized to store the spherical activated carbon pellets⁴⁸.

---

To size the adsorption columns, it is necessary to determine the cycle time for the VPSA process, the net amount of carbon dioxide that will be removed per cycle, and the density of the activated carbon being used. The bed porosity, another important factor in column sizing, can be determined based on the density, shape, and pore structure of the activated carbon in the bed. In practice, the minimum value of the porosity can be determined by packing the bed with a known mass of activated carbon and dividing this mass by the true density of the activated carbon, which yields the volume taken up by the adsorbent. The remaining volume of the column divided by the total volume yields the bed porosity.

While this lowest bed porosity may minimize the size of the column, if pressure losses from fluid flow in the packed bed are significant (determined by the Ergun equation), it is possible that the minimum cost may lie at a higher bed porosity to reduce the pressure drop. Basic calculations using the Ergun equation and costing methods for packed beds showed that the cost per ton of carbon dioxide was minimized at the lowest bed porosity.49

The cycle times for the adsorption/desorption process are necessary to determine the size of the column since, given a certain flow rate of carbon dioxide, the mass of activated carbon ($M_{AC}$) can be determined by equation 4, which is a function of the activated carbon’s working capacity of carbon dioxide ($WC_{CO_2}$), which is a function of the input temperature, pressure of adsorption and pressure of desorption. The amount of activated carbon also depends on $t_{ads}$, the time of the adsorption step of the cycle, and $n_{CO_2}$, the molar flow rate of carbon dioxide.

$$M_{AC} = \frac{t_{ads}n_{CO_2}}{WC_{CO_2}} \quad \text{Eq. 4}$$

---

49 Using costing optimization described in Section 5 and MATLAB code found in Appendix B
This equation assumes instant equilibrium\textsuperscript{50} and 100\% capture of carbon dioxide as noted in Section 7, model description. In laboratory experiments using vacuum pressure swing adsorption, capture rates (also referred to as recoveries) were typically around 85\%, which was assumed to be the recovery in each of the two stages of adsorption\textsuperscript{51}. This assumption makes requisite flow rates and corresponding sizes of equipment, as well as associated utilities closer to their values under non-idealized conditions, thus improving cost estimates.

After the mass of activated carbon is determined, the volume of the activated carbon can be found by dividing its mass by the true density of the activated carbon ($\rho_{AC}$) and the volume of the bed is equal to this volume divided by one minus the bed porosity, as shown in equation 5 below.

\begin{equation}
V_{bed} = \frac{MA_C}{\rho_{AC}} \frac{1}{1-\epsilon_{bed}} \tag{Eq. 5}
\end{equation}

Subsequently, the diameter and height of the column can be determined using the 2:1 height to diameter ratio heuristic, combined with the equation for the volume of a cylinder. Accordingly, the inner diameter of the bed is found by equation 6 below, with the height equal to 2*\(d_{bed}\).

\begin{equation}
d_{bed} = \frac{3}{\pi} \sqrt{\frac{2V_{bed}}{\pi}} \tag{Eq. 6}
\end{equation}

Thus, using these sizing equations in tandem with the model described in Section 7, the optimal size and cost of the columns can be determined while also meeting the purity requirements for EOR.

\textsuperscript{50} Described in Section 7, Model Description
**Heat Exchanger 1**

Unit ID: HX-1

Type: Shell-In-Tube Fixed Head Heat Exchanger

Material: Carbon steel, carbon steel

Size: 20 feet long, 400 ft$^2$ surface area

Cold Stream: Cooling water (25 °C)         Hot Stream: Flue gas (54.5 °C)
Entering Mass Flow Rate: 10,999 kg/hr     Entering Mass Flow Rate: 20,140 kg/hr
Final Temperature: 35 °C ($\Delta T = 10$ °C) Final Temperature: 35 °C ($\Delta T = 19.5$ °C)

Gas Stream Mass Flow Rate: 19,690 kg/hr

Water Stream Mass Flow Rate: 450 kg/hr

Total Heat Exchanged: 460,191 kJ/hr

This heat exchanger uses cooling water to condense water out of the entering flue gas stream and prepare the flue gas for adsorption. The heat exchanger lowers the water content in the flue gas stream from 7.7% to 4.2% H$_2$O by volume.
Heat Exchanger 2

Unit ID: HX-1
Type: Shell-In-Tube Fixed Head Heat Exchanger
Material: Carbon steel, carbon steel
Size: 20 feet long, 15 ft\(^2\) surface area

Cold Stream: Chilled water (4 °C)  
Entering Mass Flow Rate: 8,946 kg/hr  
Final Temperature: 14 °C (\(\Delta T = 10 °C\))

Hot Stream: Flue gas (35 °C)  
Entering Mass Flow Rate: 19,690 kg/hr  
Final Temperature: 20 °C (\(\Delta T = 15 °C\))

Gas Stream Mass Flow Rate: 19,388 kg/hr  
Water Stream Mass Flow Rate: 302 kg/hr

Total Heat Exchanged: 354,780 btu/hr

The second heat exchanger in the cooling process uses chilled water to both prepare the flue gas for adsorption and to further dehydrate the flue gas stream. The heat exchanger lowers the water content in the flue gas stream from 4.2% to 1.7% H\(_2\)O by volume.
Pressurizing Blower 1

Unit ID: B-1
Type: Positive Displacement Blower
Material: Cast iron

Motor Efficiency: 0.9
Blower Efficiency: 0.7
Power Usage: 70 kW
Volumetric Flow: 9050 ft³/min
Pressure in: 1 bar
Pressure out: 1.11 bar

The first blower pressurizes the flue gas to prepare for adsorption and do a final dehydration on the flue gas stream. The flue gas dehydrates from 1.7% to 1.1% H₂O by volume. The pressurization to 1.11 bar, was chosen as an economic optimum between purity and capture of carbon dioxide and cost of scaling. Higher pressures would result in a larger capture rate, smaller amount of activated carbon, and smaller adsorption column, but at the cost of carbon dioxide purity.
Vacuum Blower 1

Unit ID: B-1
Type: Positive Displacement Blower
Material: Cast iron

Motor Efficiency: 0.9
Blower Efficiency: 0.7
Power Usage: 101.3 kW
Volumetric Flow: 1811 ft³/min
Pressure in: 1 bar
Pressure out: 0.5 bar

This blower lowers the pressure inside the packed column in order to desorb the captured carbon dioxide and N₂. On the advice of Dr. Targett, the vacuum blower was modelled a normal blower with twice the pressure differential. In this case, the blower was modelled as a pressure swing from 1 bar to 2 bar. The lower the desorption pressure, the more carbon dioxide and N₂ is desorbed, and at a greater purity. However, the equipment and operating costs increase in order to decrease the pressure. The economic optimization process suggests a more powerful blower that could give a lower desorption pressure would have better economic returns, but blowers typically do not give pressure differentials more than 1 bar when pressurizing and 0.5 bar when depressurizing.
Pressurizing Blower 2

Unit ID: B-1
Type: Positive Displacement Blower
Material: Cast iron

Motor Efficiency: 0.9
Blower Efficiency: 0.7
Power Usage: 50.7 kW
Volumetric Flow: 1811 ft³/min
Pressure in: 0.5 bar
Pressure out: 1 bar

This second pressurization blower increases the pressure to significantly less than that of the first pressurizing blower. This is likely because the second blower seems to be geared toward raising the purity through a regime that is harder to purify. Because the isotherm follows a half-order fit, the adsorption pressure must be lower in order to desorb a greater purity carbon dioxide stream.
Vacuum Blower 2

Unit ID: B-1

Type: Positive Displacement Blower

Material: Cast iron

Motor Efficiency: 0.9
Blower Efficiency: 0.7
Power Usage: 78.5 kW
Volumetric Flow: 1461 ft³/min
Pressure in: 1 bar
Pressure out: 0.52 bar

This second vacuum blower is modelled the same way as the first: a pressurizing blower with double the pressure differential: from 1 bar to 1.96 bar.
### Section 12: Specification Sheets

#### Table 12.1: Blower B-1 Specifications and Costing

<table>
<thead>
<tr>
<th>Equipment Label</th>
<th>B-1</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Function</strong></td>
<td>To increase the pressure of the water-lean flue gas stream S-6 from the water removal process to yield stream S-8 into the VPSA process, as well as another outlet water stream S-7.</td>
</tr>
<tr>
<td><strong>Design Data</strong></td>
<td></td>
</tr>
<tr>
<td>Type</td>
<td>Rotary Straight-Lobe</td>
</tr>
<tr>
<td>Mechanical Efficiency, $\eta_B$</td>
<td>60%</td>
</tr>
<tr>
<td>Motor Efficiency, $\eta_M$ (Hp)</td>
<td>0.93</td>
</tr>
<tr>
<td>Material</td>
<td>Cast Iron</td>
</tr>
<tr>
<td>Size Factor; Brake Horse Power (Hp)</td>
<td>410</td>
</tr>
<tr>
<td>Power Consumption (Hp)</td>
<td>443</td>
</tr>
<tr>
<td><strong>Stream Data</strong></td>
<td></td>
</tr>
<tr>
<td>Flow Rate ($ft^3/min$)</td>
<td>9050</td>
</tr>
<tr>
<td>Inlet Pressure (lb$_f$/in$^2$)</td>
<td>14.5</td>
</tr>
<tr>
<td>Outlet Pressure (lb$_f$/in$^2$)</td>
<td>21.8</td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>1.3</td>
</tr>
<tr>
<td>Specific Heat Ratio</td>
<td>1.4</td>
</tr>
<tr>
<td><strong>Total Purchase Cost</strong></td>
<td>$185,000</td>
</tr>
<tr>
<td><strong>Total Installed Cost</strong></td>
<td>$398,000</td>
</tr>
</tbody>
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#### Table 12.2: Blower B-2 Specifications and Costing

<table>
<thead>
<tr>
<th>Equipment Label</th>
<th>B-2</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Function</strong></td>
<td>To increase the pressure of streams from the first adsorption process to allow the columns to desorb.</td>
</tr>
<tr>
<td><strong>Design Data</strong></td>
<td></td>
</tr>
<tr>
<td>Type</td>
<td>Rotary Straight-Lobe</td>
</tr>
<tr>
<td>Mechanical Efficiency, $\eta_B$</td>
<td>60%</td>
</tr>
<tr>
<td>Motor Efficiency, $\eta_M$ (Hp)</td>
<td>0.91</td>
</tr>
<tr>
<td>Material</td>
<td>Cast Iron</td>
</tr>
<tr>
<td>Size Factor; Brake Horse Power (Hp)</td>
<td>110</td>
</tr>
<tr>
<td>Power Consumption (Hp)</td>
<td>121</td>
</tr>
<tr>
<td><strong>Stream Data</strong></td>
<td></td>
</tr>
<tr>
<td>Flow Rate ($ft^3/min$)</td>
<td>1370</td>
</tr>
<tr>
<td>Inlet Pressure (lb$_f$/in$^2$)</td>
<td>14.5</td>
</tr>
<tr>
<td>Outlet Pressure (lb$_f$/in$^2$)</td>
<td>29</td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>1.3</td>
</tr>
<tr>
<td>Specific Heat Ratio</td>
<td>1.4</td>
</tr>
<tr>
<td><strong>Total Purchase Cost</strong></td>
<td>$79,500</td>
</tr>
<tr>
<td><strong>Total Installed Cost</strong></td>
<td>$171,000</td>
</tr>
</tbody>
</table>
### Table 12.3: Blower B-3 Specifications and Costing

<table>
<thead>
<tr>
<th>Equipment Label</th>
<th>B-3</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Function</strong></td>
<td>To pressurize stream S-23 for the second VPSA process.</td>
</tr>
<tr>
<td><strong>Design Data</strong></td>
<td></td>
</tr>
<tr>
<td>Type</td>
<td>Rotary Straight-Lobe</td>
</tr>
<tr>
<td>Mechanical Efficiency, $\eta_B$</td>
<td>60%</td>
</tr>
<tr>
<td>Motor Efficiency, $\eta_M$ (Hp)</td>
<td>0.91</td>
</tr>
<tr>
<td>Material</td>
<td>Cast Iron</td>
</tr>
<tr>
<td>Size Factor; Brake Horse Power (Hp)</td>
<td>56</td>
</tr>
<tr>
<td>Power Consumption (Hp)</td>
<td>63</td>
</tr>
<tr>
<td><strong>Stream Data</strong></td>
<td></td>
</tr>
<tr>
<td>Flow Rate (ft³/min)</td>
<td>1370</td>
</tr>
<tr>
<td>Inlet Pressure (lb/in²)</td>
<td>14.5</td>
</tr>
<tr>
<td>Outlet Pressure (lb/in²)</td>
<td>21</td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>1.3</td>
</tr>
<tr>
<td>Specific Heat Ratio</td>
<td>1.4</td>
</tr>
<tr>
<td><strong>Total Purchase Cost</strong></td>
<td>$50,700</td>
</tr>
<tr>
<td><strong>Total Installed Cost</strong></td>
<td>$109,000</td>
</tr>
</tbody>
</table>

### Table 12.4: Blower B-4 Specifications and Costing

<table>
<thead>
<tr>
<th>Equipment Label</th>
<th>B-4</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Function</strong></td>
<td>To increase the pressure of streams from the second adsorption process to allow the columns to desorb.</td>
</tr>
<tr>
<td><strong>Design Data</strong></td>
<td></td>
</tr>
<tr>
<td>Type</td>
<td>Rotary Straight-Lobe</td>
</tr>
<tr>
<td>Mechanical Efficiency, $\eta_B$</td>
<td>60%</td>
</tr>
<tr>
<td>Motor Efficiency, $\eta_M$ (Hp)</td>
<td>0.77</td>
</tr>
<tr>
<td>Material</td>
<td>Cast Iron</td>
</tr>
<tr>
<td>Size Factor; Brake Horse Power (Hp)</td>
<td>113</td>
</tr>
<tr>
<td>Power Consumption (Hp)</td>
<td>124</td>
</tr>
<tr>
<td><strong>Stream Data</strong></td>
<td></td>
</tr>
<tr>
<td>Flow Rate (ft³/min)</td>
<td>1467</td>
</tr>
<tr>
<td>Inlet Pressure (lb/in²)</td>
<td>14.5</td>
</tr>
<tr>
<td>Outlet Pressure (lb/in²)</td>
<td>28</td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>1.3</td>
</tr>
<tr>
<td>Specific Heat Ratio</td>
<td>1.4</td>
</tr>
<tr>
<td><strong>Total Purchase Cost</strong></td>
<td>$81,000</td>
</tr>
<tr>
<td><strong>Total Installed Cost</strong></td>
<td>$174,000</td>
</tr>
</tbody>
</table>
### Table 12.5: Adsorption Column A-1 and A-2 Specifications and Costing

<table>
<thead>
<tr>
<th>Equipment Label</th>
<th>A-1, A-2</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Required</td>
<td>2</td>
</tr>
<tr>
<td>Function</td>
<td>House the AC adsorbent where the first VPSA process occurs. Adsorb CO₂ from inlet stream, desorb CO₂ into CO₂-rich stream, and allow CO₂-lean stream to exit into the environment.</td>
</tr>
<tr>
<td>Design Data</td>
<td></td>
</tr>
<tr>
<td>Type</td>
<td>Packed Column</td>
</tr>
<tr>
<td>Material</td>
<td>Carbon-steel</td>
</tr>
<tr>
<td>Inner Diameter (ft)</td>
<td>5.79</td>
</tr>
<tr>
<td>Height (ft)</td>
<td>11.6</td>
</tr>
<tr>
<td>Wall thickness (ft)</td>
<td>0.00047</td>
</tr>
<tr>
<td>Design Pressure (psig)</td>
<td>10.5</td>
</tr>
<tr>
<td>Weld Efficiency</td>
<td>0.85</td>
</tr>
<tr>
<td>Stress (psi)</td>
<td>13750</td>
</tr>
<tr>
<td>Bulk Volume (ft³)</td>
<td>304</td>
</tr>
<tr>
<td>Adsorbent Data</td>
<td></td>
</tr>
<tr>
<td>Packing Classfication</td>
<td>Structured</td>
</tr>
<tr>
<td>Amount of AC per column (ft³)</td>
<td>150</td>
</tr>
<tr>
<td>Cost of AC per Column</td>
<td>$12,500</td>
</tr>
<tr>
<td>Cost per Empty Column</td>
<td>$92,897</td>
</tr>
<tr>
<td>Total Purchase Cost</td>
<td>$105,400</td>
</tr>
<tr>
<td>Total Installed Cost</td>
<td>$386,400</td>
</tr>
</tbody>
</table>

### Table 12.6: Adsorption Column A-3 and A-4 Specifications and Costing

<table>
<thead>
<tr>
<th>Equipment Label</th>
<th>A-3, A-4</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Required</td>
<td>2</td>
</tr>
<tr>
<td>Function</td>
<td>House the AC adsorbent where the second VPSA process occurs. Adsorb CO₂ from inlet stream, desorb CO₂ into CO₂-rich stream, and allow CO₂-lean stream to exit into the environment.</td>
</tr>
<tr>
<td>Design Data</td>
<td></td>
</tr>
<tr>
<td>Type</td>
<td>Packed Column</td>
</tr>
<tr>
<td>Material</td>
<td>Carbon-steel</td>
</tr>
<tr>
<td>Inner Diameter (ft)</td>
<td>2.79</td>
</tr>
<tr>
<td>Height (ft)</td>
<td>5.57</td>
</tr>
<tr>
<td>Wall thickness (ft)</td>
<td>0.00027</td>
</tr>
<tr>
<td>Design Pressure (psig)</td>
<td>0</td>
</tr>
<tr>
<td>Weld Efficiency</td>
<td>0.85</td>
</tr>
<tr>
<td>Stress (psi)</td>
<td>13750</td>
</tr>
<tr>
<td>Bulk Volume (ft³)</td>
<td>34.0</td>
</tr>
<tr>
<td>Adsorbent Data</td>
<td></td>
</tr>
<tr>
<td>Packing Classfication</td>
<td>Structured</td>
</tr>
<tr>
<td>Amount of AC per column (ft³)</td>
<td>24</td>
</tr>
<tr>
<td>Cost of AC per Column</td>
<td>$1,400</td>
</tr>
<tr>
<td>Cost per Empty Column</td>
<td>$30,600</td>
</tr>
<tr>
<td>Total Purchase Cost</td>
<td>$320,000</td>
</tr>
<tr>
<td>Total Installed Cost</td>
<td>$258,800</td>
</tr>
</tbody>
</table>
Table 12.7: Heat Exchanger HX-1 Specifications and Costing

<table>
<thead>
<tr>
<th>Equipment Label</th>
<th>HX-1</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Required</td>
<td>1</td>
</tr>
<tr>
<td>Function</td>
<td>Cool and condense water from the inlet flue gas stream S-1.</td>
</tr>
<tr>
<td>Operation</td>
<td>Continuous</td>
</tr>
<tr>
<td>Type</td>
<td>Shell and Tube, Floating Head</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stream ID</th>
<th>Tube Side</th>
<th>Shell Side</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet</td>
<td>Cooled Water</td>
<td>S-1</td>
</tr>
<tr>
<td>Outlet</td>
<td>Cooled Water</td>
<td>S-2</td>
</tr>
<tr>
<td>Flow rate (kg/hr)</td>
<td>40600</td>
<td>19,500</td>
</tr>
<tr>
<td>Inlet Temperature (°C)</td>
<td>20</td>
<td>120</td>
</tr>
<tr>
<td>Outlet Temperature (°C)</td>
<td>30</td>
<td>35</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Design Data</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Surface Area (m²)</strong></td>
<td>37</td>
</tr>
<tr>
<td><strong>Length (m)</strong></td>
<td>6.1</td>
</tr>
<tr>
<td><strong>U (W/m²·C)</strong></td>
<td>909</td>
</tr>
<tr>
<td><strong>LMTD (°C)</strong></td>
<td>35</td>
</tr>
<tr>
<td><strong>Fouling Resistance (m²·°C/W)</strong></td>
<td>0</td>
</tr>
<tr>
<td><strong>Construction Materials</strong></td>
<td>Carbon Steel</td>
</tr>
<tr>
<td><strong>Utilities Required/Year (kWh)</strong></td>
<td>700</td>
</tr>
<tr>
<td><strong>Purchase Cost</strong></td>
<td>$11,800</td>
</tr>
<tr>
<td><strong>Bare Module Cost</strong></td>
<td>$37,300</td>
</tr>
</tbody>
</table>
Table 12.8: Heat Exchanger HX-2 Specifications and Costing

<table>
<thead>
<tr>
<th>Equipment Label</th>
<th>HX-2</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Required</td>
<td>1</td>
</tr>
<tr>
<td>Function</td>
<td>Cool and condense the inlet gas stream S-2 from heat exchanger HX-1 to desired operating conditions.</td>
</tr>
<tr>
<td>Operation</td>
<td>Continuous</td>
</tr>
<tr>
<td>Type</td>
<td>Shell and Tube, Floating Head</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Stream ID</th>
<th>Tube Side</th>
<th>Shell Side</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet</td>
<td>Chilled Water</td>
<td>S-2</td>
</tr>
<tr>
<td>Outlet</td>
<td>Chilled Water</td>
<td>S-4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Flow rate (kg/hr)</th>
<th>Tube Side</th>
<th>Shell Side</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet Temperature (°C)</td>
<td>4</td>
<td>35</td>
</tr>
<tr>
<td>Outlet Temperature (°C)</td>
<td>14</td>
<td>20</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Design Data</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface Area (m$^3$)</td>
<td>0.43</td>
</tr>
<tr>
<td>Length (m)</td>
<td>6.1</td>
</tr>
<tr>
<td>U (W/m$^2$-°C)</td>
<td>909</td>
</tr>
<tr>
<td>LMTD (°C)</td>
<td>18</td>
</tr>
<tr>
<td>Fouling Resistance (m$^2$-°C/W)</td>
<td>0</td>
</tr>
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<table>
<thead>
<tr>
<th>Construction Materials</th>
<th>Carbon Steel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Utilities Required/Year (kWh)</td>
<td>100</td>
</tr>
<tr>
<td>Purchase Cost</td>
<td>$14,600</td>
</tr>
<tr>
<td>Bare Module Cost</td>
<td>$46,200</td>
</tr>
</tbody>
</table>
Section 13: Equipment Cost and Fixed-capital Investment Summary

The estimated equipment cost summary is given by Table 12.1 which contains the capital investment and purchase costs for each equipment unit included in the process flow diagram, as related by the bare module factor. As indicated by the table, the source of each price comes from tabulated cost data, specifically from equations found in Seider et al. The estimated purchase and installed costs for each adsorption column includes the cost of the activated carbon adsorbent packing corresponding to each. The annual equipment cost per tonne of carbon dioxide captured was calculated assuming that the equipment would be paid off over five years. Table 12.2 gives a summary of the investment information as calculated using Brian Downey’s “Profitability Analysis” Spreadsheet (2008). This spreadsheet included the installed equipment costs (and therefore bare-module costs). Site preparations and cost of service facilities were estimated at 5% of the total bare-module cost. The sum of these two costs yielded a direct permanent investment of $2,860,000. The cost of contingencies and contractor fees was estimated at 18% of the direct permanent investment. Summed to the direct permanent investment, this cost gives the depreciable capital cost of $3,360,000. The cost of land was taken to be zero since the process will be added to an existing plant. The cost of startup of the process was taken to be 10% of the depreciable capital, giving $338,000. There are no known royalties for this process at this time.
<table>
<thead>
<tr>
<th>Unit Number</th>
<th>Equipment Name</th>
<th>Estimated Purchase cost</th>
<th>Bare Module Factor</th>
<th>Estimated Capital Investment</th>
<th>Price Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>B-1</td>
<td>Positive Displacement Blower</td>
<td>$185,000</td>
<td>2.15</td>
<td>$398,000</td>
<td>Tabulated Cost data</td>
</tr>
<tr>
<td>B-2</td>
<td>Positive Displacement Blower</td>
<td>$79,500</td>
<td>2.15</td>
<td>$171,000</td>
<td>Tabulated Cost data</td>
</tr>
<tr>
<td>B-3</td>
<td>Positive Displacement Blower</td>
<td>$50,700</td>
<td>2.15</td>
<td>$109,000</td>
<td>Tabulated Cost data</td>
</tr>
<tr>
<td>B-4</td>
<td>Positive Displacement Blower</td>
<td>$81,000</td>
<td>2.15</td>
<td>$174,000</td>
<td>Tabulated Cost data</td>
</tr>
<tr>
<td>A-1</td>
<td>Packed Bed Adsorption Column</td>
<td>$105,400</td>
<td>4.16</td>
<td>$386,400</td>
<td>Tabulated Cost data</td>
</tr>
<tr>
<td>A-2</td>
<td>Packed Bed Adsorption Column</td>
<td>$105,400</td>
<td>4.16</td>
<td>$386,400</td>
<td>Tabulated Cost data</td>
</tr>
<tr>
<td>A-3</td>
<td>Packed Bed Adsorption Column</td>
<td>$32,000</td>
<td>4.16</td>
<td>$129,000</td>
<td>Tabulated Cost data</td>
</tr>
<tr>
<td>A-4</td>
<td>Packed Bed Adsorption Column</td>
<td>$32,000</td>
<td>4.16</td>
<td>$129,000</td>
<td>Tabulated Cost data</td>
</tr>
<tr>
<td>HX-1</td>
<td>Shell and Tube Heat Exchanger</td>
<td>$11,800</td>
<td>3.17</td>
<td>$37,300</td>
<td>Tabulated Cost data</td>
</tr>
<tr>
<td>HX-2</td>
<td>Shell and Tube Heat Exchanger</td>
<td>$14,600</td>
<td>3.17</td>
<td>$46,200</td>
<td>Tabulated Cost data</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td></td>
<td><strong>$697,400</strong></td>
<td></td>
<td><strong>$1,943,000</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Equipment Cost per tonne/CO₂</strong></td>
<td></td>
<td></td>
<td></td>
<td><strong>$10.87</strong></td>
<td></td>
</tr>
</tbody>
</table>
## Table 13.2: Investment Summary

### Investment Summary

#### Installed Equipment Costs:

- Total Direct Materials and Labor Costs: $100,500
- Miscellaneous Installation Costs: $2,500,300
- Material and Labor G&A Overhead and Contractor Fees: $-
- Contractor Engineering Costs: $-
- Indirect Costs: $-

**Total:** $2,600,800

#### Direct Permanent Investment

- Cost of Site Preparations: $130,040
- Cost of Service Facilities: $130,040

**Direct Permanent Investment:** $2,860,880

#### Total Depreciable Capital

- Cost of Contingencies & Contractor Fees: $514,958

**Total Depreciable Capital:** $3,375,838

#### Total Permanent Investment

- Cost of Land: $-
- Cost of Royalties: $-
- Cost of Plant Start-Up: $337,584

**Total Permanent Investment - Unadjusted:** $3,713,422

Site Factor: 1.00

**Total Permanent Investment:** $3,713,422
Section 14: Operating Cost – Cost of Manufacture

Components that contribute to the operating cost of the process include utilities and operations/maintenance. Table 13.1 shows the estimated utilities cost for each relevant equipment unit in the process flow diagram. The adsorption columns and storage tank are not included as they are assumed to have no utility requirements. Utility costs for electricity, cooling water, and chilling water were taken from Seider et al.’s Product and Process Design Principles. Table 13.2 shows the price of each required utility as well as the ratio of use in the process. Operations and maintenance (fixed costs) were found using Brian Downey’s “Profitability Analysis” Spreadsheet and can be seen in Table 13.3. Maintenance wages and benefits were taken to be 4.50% of the total depreciable capital. Operating overhead costs were taken to be 7.10% of maintenance and operations wages and benefits. Property taxes and insurance were assumed to be 2.00% of the total depreciable capital. Rental fees for office and laboratory space were taken to be zero since the process will be added to an existing plant. Similarly, it was estimated that an average of half of an operator, at $40/hr in wages and benefits, would be required to oversee the carbon capture process. This means that one of the plant’s existing operators would likely spend a maximum of half of their time overseeing carbon capture, and half to do other duties at the plant.
### Table 14.1: Estimated Unit Utilities Cost Summary

<table>
<thead>
<tr>
<th>Unit Number</th>
<th>Equipment Name</th>
<th>Utility</th>
<th>Amount of Utility Required</th>
<th>Utility Cost</th>
<th>Yearly Cost of Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>B-1</td>
<td>Positive Displacement Blower</td>
<td>Electric Power</td>
<td>285 kW</td>
<td>$0.07/kWh</td>
<td>$177,000</td>
</tr>
<tr>
<td>B-2</td>
<td>Positive Displacement Blower</td>
<td>Electric Power</td>
<td>76.4 kW</td>
<td>$0.07/kWh</td>
<td>$46,600</td>
</tr>
<tr>
<td>B-3</td>
<td>Positive Displacement Blower</td>
<td>Electric Power</td>
<td>38.2 kW</td>
<td>$0.07/kWh</td>
<td>$23,000</td>
</tr>
<tr>
<td>B-4</td>
<td>Positive Displacement Blower</td>
<td>Electric Power</td>
<td>78.8 kW</td>
<td>$0.07/kWh</td>
<td>$48,000</td>
</tr>
<tr>
<td>HX-1</td>
<td>Shell and Tube Heat Exchanger</td>
<td>Electric Power;</td>
<td>480 kW; 21,500 lb/tonne CO₂</td>
<td>$0.10/1000</td>
<td>$79,000</td>
</tr>
<tr>
<td>HX-2</td>
<td>Shell and Tube Heat Exchanger</td>
<td>Electric Power;</td>
<td>97 kW; 0.0838 kWh/tonne CO₂</td>
<td>$5.00/GJ</td>
<td>$63,800</td>
</tr>
</tbody>
</table>

**Process Total** $437,000

### Table 14.2: Prices and Amounts of Utilities for Overall Process

<table>
<thead>
<tr>
<th>Utility</th>
<th>Cost of Utility</th>
<th>Amount of Utility Required</th>
<th>Total Yearly Cost of Utility</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electricity</td>
<td>$0.07/kWh</td>
<td>1.61 kWh/tonne CO₂</td>
<td>$419,000</td>
</tr>
<tr>
<td>Cooling Water</td>
<td>$0.10/1000 gal</td>
<td>21,500 lb/tonne CO₂</td>
<td>$2,550</td>
</tr>
<tr>
<td>Chilling Water</td>
<td>$5.00/GJ</td>
<td>0.0838 kWh/tonne CO₂</td>
<td>$15,300</td>
</tr>
</tbody>
</table>

**Cost of Utilities per tonne of CO₂** $10.78
<table>
<thead>
<tr>
<th>Fixed Cost Summary</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Operations</strong></td>
<td></td>
</tr>
<tr>
<td>Direct Wages and Benefits</td>
<td>$208,000</td>
</tr>
<tr>
<td>Direct Salaries and Benefits</td>
<td>$31,200</td>
</tr>
<tr>
<td>Operating Supplies and Services</td>
<td>$12,480</td>
</tr>
<tr>
<td>Technical Assistance to Manufacturing</td>
<td>$150,000</td>
</tr>
<tr>
<td>Control Laboratory</td>
<td>$162,500</td>
</tr>
<tr>
<td><strong>Total Operations</strong></td>
<td>$564,180</td>
</tr>
<tr>
<td><strong>Maintenance</strong></td>
<td></td>
</tr>
<tr>
<td>Wages and Benefits</td>
<td>$151,913</td>
</tr>
<tr>
<td>Salaries and Benefits</td>
<td>$37,978</td>
</tr>
<tr>
<td>Materials and Services</td>
<td>$151,913</td>
</tr>
<tr>
<td>Maintenance Overhead</td>
<td>$7,596</td>
</tr>
<tr>
<td><strong>Total Maintenance</strong></td>
<td>$349,399</td>
</tr>
<tr>
<td><strong>Operating Overhead</strong></td>
<td></td>
</tr>
<tr>
<td>General Plant Overhead</td>
<td>$30,465</td>
</tr>
<tr>
<td>Mechanical Department Services</td>
<td>$10,298</td>
</tr>
<tr>
<td>Employee Relations Department</td>
<td>$31,753</td>
</tr>
<tr>
<td><strong>Total Operating Overhead</strong></td>
<td>$72,516</td>
</tr>
<tr>
<td><strong>Property Taxes and Insurance</strong></td>
<td></td>
</tr>
<tr>
<td>Property Taxes and Insurance</td>
<td>$67,517</td>
</tr>
<tr>
<td><strong>Other Annual Expenses</strong></td>
<td></td>
</tr>
<tr>
<td>Rental Fees (Office and Laboratory Space)</td>
<td>$-</td>
</tr>
<tr>
<td>Licensing Fees</td>
<td>$-</td>
</tr>
<tr>
<td>Miscellaneous</td>
<td>$-</td>
</tr>
<tr>
<td><strong>Total Other Annual Expenses</strong></td>
<td>$-</td>
</tr>
<tr>
<td><strong>Total Fixed Costs</strong></td>
<td>$1,053,612</td>
</tr>
<tr>
<td><strong>Fixed Costs per tonne of CO₂</strong></td>
<td>$28.87</td>
</tr>
</tbody>
</table>
Section 15: Environmental Considerations

Although the primary goal of this process is to optimize the VPSA process for carbon dioxide removal, the ultimate purpose of carbon capture using activated carbon is to prevent carbon dioxide from harming the environment (global warming, ocean acidification, and the like) by removing it from the gases escaping to the atmosphere. For the purposes of setting a baseline value for the cost per tonne of carbon dioxide captured, a removal rate of 65% was chosen, but this capture rate was somewhat arbitrary, though 52. The VPSA process could theoretically remove even greater amounts of carbon dioxide from flue gases; however, as more carbon dioxide is captured, a greater fraction of the power plant’s energy produced will be consumed by the process and the cost per tonne of carbon dioxide captured will increase. The cost will increase because the process will not only have to yield high purities of carbon dioxide to allow for selling for enhanced oil recovery, but will also have to be designed to minimize carbon dioxide losses through use of a larger column to better approach equilibrium or by adding more VPSA steps to capture carbon dioxide leaking into the atmosphere through the bed.

Section 16: Profitability Analysis

The “Profitability Analysis” spreadsheet by Brian K. Downey (2008) was used to analyze the process from an economic standpoint. The primary goal of this project is to design the most cost-efficient carbon dioxide removal process from the flue gas of a power plant to reduce emissions of this harmful greenhouse gas, so designing the process to be profitable would be extremely difficult, if not impossible, with existing technologies. However, selling the captured carbon dioxide for the purposes of enhanced oil recovery reduces costs by 40%. The final cost per ton of carbon dioxide removed for this process is $28.16 (after taking the sale of the carbon dioxide into account). Table 15.1 shows the final cost per tonne of carbon dioxide, and how each component contributes.

<table>
<thead>
<tr>
<th>Classification of Cost</th>
<th>Cost per tonne of CO₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Operating Costs</td>
<td></td>
</tr>
<tr>
<td>Utility Costs</td>
<td>$10.78</td>
</tr>
<tr>
<td>Fixed Costs</td>
<td>$28.87</td>
</tr>
<tr>
<td>Equipment Costs</td>
<td>$11.56</td>
</tr>
<tr>
<td>Selling Price of CO₂</td>
<td>($20.00)</td>
</tr>
<tr>
<td>Process Total</td>
<td>$28.16</td>
</tr>
</tbody>
</table>

The plant is assumed to operate 24 hours a day, seven days a week, every day of the year. Since it is a power plant, it will not shut down. If there is a problem with the process, storage tanks may be used in place of one of the adsorption processes to allow for repairs without shutting the process down. A general inflation rate of 1.7% was obtained from Taborda. A 5 year MACRS depreciation schedule was implemented for the equipment depreciation. The project start date was assumed to be 2018. Projected prices for the carbon dioxide market were obtained from Luckow and can be found in Figure A-15.1 in the Appendix. The current US political climate makes it difficult to predict exactly what kinds of incentives companies will have for
reducing their carbon footprint by the time the process was ready. Therefore, a conservative assumption was made to omit any potential carbon credits or tax benefits, but to assume there would be no income tax because of the sale of the captured carbon dioxide.

Table 16.2 shows some of the inputs for which the profitability analysis was conducted over. Table 16.3 summarizes some of the important profitability results. As expected, the process is not profitable. The net present value is -$7M, at an ROI after three years of production of -27%.

Table 16.2: Profitability Inputs

```
<table>
<thead>
<tr>
<th>Year</th>
<th>Action</th>
<th>Distribution of Permanent Investment</th>
<th>Production Capacity</th>
<th>Depreciation 5 year MACRS</th>
<th>Product Price</th>
</tr>
</thead>
<tbody>
<tr>
<td>2018</td>
<td>Design</td>
<td>100%</td>
<td>0.0%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2019</td>
<td>Construction</td>
<td>0%</td>
<td>0.0%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2020</td>
<td>Production</td>
<td>45.0%</td>
<td>90.0%</td>
<td>20.00%</td>
<td>$29.00</td>
</tr>
<tr>
<td>2021</td>
<td>Production</td>
<td>32.00%</td>
<td>90.0%</td>
<td>19.20%</td>
<td>$20.00</td>
</tr>
<tr>
<td>2022</td>
<td>Production</td>
<td>11.62%</td>
<td>90.0%</td>
<td>11.62%</td>
<td>$20.00</td>
</tr>
<tr>
<td>2023</td>
<td>Production</td>
<td>5.76%</td>
<td>90.0%</td>
<td>5.76%</td>
<td>$21.00</td>
</tr>
<tr>
<td>2024</td>
<td>Production</td>
<td>9.00%</td>
<td>90.0%</td>
<td></td>
<td>$22.00</td>
</tr>
<tr>
<td>2025</td>
<td>Production</td>
<td>9.00%</td>
<td>90.0%</td>
<td></td>
<td>$24.00</td>
</tr>
<tr>
<td>2026</td>
<td>Production</td>
<td>9.00%</td>
<td>90.0%</td>
<td></td>
<td>$25.00</td>
</tr>
<tr>
<td>2027</td>
<td>Production</td>
<td>9.00%</td>
<td>90.0%</td>
<td></td>
<td>$27.00</td>
</tr>
<tr>
<td>2028</td>
<td>Production</td>
<td>9.00%</td>
<td>90.0%</td>
<td></td>
<td>$28.00</td>
</tr>
<tr>
<td>2029</td>
<td>Production</td>
<td>9.00%</td>
<td>90.0%</td>
<td></td>
<td>$30.00</td>
</tr>
<tr>
<td>2030</td>
<td>Production</td>
<td>9.00%</td>
<td>90.0%</td>
<td></td>
<td>$31.00</td>
</tr>
<tr>
<td>2031</td>
<td>Production</td>
<td>9.00%</td>
<td>90.0%</td>
<td></td>
<td>$34.00</td>
</tr>
<tr>
<td>2032</td>
<td>Production</td>
<td>9.00%</td>
<td>90.0%</td>
<td></td>
<td>$38.00</td>
</tr>
</tbody>
</table>
```
# Table 16.3: Profitably Results Summary

## Profitability Measures

The Internal Rate of Return (IRR) for this project is **Negative IRR**

The Net Present Value (NPV) of this project in 2018 is **$(7,118,800)$**

## ROI Analysis (Third Production Year)

<table>
<thead>
<tr>
<th>Item</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Annual Sales</td>
<td>657,000</td>
</tr>
<tr>
<td>Annual Costs</td>
<td>(1,395,003)</td>
</tr>
<tr>
<td>Depreciation</td>
<td>(297,074)</td>
</tr>
<tr>
<td>Income Tax</td>
<td>-</td>
</tr>
<tr>
<td>Net Earnings</td>
<td>(1,035,077)</td>
</tr>
<tr>
<td>Total Capital Investment</td>
<td>3,852,561</td>
</tr>
<tr>
<td>ROI</td>
<td>-26.87%</td>
</tr>
</tbody>
</table>
Section 17: Conclusions and Recommendations

From a cost perspective, carbon capture using VPSA on activated carbon is a viable option to reduce global emissions of carbon dioxide and mitigate its negative side effects. The results of the cost optimization performed in this project show that the lowest achievable cost to capture 100 tons of carbon dioxide a day for VPSA-based carbon capture for coal-fired power plants is $28 per tonne of carbon dioxide removed (at a 65% capture rate and 93% purity), while using approximately 12% of the power plant’s energy output.

While the results of this study demonstrate that activated carbon-based capture using VPSA provides promising economics and energy consumption, it will still compete with established industry standards including amine-based capture and membrane capture, as well as zeolite-based capture, another promising adsorption-based carbon capture process.

Amine-based carbon capture is an absorption process that involves contacting the gas phase containing carbon dioxide with a solvent capable of removing (via absorption into the liquid phase) the carbon dioxide53. Amine-based capture methods consistently remove over 90% of the carbon dioxide from flue gas streams at purities above 99% and can also be regenerated reliably; however, the capture procedure takes up to 41% of the power plant’s energy.54 Aside from its energy consumption great, amine-based carbon capture also costs $47 per tonne of carbon dioxide removed (after taking profits from enhanced oil recovery carbon dioxide sales into consideration), which is much greater than the cost for VPSA capture.55

——

55 Radosz et al., “Flue-Gas Carbon Capture on Carbonaceous Sorbents.”
Membrane separations remove the carbon dioxide by allowing solution, diffusion, and/or ionic transport through the membrane into a separate stream\textsuperscript{56} and, though cost-efficient, the removal processes cannot easily yield carbon dioxide streams greater than 90\% purity. To achieve purity levels in the 90-100\% range, more extreme pressure gradients must be generated across the membrane, which, in turn, requires either more resilient membranes or multiple membrane separation stages. When achieving carbon dioxide purities of greater than 90\%, the cost per tonne of carbon dioxide removed is $47.40.\textsuperscript{57}

Carbon capture using zeolites, which involves adsorption processes similar to those used with activated carbon-based capture, has some advantages over capture processes that use activated-carbon, such as higher selectivity of carbon dioxide over nitrogen, which leads to extremely pure carbon dioxide streams. However, zeolites require temperatures over 300 °C during recovery to remove adsorbed water, or, alternatively, require extensive and expensive water removal processes prior to adsorption.\textsuperscript{58} - Zeolites are also extremely expensive relative to activated carbon, and ultimately end up costing approximately $51 per tonne carbon dioxide captured.

Temperature swing adsorption (TSA) and pressure swing adsorption (PSA) recovery methods are other adsorption alternatives to VPSA that can also use activated carbon as the sorbent in the system. TSA could theoretically prove almost as effective, if not more effective, as VPSA, but the process requires both steam heating and air/water cooling, both of which


\textsuperscript{57} Maas et al., “Energetic and Economic Evaluation of Membrane-Based Carbon Capture Routes for Power Plant Processes.”

significantly increase operating costs. Not only that, but TSA has much longer cycle times than VPSA, which translates to much needing more activated carbon and thus larger columns. When designing future processes, however, temperature swings may assist the VPSA process by increasing working capacity (since less carbon dioxide will remain on the adsorbent at higher temperatures). PSA functions similarly to VPSA, but without the advantage of higher selectivity at lower desorption pressures. As a result, more stages of VPSA are necessary to achieve the desired 92% (or greater) purity. Even discounting equipment and material costs, the two processes (TSA and PSA) cost at least $37 per tonne carbon dioxide captured. A summary of the costs of carbon capture using different capture methods are presented in in Table 17.1 below.

<table>
<thead>
<tr>
<th>Capture Method</th>
<th>Amine-Based</th>
<th>Membrane</th>
<th>Zeolite</th>
<th>Activated Carbon TSA/PSA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost per tonne CO₂ avoided ($)</td>
<td>$47</td>
<td>$47.4</td>
<td>$51</td>
<td>$37</td>
</tr>
</tbody>
</table>

Although this process optimization swept over a wide range of temperatures, pressures of adsorption and desorption, and also considered alternative units for water removal and pressurization, there are still more considerations that can further improve the process to both minimize cost and better model the VPSA process. Costs could potentially be reduced through implementation of a more complex Skarstom cycle, which could utilize more columns to reduce blower requirements further since pressure equalization would be more complete (pressurization of third column during equalization of the other two).

A large area of importance that was not explored in detail during this process optimization was the role of kinetics, which, if implemented into the model, will provide
estimates of capture rates and cycle times more accurately than when operating under assumed equilibrium conditions. Similarly, though the temperature changes during adsorption and desorption are negligible, introducing thermal considerations will also enhance the accuracy of the model and thus will make pricing and cost estimates even more precise than in the analysis performed in this study.

More broadly, this report relates to the potential impact it may have on reduction in carbon dioxide emissions (and its associated harmful effects on the environment). The Princeton Environmental Institute published a report in July of 2005, which identified several methods through which “wedges” of 1 billion tons of carbon dioxide emissions can be avoided over the next 50 years to stabilize atmospheric carbon dioxide levels. One of those wedges can be accomplished by performing carbon capture and storage on 800 large coal-fired power plants by 2055,59 which could be more possible with activated carbon-based carbon dioxide capture using VPSA, which this report demonstrates can be both cost and energy effective. Although the current sizing and cycle optimization was performed for the capture of 100 tonnes of carbon dioxide per day, the same equations and principles could be applied to larger plants to aid in the effort to mitigate carbon dioxide emissions.

---

Section 18: Bibliography


[55] Targett, Matthew “Senior Design Meetings.”


Section 19: Acknowledgements

Thank you to Dr. Talid Sinno, Dr. Matthew Targett (LP Amina), Dr. Bruce Vrana, Dr. Warren Seider, Dr. Sue Ann Bidstrup-Allen, Dr. Raymond Gorte, Dr. Leonard Fabiano, and all of the industrial consultants who attended our meetings, especially Dr. Adam Brostow. Without the help of these knowledgeable and experienced professionals, this project would not have been possible.
Appendix A: Water Removal Aspen Simulations

The following are the Aspen simulations for the water removal processes. Part 1 outlines the simulation run for the initial water removal in streams 1-8. Part 2 outline the secondary water removal in streams 22-24.

Part 1:

Block Report:

BLOCK:  B-1      MODEL: FLASH2
-------------------------------
INLET STREAM:          FLUE3
OUTLET VAPOR STREAM:   FLUE4
OUTLET LIQUID STREAM:  WATER3
PROPERTY OPTION SET:   RK-SOAVE  STANDARD RKS EQUATION OF STATE

***  MASS AND ENERGY BALANCE  ***

<table>
<thead>
<tr>
<th></th>
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*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E 4167.59 KG/HR
PRODUCT STREAMS CO2E 4167.59 KG/HR
NET STREAMS CO2E PRODUCTION 0.00000 KG/HR
UTILITIES CO2E PRODUCTION 0.00000 KG/HR
TOTAL CO2E PRODUCTION 0.00000 KG/HR

*** INPUT DATA ***

TWO PHASE TP FLASH
SPECIFIED TEMPERATURE C 20.0000
SPECIFIED PRESSURE BAR 1.11000
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000
*** RESULTS ***

OUTLET TEMPERATURE  C  20.000
OUTLET PRESSURE     BAR  1.1100
HEAT DUTY          CAL/SEC -6847.4
VAPOR FRACTION     0.99667

V-L PHASE EQUILIBRIUM:

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BLOCK: HX-1    MODEL: FLASH2

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INLET STREAM: FLUE1
OUTLET VAPOR STREAM: FLUE2
OUTLET LIQUID STREAM: WATER1
PROPERTY OPTION SET: RK-SOAVE STANDARD RKS EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

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*** CO2 EQUIVALENT SUMMARY ***

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<td>NET STREAMS CO2E PRODUCTION</td>
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<td>UTILITIES CO2E PRODUCTION</td>
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<td>TOTAL CO2E PRODUCTION</td>
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*** INPUT DATA ***

TWO PHASE TP FLASH
SPECIFIED TEMPERATURE C  35.0000
SPECIFIED PRESSURE      BAR  1.00000
MAXIMUM NO. ITERATIONS  30
CONVERGENCE TOLERANCE   0.000100000

*** RESULTS ***

OUTLET TEMPERATURE  C  35.000
OUTLET PRESSURE     BAR  1.0000
HEAT DUTY          CAL/SEC -1.0362E+06
VAPOR FRACTION     0.96393

V-L PHASE EQUILIBRIUM:

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BLOCK: HX-2    MODEL: FLASH2

INLET STREAM:       FLUE2
OUTLET VAPOR STREAM: FLUE3
OUTLET LIQUID STREAM: WATER2
PROPERTY OPTION SET:  RK-SOAVE  STANDARD RK-S EQUATION OF STATE

*** MASS AND ENERGY BALANCE ***

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<th>RELATIVE DIFF.</th>
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*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E 4167.59 KG/HR
PRODUCT STREAMS CO2E 4167.59 KG/HR
NET STREAMS CO2E PRODUCTION 0.00000 KG/HR
UTILITIES CO2E PRODUCTION 0.00000 KG/HR
TOTAL CO2E PRODUCTION 0.00000 KG/HR

*** INPUT DATA ***
TWO PHASE TP FLASH
SPECIFIED TEMPERATURE C 20.0000
SPECIFIED PRESSURE BAR 1.00000
MAXIMUM NO. ITERATIONS 30
CONVERGENCE TOLERANCE 0.000100000

*** RESULTS ***
OUTLET TEMPERATURE C 20.000
OUTLET PRESSURE BAR 1.0000
HEAT DUTY CAL/SEC -74659.
VAPOR FRACTION 0.97369

V-L PHASE EQUILIBRIUM :

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Stream Report:

**FLUE1**

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<td>TO :</td>
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**SUBSTREAM: MIXED**

**PHASE:** VAPOR

**COMPONENTS:** KMOL/HR

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**TOTAL FLOW:**

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**STATE VARIABLES:**

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**ENTHALPY:**

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**ENTROPY:**

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**FLUE2**

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**SUBSTREAM: MIXED**

**PHASE:** VAPOR

**COMPONENTS:** KMOL/HR

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**TOTAL FLOW:**

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**STATE VARIABLES:**

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**ENTHALPY:**

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**STREAM ID**: WATER3  
**FROM**: B-1  
**TO**: ----  
**SUBSTREAM**: MIXED  
**PHASE**: LIQUID  
**COMPONENTS**: KMOL/HR  
- **H2O**: 2.1394  
- **N2**: 1.0016-07  
- **CO2**: 7.3633-06  
**TOTAL FLOW**:  
- **KMOL/HR**: 2.1394  
- **KG/HR**: 38.5416  
- **L/MIN**: 0.6432  

**STATE VARIABLES**:  
- **TEMP C**: 20.0000  
- **PRES BAR**: 1.1100  
- **VFRAC**: 0.0  
- **LFRAC**: 1.0000  
- **SFRAC**: 0.0  

**ENTHALPY**:  
- **CAL/MOL**: -6.9142+04  
- **CAL/GM**: -3837.9230  
- **CAL/SEC**: -4.1089+04  

**ENTROPY**:  
- **CAL/MOL-K**: -41.2624  
- **CAL/GM-K**: -2.2904  

**DENSITY**:  
- **MOL/CC**: 5.5440-02  
- **GM/CC**: 0.9988  
- **AVG MW**: 18.0154

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**Part 2:**

---
Block Report

BLOCK:  B1       MODEL:  FLASH2

INLET STREAM:      S2
OUTLET VAPOR STREAM:  S3
OUTLET LIQUID STREAM:  S4
PROPERTY OPTION SET:  RK-SOAVE  STANDARD RKS EQUATION OF STATE

***  MASS AND ENERGY BALANCE  ***

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<tr>
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<th>IN</th>
<th>OUT</th>
<th>RELATIVE DIFF.</th>
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***  CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E             4161.39      KG/HR
PRODUCT STREAMS CO2E          4161.39      KG/HR
NET STREAMS CO2E PRODUCTION   0.00000      KG/HR
UTILITIES CO2E PRODUCTION     0.00000      KG/HR
TOTAL CO2E PRODUCTION         0.00000      KG/HR

***  INPUT DATA  ***

TWO PHASE  TP  FLASH
SPECIFIED TEMPERATURE C                                  20.0000
SPECIFIED PRESSURE    BAR                                 1.00000
MAXIMUM NO. ITERATIONS                                   30
CONVERGENCE TOLERANCE                                     0.000100000

***  RESULTS  ***

OUTLET TEMPERATURE    C                                    20.000
OUTLET PRESSURE       BAR                                  1.0000
HEAT DUTY             CAL/SEC                               -7303.9
VAPOR FRACTION        0.95692

V-L PHASE EQUILIBRIUM :

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<th>X(I)</th>
<th>Y(I)</th>
<th>K(I)</th>
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Stream Report

S2  S3  S4

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SUBSTREAM: MIXED

PHASE:

COMPONENTS: KMOL/HR

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<th>S4</th>
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<tr>
<td>H2O</td>
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</tr>
<tr>
<td>N2</td>
<td>37.1840</td>
<td>37.1840</td>
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<tr>
<td>CO2</td>
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<td>94.5559</td>
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<tr>
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STATE VARIABLES:

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<td>20.0000</td>
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<td>LFRAC</td>
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**SUBSTREAM: MIXED**

**PHASE:** MIXED

**COMPONENTS: KMOL/HR**

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<td>N2</td>
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<td>CO2</td>
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**SUBSTREAM: MIXED**

**PHASE:** --

**COMPONENTS: KMOL/HR**

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<tbody>
<tr>
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<td>N2</td>
<td>37.1840</td>
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<tr>
<td>CO2</td>
<td>94.5559</td>
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**TOTAL FLOW:**

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**STATE VARIABLES:**

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TO   :              ----

SUBSTREAM: MIXED

PHASE: LIQUID

COMPONENTS: KMOL/HR

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<tr>
<td>CO2</td>
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TOTAL FLOW:

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STATE VARIABLES:

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<tr>
<td>LFRAC</td>
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ENTHALPY:

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<td>CAL/GM</td>
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DENSITY:

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<td>GM/CC</td>
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<tr>
<td>AVG MW</td>
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</table>
Appendix B: MATLAB Code
This section contains the MATLAB code used for process modeling, equipment sizing, and costing. Also note
that commented out code or information may be a relic of previous iterations and does not necessarily hold for the
actual treatment of the process

Half-Order Function

```matlab
function y = half_order(a,xdata);

y = a(1).*xdata.^(1/2)+a(2).*xdata;

end
```
Carbon Dioxide Adsorption Isotherm Fitting Script

CO2_20 = csvread('co2_20.csv',1);
CO2_40 = csvread('co2_40.csv',1);
CO2_20_pres = CO2_20(:,1);
CO2_20_loading = CO2_20(:,2);
CO2_40_pres = CO2_40(:,1);
CO2_40_loading = CO2_40(:,2);

% CO2_20_poly = polyfit(CO2_20_pres,CO2_20_loading,2);
% CO2_40_poly = polyfit(CO2_40_pres,CO2_40_loading,2);

starting_guess = [1; 1];
[coeffs_20] = lsqcurvefit(@half_order,starting_guess,CO2_20_pres,CO2_20_loading);
[coeffs_40] = lsqcurvefit(@half_order,starting_guess,CO2_40_pres,CO2_40_loading);

x = 0:1:200;

CO2_20_fit = coeffs_20(1).*x.^(1/2)+coeffs_20(2).*x;
CO2_40_fit = coeffs_40(1).*x.^(1/2)+coeffs_40(2).*x;

figure
hold on
p1=plot(CO2_20_pres,CO2_20_loading,'*');
p2=plot(CO2_40_pres,CO2_40_loading,'o');
p3=plot(x,CO2_20_fit);
p4=plot(x,CO2_40_fit);
xaxis = xlabel('Partial Pressure of CO2 (kPa)');
yaxis = ylabel('Loading (mol CO2/kg AC)');
xaxis.FontSize = 16;
yaxis.FontSize = 16;
t=title('Extrapolated Adsorption Isotherms for CO2 on Activated Carbon');
t.FontSize = 16;
leg=legend('CO2 lit data 20 C','CO2 lit data 40 C','CO2 data fit 20 C', 'CO2 data fit 40 C');
leg.FontSize = 12;
Nitrogen Adsorption Isotherm Fitting Script

N2_20 = csvread('n2_20.csv',1)
N2_60 = csvread('n2_60.csv',1)
N2_20_pres = N2_20(:,1);
N2_20_loading = N2_20(:,2);
N2_60_pres = N2_60(:,1);
N2_60_loading = N2_60(:,2);

% CO2_20_poly = polyfit(CO2_20_pres,CO2_20_loading,2);
% CO2_40_poly = polyfit(CO2_40_pres,CO2_40_loading,2);

starting_guess = [1; 1];

[coeffs_20] = lsqcurvefit(@half_order,starting_guess,N2_20_pres,N2_20_loading);
[coeffs_40] = lsqcurvefit(@half_order,starting_guess,N2_60_pres,N2_60_loading);

x = 0:1:200;
N2_20_fit = coeffs_20(1).*x.^(1/2)+coeffs_20(2).*x;
N2_40_fit = coeffs_40(1).*x.^(1/2)+coeffs_40(2).*x;

figure
hold on
plot(N2_20_pres,N2_20_loading,'*');
plot(N2_60_pres,N2_60>Loading,'o');
plot(x,N2_20_fit);
plot(x,N2_40_fit);
xaxis = xlabel('Partial Pressure of N2 (kPa)');
yaxis = ylabel('Loading (mol N2/kg AC)');
xaxis.FontSize = 16;
yaxis.FontSize = 16;
t = title('Extrapolated Adsorption Isotherms for N2 on Activated Carbon');
t.FontSize = 16;
leg = legend('N2 lit data 20 C','N2 lit data 40 C','N2 data fit 20 C', 'N2 data fit 40 C');
leg.FontSize = 12;
Carbon Dioxide Viscosity Function

```matlab
function [mu_CO2] = CO2_viscosity(T)
%Input T in Celsius, get output of viscosity in kg/(m*s)
To = 527.67; %Reference temperature in Rankine
T_R = T*1.8+491.67; %Temperature in Rankine
C = 240; %Sutherland constant
mu_o = 0.01480; %reference viscosity (cP)
a = 0.555*To+C;
b = 0.555*T_R+C;
mu_cP = mu_o*(a/b)*(T_R/To)^(3/2);
[mu_CO2] = mu_cP*10^-3;%units of kg/(m*s)
end
```
Nitrogen Viscosity Script

function [mu_N2] = N2_viscosity(T)
%Input T in Celsius, get output of viscosity in kg/(m*s)
To = 540.99; %Reference temperature in Rankine
T_R = T*1.8+491.67; %Temperature in Rankine
C = 111; %Sutherland constant
mu_o = 0.01781; %reference viscosity (cP)
a = 0.555*To+C;
b = 0.555*T_R+C;
mu_cP = mu_o*(a/b)*(T_R/To)^(3/2);
[mu_N2] = mu_cP*10^-3; %units of kg/(m*s)
end
Adsorption/Desorption Amount Function without Purity Input

```matlab
function [sel,AA_CO2,AA_N2] = selectivityIP4(T,P)
% chem is the chemical, either 'CO2' or 'N2'
% temp is the temperature in Celsius
% pres is the pressure in kPa
% adjust these volume percentages based on the input flue gas
PercentCO2 = 15;
PercentN2 = 85;
FracCO2 = PercentCO2/100; %volume fraction CO2
FracN2 = PercentN2/100; % volume fraction N2
PPC = FracCO2*P; %partial pressure of CO2
PPN = FracN2*P; %partial pressure of N2

if T < 20
    [AA_CO2] = 0;
    [AA_N2] = 0;
end
if T >=20 && T<40
    if P <= 400 %low pressure
        CO2_20 = 0.2391*PPC^(0.5) + 0.0094*PPC;
        CO2_40 = 0.1553*PPC^(0.5) + 0.0093*PPC;
        [AA_CO2] = CO2_20 + (CO2_40 - CO2_20)*(T-20)/20;
        N2_20 = 0.0109*PPN^(0.5) + 0.0031*PPN;
        N2_60 = 0.0045*PPN^(0.5) + 0.0017*PPN;
        [AA_N2] = N2_20 + (N2_60 - N2_20)*(T-20)/40;
    end
end
if T > 150
    disp 'No data above 150 C'
end
%[sel] = [AA_CO2]/([AA_CO2]+[AA_N2])*100;
[sel]=1;
end
```


Adsorption/Desorption Amount Function with Purity Input

function [sel,AA_CO2,AA_N2] = selectivityIP5(T,P,purity_CO2)
% chem is the chemical, either 'CO2' or 'N2'
% temp is the temperature in Celsius
% pres is the pressure in kPa
% adjust these volume percentages based on the input flue gas
PPC = purity_CO2*P;  %partial pressure of CO2
PPN = (1-purity_CO2)*P;  %partial pressure of N2
if T < 20
    [AA_CO2] = 0;
    [AA_N2] = 0;
end
if T >=20 && T<40
    if P <= 400  %low pressure
        CO2_20 = 0.2391*PPC^(0.5) + 0.0094*PPC;
        CO2_40 = 0.1553*PPC^(0.5) + 0.0093*PPC;
        [AA_CO2] = CO2_20 + (CO2_40 - CO2_20)*(T-20)/20;
        N2_20 = 0.0109*PPN^(0.5) + 0.0031*PPN;
        N2_60 = 0.0045*PPN^(0.5) + 0.0017*PPN;
        [AA_N2] = N2_20 + (N2_60 - N2_20)*(T-20)/40;
    end
end
if T > 150
    disp 'No data above 150 C'
end
[sel] = [AA_CO2]/([AA_CO2]+[AA_N2])*100;
end
**Column 1 Sizing Script**

% Size Determination of columns
% ASSUMPTIONS
% 1. Instant equilibrium
% 2. 24/7 operation
% 3. 2:1 aspect ratio (h to D)
% 4. 10 minute cycle time
% 5. 5 minutes adsorbing, 5 minutes desorbing
% 6. Ideal gas
% 7. Density of AC assumed from paper
% 10. Isothermal

% Process constants
MMCO₂ = 44.01/1000; % kg Co₂/mol
R = 8.314; % ideal gas constant for SI units
Rho_AC = 984; % density of activated carbon, kg/m³
ε_b = 0.5; % bed porosity

% INPUTS
CO₂_capture_tons = 100; % CO₂ capture per day in tons
CO₂_capture_rate = 1; % Fraction of CO₂ captured
Run_time_daily = 24; % hours of capture per day
Gas_in_fracCO₂ = 0.15; % mole fraction CO₂ in inlet flue gas stream
Inlet_P = P_ads_1*10^5; % 1 bar inlet in Pa
Inlet_T = T_1+273; % T Kelvin for inlet
T_ads_min = 5; % minutes of adsorption
T_des_min = 5; % minutes of desorption

% Intermediates
CO₂_capture_kg = CO₂_capture_tons*1000; % CO₂ capture per day in tons
CO₂_molar_flow_daily = CO₂_capture_kg/MMCO₂; % daily moles of CO₂ in (captured)
Op_time = Run_time_daily*3600; % seconds of operation daily
CO₂_molar_flow_cap = CO₂_molar_flow_daily/Op_time; % molar flow of CO₂/s (captured)
CO₂_molar_flow = CO₂_molar_flow_cap/CO₂_capture_rate; % molar flow of CO₂/s (total)
Gas_molar_flow = CO₂_molar_flow/Gas_in_fracCO₂/CO₂_capture_rate; % total molar flow rate of gas/s (total)

Volumetric_gas = Gas_molar_flow*R*Inlet_T/Inlet_P; % volumetric flow rate of gas (total)
t_ads = t_ads_min*60; % seconds of adsorption
t_des = t_des_min*60; % seconds of desorption

% Capture of CO₂ (based on 1.5 bar adsorption, 0.5 bar desorption)
P_ads = P_ads_1; % bar
P_ads_kPa = P_ads_1*100; % kPa
PPC_ads_kPa = P_ads_kPa*Gas_in_fracCO₂; % partial pressure CO₂ in kPa
P_des = P_des_1; % bar
P_des_kPa = P_des_1*100; % kPa
PPC_des_kPa = P_des_kPa*Gas_in_fracCO₂; % partial pressure CO₂ in kPa (assume pure CO₂)
% DOUBLE CHECK THIS DESORPTION THING
T_ads = Inlet_T-273; % Celsius
T_des = Inlet_T-273; % Celsius
% Selectivity IP4
[sel_ads, AA_CO2_ads, AA_N2_ads] = selectivityIP4(T_ads, P_ads_kPa); % programmed in function
with 15% CO2 and some input P in kPa
purity_ads = AA_CO2_ads/(AA_CO2_ads+AA_N2_ads);
% [sel_des, AA_CO2_des, AA_N2_des] = selectivityIP3(T_des, P_des_kPa, purity_ads); % programmed with
[sel_des, AA_CO2_des, AA_N2_des] = selectivityIP4(T_des, P_des_kPa); % programmed with
Net_CO2 = AA_CO2_ads - AA_CO2_des; % net CO2 captured (mol/kg AC)

% Deliverables/Outputs
kg_AC = t_ads*CO2_molar_flow_cap/Net_CO2; % Mass of AC needed for capture (kg)
V_AC = kg_AC/Rho_AC; % volume of AC in m^3
V_bed = V_AC/(1-e_b); % volume of bed in m^3
D_bed = (V_bed*4/3/pi)^(1/3);
h_bed = D_bed*2;
disp(['The diameter of the bed is ', num2str(D_bed), ' m'])
disp(['The height of the bed is ', num2str(h_bed), ' m'])
Column 2 Sizing Script

% Size Determination of columns
% ASSUMPTIONS
% 1. Instant equilibrium
% 2. 24/7 operation
% 3. 2:1 aspect ratio (h to D)
% 4. 10 minute cycle time
% 5. 5 minutes adsorbing, 5 minutes desorbing
% 6. Ideal gas
% 7. Density of AC assumed from paper
% 8. For modeling purposes, used input P of 1.5 bar and desorption P of 0.5 bar for amount captured
% 9. No N2 or H2O adsorbed
% 10. Isothermal
% 11. Bed porosity of 0.5

% Process constants
MMCO2 = 44.01/1000; % kg Co2/mol
R = 8.314; % ideal gas constant for SI units
Rho_AC = 984; % density of activated carbon, kg/m^3
e_b = 0.5; % bed porosity

% INPUTS
CO2_capture_tons = 100; % CO2 capture per day in tons

% Assume venting off of 0.25, capture 100% of remaining
CO2_capture_rate = 1; % Fraction of CO2 captured

Run_time_daily = 24; % hours of capture per day
Gas_in_fracCO2_2 = Purity_col1; % mole fraction CO2 in inlet flue gas stream
Inlet_P_2 = 1.3*10^5; % 1 bar inlet in Pa
Inlet_T = 303; % 30 Celsius in Kelvin for inlet
in_t_ads_min = 2; % minutes of adsorption
Inlet_T = 303; % 30 Celsius in Kelvin for inlet
in_t_des_min = 2; % minutes of desorption

% Intermediates
CO2_capture_kg = CO2_capture_tons*1000; % CO2 capture per day in tons
CO2_molar_flow_daily = CO2_capture_kg/MMCO2; % daily moles of CO2 in (captured)
Op_time = Run_time_daily*3600; % seconds of operation daily
CO2_molar_flow_cap = CO2_molar_flow_daily/Op_time; % molar flow of CO2/s (captured)
CO2_molar_flow = CO2_molar_flow_cap/CO2_capture_rate; % molar flow of CO2/s (total)
Gas_molar_flow = CO2_molar_flow/Gas_in_fracCO2_2/CO2_capture_rate; % total molar flow rate of gas/s (total)

Volumetric_gas = Gas_molar_flow*R*Inlet_T/Inlet_P_2; % volumetric flow rate of gas (total)

% Capture of CO2 (based on 1.5 bar adsorption, 0.5 bar desorption)
P_ads_2 = 1.3; % bar
P_ads_kPa_2 = P_ads_2*100; % kPa
PPC_ads_kPa_2 = P_ads_kPa_2*Gas_in_fracCO2_2; % partial pressure CO2 in kPa
P_des_2 = P_des_2; %bar
P_des_kPa_2 = P_des_2*100; %kPa
PPC_des_kPa_2 = P_des_kPa_2*Gas_in_fracCO2_2; %partial pressure CO2 in kPa (assume pure CO2)

%DOUBLE CHECK THIS DESORPTION THING
T_ads = Inlet_T-273; %Celsius
T_des = Inlet_T-273; %Celsius
[sel_ads,AA_CO2_ads_2,AA_N2_ads_2] = selectivityIP5(T_ads, P_ads_kPa_2,Purity_col1);
%programmed in function with 15% CO2 and some input P in kPa
%purity_ads = AA_CO2_ads/(AA_CO2_ads+AA_N2_ads);

%DOUBLE CHECK THIS ADSORPTION THING
[sel_des,AA_CO2_des_2,AA_N2_des_2] = selectivityIP3(T_des, P_des_kPa_2,purity_ads);
%programmed with

Net_CO2_2 = AA_CO2_ads-AA_CO2_des; %net CO2 captured (mol/kg AC)

%Deliverables/Outputs
kg_AC_2 = t_ads*CO2_molar_flow_cap/Net_CO2_2; %Mass of AC needed for capture (kg)
V_AC_2 = kg_AC/Rho_AC; %volume of AC in m^3
V_bed_2 = V_AC/(1-e_b); %volume of bed in m^3
D_bed_2 = (V_bed*4/2/pi)^(1/3);
h_bed_2 = D_bed*2;
disp(['The diameter of the bed is ', num2str(D_bed_2), ' m'])
disp(['The height of the bed is ', num2str(h_bed_2), ' m'])
Column 1 Sizing Script with no Display

% Size Determination of columns
% ASSUMPTIONS
% 1. Instant equilibrium
% 2. 24/7 operation
% 3. 2:1 aspect ratio (h to D)
% 4. 10 minute cycle time
% 5. 5 minutes adsorbing, 5 minutes desorbing
% 6. Ideal gas
% 7. Density of AC assumed from paper
% 8. For modeling purposes, used input P of 1.5 bar and desorption P of 0.5 bar for amount captured
% 9. No N2 or H2O adsorbed
% 10. Isothermal
% 11. Bed porosity of 0.5

%Process constants
MMCO2 = 44.01/1000; %kg Co2/mol
R = 8.314; %ideal gas constant for SI units
Rho_AC = 984; %density of activated carbon, kg/m^3
e_b = 0.5; %bed porosity

% INPUTS
CO2_capture_tons = 100; %CO2 capture per day in tons

%Assume venting off of 0.25, capture 100% of remaining
CO2_capture_rate = 1; %Fraction of CO2 captured

Run_time_daily = 24; %hours of capture per day
Gas_in_fracCO2 = 0.15; %mole fraction CO2 in inlet flue gas stream
Inlet_P = P_ads_1*10^5; %1 bar inlet in Pa
Inlet_T = T_1+273; %T Kelvin for inlet
t_ads_min = 5; %minutes of adsorption
t_des_min = 5; %minutes of desorption

%Intermediates
CO2_capture_kg = CO2_capture_tons*1000; %CO2 capture per day in tons
CO2_molar_flow_daily = CO2_capture_kg/MMCO2; %daily moles of CO2 in (captured)
Op_time = Run_time_daily*3600; %seconds of operation daily
CO2_molar_flow_cap = CO2_molar_flow_daily/Op_time; %molar flow of CO2/s (captured)
CO2_molar_flow = CO2_molar_flow_cap/CO2_capture_rate; %molar flow of CO2/s (total)
Gas_molar_flow = CO2_molar_flow/Gas_in_fracCO2/CO2_capture_rate; %total molar flow rate of gas/s (total)
Volumetric_gas = Gas_molar_flow*R*Inlet_T/Inlet_P; %volumetric flow rate of gas (total)
t_ads = t_ads_min*60; %seconds of adsorption
t_des = t_des_min*60; %seconds of desorption

%Capture of CO2 (based on 1.5 bar adsorption, 0.5 bar desorption)
\[
P_{\text{ads}} = P_{\text{ads}_1}; \quad \text{\%bar}
\]
\[
P_{\text{ads}} \text{ kPa} = P_{\text{ads}} \times 100; \quad \text{\%kPa}
\]
\[
P_{\text{PPC_ads}} \text{ kPa} = P_{\text{PPC_ads}} \times \text{Gas in frac CO2}; \quad \text{\%partial pressure CO2 in kPa}
\]
\[
P_{\text{des}} = P_{\text{des}_1}; \quad \text{\%bar}
\]
\[
P_{\text{des}} \text{ kPa} = P_{\text{des}} \times 100; \quad \text{\%kPa}
\]
\[
P_{\text{PPC_des}} \text{ kPa} = P_{\text{PPC_des}} \times \text{Gas in frac CO2}; \quad \text{\%partial pressure CO2 in kPa (assume pure CO2)}
\]
\[
\text{\%DOUBLE CHECK THIS DESORPTION THING}
\]
\[
T_{\text{ads}} = \text{Inlet T} - 273; \quad \text{\%Celsius}
\]
\[
T_{\text{des}} = \text{Inlet T} - 273; \quad \text{\%Celsius}
\]
\[
[\text{sel_ads,AA CO2_ads,AA N2_ads}] = \text{selectivityIP4}(T_{\text{ads}}, P_{\text{ads}} \text{ kPa}); \quad \text{\%programmed in function with 15\% CO2 and some input P in kPa}
\]
\[
% \text{purity_ads} = AA CO2_ads / (AA CO2_ads + AA N2_ads);
\]
\[
[\text{sel_des,AA CO2_des,AA N2_des}] = \text{selectivityIP3}(T_{\text{des}}, P_{\text{des}} \text{ kPa, purity_ads}); \quad \text{\%programmed with}
\]
\[
[\text{sel_des,AA CO2_des,AA N2_des}] = \text{selectivityIP4}(T_{\text{des}}, P_{\text{des}} \text{ kPa}); \quad \text{\%programmed with}
\]
\[
\text{Net CO2} = AA CO2_ads - AA CO2_des; \quad \text{\%net CO2 captured (mol/kg AC)}
\]
\[
% \text{Deliverables/Outputs}
\]
\[
\text{kg AC} = t_{\text{ads}} \times \text{CO2 molar_flow_cap} / \text{Net CO2}; \quad \text{\%Mass of AC needed for capture (kg)}
\]
\[
V_{\text{AC}} = \text{kg AC/Rho AC}; \quad \text{\%volume of AC in m}^3
\]
\[
V_{\text{bed}} = V_{\text{AC}} / (1-e_b); \quad \text{\%volume of bed in m}^3
\]
\[
D_{\text{bed}} = (V_{\text{bed}} \times 4 / 2 \pi)^{(1/3)};
\]
\[
h_{\text{bed}} = D_{\text{bed}} \times 2;
\]
\[
% \text{disp([''The diameter of the bed is '', num2str(D_{\text{bed}}), ' m'])}
\]
\[
% \text{disp([''The height of the bed is '', num2str(h_{\text{bed}}), ' m'])}
\]
% Size Determination of columns
% ASSUMPTIONS
% 1. Instant equilibrium
% 2. 24/7 operation
% 3. 2:1 aspect ratio (h to D)
% 4. 10 minute cycle time
% 5. 5 minutes adsorbing, 5 minutes desorbing
% 6. Ideal gas
% 7. Density of AC assumed from paper
% 8. For modeling purposes, used input P of 1.5 bar and desorption P of 0.5
% bar for amount captured
% 9. No N2 or H2O adsorbed
% 10. Isothermal
% 11. Bed porosity of 0.5

% Process constants
MMCO2 = 44.01/1000; % kg Co2/mol
R = 8.314; % ideal gas constant for SI units
Rho_AC = 984; % density of activated carbon, kg/m^3
epsilon_b = 0.5; % bed porosity

% INPUTS
CO2_capture_tons = 100; % CO2 capture per day in tons
CO2_capture_rate = 1; % Fraction of CO2 captured
Run_time_daily = 24; % hours of capture per day
Gas_in_fracCO2_2 = Purity_col1; % mole fraction CO2 in inlet flue gas stream
Inlet_P_2 = 1.3*10^5; % 1 bar inlet in Pa
Inlet_T = 303; % 30 Celsius in Kelvin for inlet
T_ads_min = 2; % minutes of adsorption
T_des_min = 2; % minutes of desorption

% Intermediates
CO2_capture_kg = CO2_capture_tons*1000; % CO2 capture per day in tons
CO2_molar_flow_daily = CO2_capture_kg/MMCO2; % daily moles of CO2 in (captured)
Op_time = Run_time_daily*3600; % seconds of operation daily
CO2_molar_flow_cap = CO2_molar_flow_daily/Op_time; % molar flow of CO2/s (captured)
CO2_molar_flow = CO2_molar_flow_cap/CO2_capture_rate; % molar flow of CO2/s (total)
Gas_molar_flow = CO2_molar_flow/Gas_in_fracCO2_2/CO2_capture_rate; % total molar flow rate of gas/s (total)
Volumetric_gas = Gas_molar_flow*R*Inlet_T/Inlet_P_2; % volumetric flow rate of gas (total)
t_ads = t_ads_min*60; % seconds of adsorption
t_des = t_des_min*60; % seconds of desorption

% Capture of CO2 (based on 1.5 bar adsorption, 0.5 bar desorption)
\[ P_{\text{ads\_2}} = 1.3; \quad \text{%bar} \]
\[ P_{\text{ads\_kPa\_2}} = P_{\text{ads\_2}} \times 100; \quad \text{%kPa} \]
\[ \text{PCC\_ads\_kPa\_2} = P_{\text{ads\_kPa\_2}} \times \text{Gas\_in\_fracCO2\_2}; \quad \text{%partial pressure CO2 in kPa} \]
\[ P_{\text{des\_2}} = P_{\text{des\_2}}; \quad \text{%bar} \]
\[ P_{\text{des\_kPa\_2}} = P_{\text{des\_2}} \times 100; \quad \text{%kPa} \]
\[ \text{PCC\_des\_kPa\_2} = P_{\text{des\_kPa\_2}} \times \text{Gas\_in\_fracCO2\_2}; \quad \text{%partial pressure CO2 in kPa (assume pure CO2)} \]

DOUBLE CHECK THIS DESORPTION THING

\[ T_{\text{ads}} = \text{Inlet\_T} - 273; \quad \text{%Celsius} \]
\[ T_{\text{des}} = \text{Inlet\_T} - 273; \quad \text{%Celsius} \]
\[ [\text{sel\_ads, AA\_CO2\_ads\_2, AA\_N2\_ads\_2}] = \text{selectivityIP5}(T_{\text{ads}}, P_{\text{ads\_kPa\_2}}, \text{Purity\_col1}); \]
\[ \text{%programmed in function with 15\% CO2 and some input P in kPa} \]
\[ \text{purity\_ads} = \frac{\text{AA\_CO2\_ads\_2}}{\text{AA\_CO2\_ads\_2} + \text{AA\_N2\_ads\_2}}; \]
\[ [\text{sel\_des, AA\_CO2\_des\_2, AA\_N2\_des\_2}] = \text{selectivityIP3}(T_{\text{des}}, P_{\text{des\_kPa}}, \text{purity\_ads}); \]
\[ \text{%programmed with} \]
\[ \text{Net\_CO2\_2} = \text{AA\_CO2\_ads\_2} - \text{AA\_CO2\_des\_2}; \quad \text{%net CO2 captured (mol/kg AC)} \]

\%Deliverables/Outputs
\[ \text{kg\_AC\_2} = \frac{\text{t\_ads} \times \text{CO2\_molar\_flow\_cap}}{\text{Net\_CO2\_2}}; \quad \text{%Mass of AC needed for capture (kg)} \]
\[ \text{V\_AC\_2} = \frac{\text{kg\_AC}}{\text{Rho\_AC}}; \quad \text{%volume of AC in m}^3 \]
\[ \text{V\_bed\_2} = \frac{\text{V\_AC}}{1 - \text{e\_b}}; \quad \text{%volume of bed in m}^3 \]
\[ \text{D\_bed\_2} = \left( \frac{\text{V\_bed\_2} \times 4/2}{\text{pi}} \right)^{1/3}; \]
\[ \text{h\_bed\_2} = D\_bed\_2 \times 2; \]
\[ \text{% disp([''The diameter of the bed is '', num2str(D\_bed\_2), ' m'])} \]
\[ \text{% disp([''The height of the bed is '', num2str(h\_bed\_2), ' m'])} \]
Column 1 Sizing Script with Bed Volumes Output

% Size Determination of columns
% ASSUMPTIONS
% 1. Instant equilibrium
% 2. 24/7 operation
% 3. 2:1 aspect ratio (h to D)
% 4. 10 minute cycle time
% 5. 5 minutes adsorbing, 5 minutes desorbing
% 6. Ideal gas
% 7. Density of AC assumed from paper
% 8. For modeling purposes, used input P of 1.5 bar and desorption P of 0.5 bar for amount captured
% 9. No N2 or H2O adsorbed
% 10. Isothermal
% 11. Bed porosity of 0.5

% Process constants
MMCO2 = 44.01/1000; % kg Co2/mol
R = 8.314; % Ideal gas constant for SI units
Rho_AC = 984; % Density of activated carbon, kg/m^3
e_b = 0.5; % Bed porosity

% INPUTS
CO2_capture_tons = 100; % CO2 capture per day in tons

% Assume venting off of 0.25, capture 100% of remaining
CO2_capture_rate = 1; % Fraction of CO2 captured

Run_time_daily = 24; % Hours of capture per day
Gas_in_fracCO2 = 0.15; % Mole fraction CO2 in inlet flue gas stream
Inlet_P = P_ads_1*10^5; % 1 bar inlet in Pa
Inlet_T = T_1+273; % T Kelvin for inlet

% Intermediates
CO2_capture_kg = CO2_capture_tons*1000; % CO2 capture per day in tons
CO2_molar_flow_daily = CO2_capture_kg/MMCO2; % Daily moles of CO2 in (captured)
Op_time = Run_time_daily*3600; % Seconds of operation daily
CO2_molar_flow_cap = CO2_molar_flow_daily/Op_time; % Molar flow of CO2/s (captured)
CO2_molar_flow = CO2_molar_flow_cap/CO2_capture_rate; % Molar flow of CO2/s (total)
Gas_molar_flow = CO2_molar_flow/Gas_in_fracCO2/CO2_capture_rate; % Total molar flow rate of gas/s (total)

Volumetric_gas = Gas_molar_flow*R*Inlet_T/Inlet_P; % Volumetric flow rate of gas (total)
t_ads = t_ads_min*60; % Seconds of adsorption

t_des = t_des_min*60; % Seconds of desorption

% Capture of CO2 (based on 1.5 bar adsorption, 0.5 bar desorption)
P_ads = P_ads_1; %bar
P_ads_kPa = P_ads*100; %kPa
PPC_ads_kPa = P_ads_kPa*Gas_in_fracCO2; %partial pressure CO2 in kPa
P_des = P_des_1; %bar
P_des_kPa = P_des*100; %kPa
PPC_des_kPa = P_des_kPa*Gas_in_fracCO2; %partial pressure CO2 in kPa (assume pure CO2)
%DOUBLE CHECK THIS DESORPTION THING
T_ads = Inlet_T-273; %Celsius
T_des = Inlet_T-273; %Celsius
[sel_ads,AA_CO2_ads,AA_N2_ads] = selectivityIP4(T_ads, P_ads_kPa); %programmed in function
%with 15% CO2 and some input P in kPa
%purity_ads = AA_CO2_ads/(AA_CO2_ads+AA_N2_ads);
[sel_des,AA_CO2_des,AA_N2_des] = selectivityIP3(T_des, P_des_kPa, purity_ads); %programmed with
[sel_des,AA_CO2_des,AA_N2_des] = selectivityIP4(T_des, P_des_kPa); %programmed with
Net_CO2 = AA_CO2_ads-AA_CO2_des; %net CO2 captured (mol/kg AC)

%Deliverables/Outputs
kg_AC = t_ads*CO2_molar_flow_cap/Net_CO2; %Mass of AC needed for capture (kg)
V_AC = kg_AC/Rho_AC; %volume of AC in m^3
V_bed = V_AC/(1-e_b); %volume of bed in m^3
D_bed = (V_bed*4/2/pi)^(1/3);
h_bed = D_bed*2;
disp(['The diameter of the bed is ', num2str(D_bed), ' m'])
disp(['The height of the bed is ', num2str(h_bed), ' m'])
Column 2 Sizing Script with Bed Volumes Output

% Size Determination of columns
% ASSUMPTIONS
% 1. Instant equilibrium
% 2. 24/7 operation
% 3. 2:1 aspect ratio (h to D)
% 4. 10 minute cycle time
% 5. 5 minutes adsorbing, 5 minutes desorbing
% 6. Ideal gas
% 7. Density of AC assumed from paper
% 8. For modeling purposes, used input P of 1.5 bar and desorption P of 0.5
% bar for amount captured
% 9. No N2 or H2O adsorbed
% 10. Isothermal
% 11. Bed porosity of 0.5

% Process constants
MMCO2 = 44.01/1000; % kg Co2/mol
R = 8.314; % ideal gas constant for SI units
Rho_AC = 984; % density of activated carbon, kg/m^3
e_b = 0.5; % bed porosity

% INPUTS
CO2_capture_tons = 100; % CO2 capture per day in tons

% Assume venting off of 0.25, capture 100% of remaining
CO2_capture_rate = 1; % fraction of CO2 captured

Run_time_daily = 24; % hours of capture per day
Gas_in_fracCO2_2 = Purity_col1; % mole fraction CO2 in inlet flue gas stream
Inlet_P_2 = P_ads_2*10^5; % 1 bar inlet in Pa
Inlet_T = T_2+273; % 30 Celsius in Kelvin for inlet
Gas_in_T_2 = T_2+273; % 30 Celsius in Kelvin for inlet
Gas_in_T_2 = T_2+273; % 30 Celsius in Kelvin for inlet
Gas_molar_flow = CO2_molar_flow/Gas_in_fracCO2_2/CO2_capture_rate; % total molar flow rate of gas/s (total)
Volumetric_gas = Gas_molar_flow*R*Inlet_T/Inlet_P_2; % volumetric flow rate of gas (total)

% Intermediates
CO2_capture_kg = CO2_capture_tons*1000; % CO2 capture per day in tons
CO2_molar_flow_daily = CO2_capture_kg/MMCO2; % daily moles of CO2 in (captured)
Op_time = Run_time_daily*3600; % seconds of operation daily
CO2_molar_flow_cap = CO2_molar_flow_daily/Op_time; % molar flow of CO2/s (captured)
CO2_molar_flow = CO2_molar_flow_cap/CO2_capture_rate; % molar flow of CO2/s (total)
Gas_molar_flow = CO2_molar_flow*Gas_in_fracCO2_2/CO2_capture_rate; % total molar flow rate of gas/s (total)
% Capture of CO2 (based on 1.5 bar adsorption, 0.5 bar desorption)
P_ads_2 = P_ads_2; % bar
P_ads_kPa_2 = P_ads_2*100; % kPa
PPC_ads_kPa_2 = P_ads_kPa_2*Gas_in_fracCO2_2; % partial pressure CO2 in kPa
P_des_2 = P_des_2; % bar
P_des_kPa_2 = P_des_2*100; % kPa
PPC_des_kPa_2 = P_des_kPa_2*Gas_in_fracCO2_2; % partial pressure CO2 in kPa (assume pure CO2)
% DOUBLE CHECK THIS DESORPTION THING
T_ads = Inlet_T-273; % Celsius
T_des = Inlet_T-273; % Celsius
[sel_ads,AA_CO2_ads_2,AA_N2_ads_2] = selectivityIP5(T_ads, P_ads_kPa_2,Purity_col1);
% programmed in function with 15% CO2 and some input P in kPa
purity_ads = AA_CO2_ads_2/(AA_CO2_ads_2+AA_N2_ads_2);
[sel_des,AA_CO2_des_2,AA_N2_des_2] = selectivityIP3(T_des, P_des_kPa_2, purity_ads); % programmed with
[sel_des,AA_CO2_des_2,AA_N2_des_2] = selectivityIP5(T_des, P_des_kPa_2,Purity_col1);
% programmed with
Net_CO2_2 = AA_CO2_ads_2-AA_CO2_des_2; % net CO2 captured (mol/kg AC)

% Deliverables/Outputs
kg_AC_2 = t_ads*CO2_molar_flow_cap/Net_CO2_2; % Mass of AC needed for capture (kg)
V_AC_2 = kg_AC/Rho_AC; % volume of AC in m^3
V_bed_2 = V_AC/(1-e_b); % volume of bed in m^3
D_bed_2 = (V_bed*4/2/pi)^(1/3);
h_bed_2 = D_bed_2;
disp(['The diameter of the bed is ', num2str(D_bed_2), ' m'])
disp(['The height of the bed is ', num2str(h_bed_2), ' m'])
Column 1 Sizing Script with Bed Volumes Output with no Display

% Size Determination of columns
% ASSUMPTIONS
% 1. Instant equilibrium
% 2. 24/7 operation
% 3. 2:1 aspect ratio (h to D)
% 4. 10 minute cycle time
% 5. 5 minutes adsorbing, 5 minutes desorbing
% 6. Ideal gas
% 7. Density of AC assumed from paper
% 8. For modeling purposes, used input P of 1.5 bar and desorption P of 0.5
% bar for amount captured
% 9. No N2 or H2O adsorbed
% 10. Isothermal
% 11. Bed porosity of 0.5

% Process constants
MMCO2 = 44.01/1000; % kg Co2/mol
R = 8.314; % ideal gas constant for SI units
Rho_AC = 984; % density of activated carbon, kg/m^3
e_b = 0.5; % bed porosity

% INPUTS
CO2_capture_tons = 100; % CO2 capture per day in tons

% Assume venting off of 0.25, capture 100% of remaining
CO2_capture_rate = 1; % Fraction of CO2 captured

Run_time_daily = 24; % hours of capture per day
Gas_in_fracCO2 = 0.15; % mole fraction CO2 in inlet flue gas stream
Inlet_P = P_ads_1*10^5; % 1 bar inlet in Pa
Inlet_T = T_1+273; % T Kelvin for inlet

% Intermediates
CO2_capture_kg = CO2_capture_tons*1000; % CO2 capture per day in tons
CO2_molar_flow_daily = CO2_capture_kg/MMCO2; % daily moles of CO2 in (captured)
Op_time = Run_time_daily*3600; % seconds of operation daily
CO2_molar_flow_cap = CO2_molar_flow_daily/Op_time; % molar flow of CO2/s (captured)
CO2_molar_flow = CO2_molar_flow_cap/CO2_capture_rate; % molar flow of CO2/s (total)
Gas_molar_flow = CO2_molar_flow/Gas_in_fracCO2/CO2_capture_rate; % total molar flow rate of gas/s (total)

Volumetric_gas = Gas_molar_flow*R*Inlet_T/Inlet_P; % volumetric flow rate of gas (total)
t_ads = t_ads_min*60; % seconds of adsorption
t_des = t_des_min * 60; % seconds of desorption

% Capture of CO2 (based on 1.5 bar adsorption, 0.5 bar desorption)
P_ads = P_ads_1; % bar
P_ads_kPa = P_ads * 100; % kPa
PPC_ads_kPa = P_ads_kPa * Gas_in_fracCO2; % partial pressure CO2 in kPa
P_des = P_des_1; % bar
P_des_kPa = P_des * 100; % kPa
PPC_des_kPa = P_des_kPa * Gas_in_fracCO2; % partial pressure CO2 in kPa (assume pure CO2)

% DOUBLE CHECK THIS DESORPTION THING
T_ads = Inlet_T - 273; % Celsius
T_des = Inlet_T - 273; % Celsius

[sel_ads, AA_CO2_ads, AA_N2_ads] = selectivityIP4(T_ads, P_ads_kPa); % programmed in function
with 15% CO2 and some input P in kPa
purity_ads = AA_CO2_ads / (AA_CO2_ads + AA_N2_ads);

[sel_des, AA_CO2_des, AA_N2_des] = selectivityIP3(T_des, P_des_kPa, purity_ads); % programmed with
Net_CO2 = AA_CO2_ads - AA_CO2_des; % net CO2 captured (mol/kg AC)

% Deliverables/Outputs
kg_AC = t_ads * CO2_molar_flow_cap / Net_CO2; % Mass of AC needed for capture (kg)
V_AC = kg_AC / Rho_AC; % volume of AC in m^3
V_bed = V_AC / (1 - e_b); % volume of bed in m^3
D_bed = (V_bed * 4 / (2 * pi))^(1/3);
h_bed = D_bed * 2;

% disp(['The diameter of the bed is ', num2str(D_bed), ' m'])
% disp(['The height of the bed is ', num2str(h_bed), ' m'])
Column 2 Sizing Script with Bed Volumes Output with no Display

% Size Determination of columns
% ASSUMPTIONS
% 1. Instant equilibrium
% 2. 24/7 operation
% 3. 2:1 aspect ratio (h to D)
% 4. 10 minute cycle time
% 5. 5 minutes adsorbing, 5 minutes desorbing
% 6. Ideal gas
% 7. Density of AC assumed from paper
% 8. For modeling purposes, used input P of 1.5 bar and desorption P of 0.5
% bar for amount captured
% 9. No N2 or H2O adsorbed
% 10. Isothermal
% 11. Bed porosity of 0.5

% Process constants
MMCO2 = 44.01/1000; % kg Co2/mol
R = 8.314; % ideal gas constant for SI units
Rho_AC = 984; % density of activated carbon, kg/m^3
e_b = 0.5; % bed porosity

% INPUTS
CO2_capture_tons = 100; % CO2 capture per day in tons

% Assume venting off of 0.25, capture 100% of remaining
CO2_capture_rate = 1; % Fraction of CO2 captured

Run_time_daily = 24; % hours of capture per day
Gas_in_fracCO2_2 = Purity_col1; % mole fraction CO2 in inlet flue gas stream
Inlet_P_2 = P_ads_2*10^5; % 1 bar inlet in Pa
Inlet_T = T_2 + 273; % 30 Celsius in Kelvin for inlet
Inlet_P_2 = P_ads_2*10^5; % 1 bar inlet in Pa
Inlet_T = T_2 + 273; % 30 Celsius in Kelvin for inlet

% Intermediates
CO2_capture_kg = CO2_capture_tons*1000; % CO2 capture per day in tons
CO2_molar_flow_daily = CO2_capture_kg/MMCO2; % daily moles of CO2 in (captured)
Op_time = Run_time_daily*3600; % seconds of operation daily
CO2_molar_flow_cap = CO2_molar_flow_daily/Op_time; % molar flow of CO2/s (captured)
CO2_molar_flow = CO2_molar_flow_cap/CO2_capture_rate; % molar flow of CO2/s (total)
Gas_molar_flow = CO2_molar_flow/Gas_in_fracCO2_2/CO2_capture_rate; % total molar flow rate of gas/s (total)
Volumetric_gas = Gas_molar_flow*R*Inlet_T/Inlet_P_2; % volumetric flow rate of gas (total)
t_ads = t_ads_min*60; % seconds of adsorption
t_des = t_des_min*60; %seconds of desorption

%Capture of CO2 (based on 1.5 bar adsorption, 0.5 bar desorption)
P_ads_2 = P_ads_2; %bar
P_ads_kPa_2 = P_ads_2*100; %kPa
PPC_ads_kPa_2 = P_ads_kPa_2*Gas_in_fracCO2_2; %partial pressure CO2 in kPa
P_des_2 = P_des_2; %bar
P_des_kPa_2 = P_des_2*100; %kPa
PPC_des_kPa_2 = P_des_kPa_2*Gas_in_fracCO2_2; %partial pressure CO2 in kPa (assume pure CO2)
%DOUBLE CHECK THIS DESORPTION THING
T_ads = Inlet_T-273; %Celsius
T_des = Inlet_T-273; %Celsius
 [sel_ads,AA_CO2_ads_2,AA_N2_ads_2] = selectivityIP5(T_ads, P_ads_kPa_2,Purity_col1);
%programmed in function with 15% CO2 and some input P in kPa
%purity_ads = AA_CO2_ads/(AA_CO2_ads+AA_N2_ads);
 [sel_des,AA_CO2_des,AA_N2_des] = selectivityIP3(T_des, P_des_kPa, purity_ads); %programmed with
 [sel_des,AA_CO2_des_2,AA_N2_des_2] = selectivityIP5(T_des, P_des_kPa_2,Purity_col1);
%programmed with
 Net_CO2_2 = AA_CO2_ads-AA_CO2_des; %net CO2 captured (mol/kg AC)

%Deliverables/Outputs
kg_AC_2 = t_ads*CO2_molar_flow_cap/Net_CO2_2; %Mass of AC needed for capture (kg)
V_AC_2 = kg_AC/Rho_AC; %volume of AC in m^3
V_bed_2 = V_AC/(1-e_b); %volume of bed in m^3
D_bed_2 = (V_bed*4/2/pi)^(1/3);
h_bed_2 = D_bed*2;
% disp(['The diameter of the bed is ', num2str(D_bed_2), ' m'])
% disp(['The height of the bed is ', num2str(h_bed_2), ' m'])
Column 1 Sizing Function

function [V_bed, V_AC, t_total] = Column_Size_f_input(e_b, t_adsorp, t_pressurization, T, P_ads, P_des)
%Input the porosity of the bed, the time in seconds of adsorption, pressurization.

% Size Determination of columns
% ASSUMPTIONS
% 1. Instant equilibrium
% 2. 24/7 operation
% 3. 2:1 aspect ratio (h to D)
% 4. 10 minute cycle time
% 5. 5 minutes adsorbing, 5 minutes desorbing
% 6. Ideal gas
% 7. Density of AC assumed from paper
% 8. For modeling purposes, used input P of 1.3 bar and desorption P of 0.6 bar for amount captured
% 9. No N2 or H2O adsorbed
% 10. Isothermal
% 11. Bed porosity of 0.5

%Process constants
MMCO2 = 44.01/1000; %kg Co2/mol
R = 8.314; %ideal gas constant for SI units
Rho_AC = 984; %density of activated carbon, kg/m^3
e_bed = e_b; %bed porosity

% INPUTS
CO2_capture_tons = 100; %CO2 capture per day in tons
%Assume venting off of 0.25, capture 100% of remaining
CO2_capture_rate = 1; %Fraction of CO2 captured
Run_time_daily = 24; %hours of capture per day
Gas_in_fracCO2 = 0.15; %mole fraction CO2 in inlet flue gas stream
Inlet_P = P_ads*10^5; %1 bar inlet in Pa
Inlet_T = T+273; %30 Celsius in Kelvin for inlet
% t_ads_min = 5; %minutes of adsorption
% t_des_min = 5; %minutes of desorption

%Intermediates
CO2_capture_kg = CO2_capture_tons*1000; %CO2 capture per day in tons
CO2_molar_flow_daily = CO2_capture_kg/MMCO2; %daily moles of CO2 in (captured)
Op_time = Run_time_daily*3600; %seconds of operation daily
CO2_molar_flow_cap = CO2_molar_flow_daily/Op_time; %molar flow of CO2/s (captured)
CO2_molar_flow = CO2_molar_flow_cap/CO2_capture_rate; %molar flow of CO2/s (total)
Gas_molar_flow = CO2_molar_flow/Gas_in_fracCO2/CO2_capture_rate; %total molar flow rate of gas/s (total)
Volumetric_gas = Gas_molar_flow*R*Inlet_T/Inlet_P; %volumetric flow rate of gas (total)
% t_ads = t_ads_min*60; %seconds of adsorption
t_ads = t_adsorp; %seconds of adsorption
t_pres = t_pressurization; %seconds of pressurization
T_des = t_des_min*60; %seconds of desorption

% Capture of CO2 (based on 1.5 bar adsorption, 0.5 bar desorption)
P_ads = P_ads; %bar
P_ads_kPa = P_ads*100; %kPa
PPC_ads_kPa = P_ads_kPa*Gas_in_fracCO2; %partial pressure CO2 in kPa
P_des = P_des; %bar
P_des_kPa = P_des*100; %kPa
PPC_des_kPa = P_des_kPa*Gas_in_fracCO2; %partial pressure CO2 in kPa (assume pure CO2)
% DOUBLE CHECK THIS DESORPTION THING
T_ads = Inlet_T-273; %Celsius
T_des = Inlet_T-273; %Celsius
[sel_ads,AA_CO2_ads,AA_N2_ads] = selectivityIP4(T_ads, P_ads_kPa); %programmed in function with 15% CO2 and some input P in kPa
%purity_ads = AA_CO2_ads/(AA_CO2_ads+AA_N2_ads);
[sel_des,AA_CO2_des,AA_N2_des] = selectivityIP3(T_des, P_des_kPa, purity_ads); %programmed with
[sel_des,AA_CO2_des,AA_N2_des] = selectivityIP4(T_des, P_des_kPa); %programmed with
Net_CO2 = AA_CO2_ads-AA_CO2_des; %net CO2 captured (mol/kg AC)

% Deliverables/Outputs
kg_AC = t_ads*CO2_molar_flow_cap/Net_CO2; %Mass of AC needed for capture (kg)
V_AC = kg_AC/Rho_AC; %volume of AC in m^3
V_bed = V_AC/(1-e_bed); %volume of bed in m^3
D_bed = (V_bed*4/2/pi)^(1/3);
h_bed = D_bed*2;
t_total = t_adsorp+t_pressurization;
% disp(['The diameter of the bed is ', num2str(D_bed), ' m'])
% disp(['The height of the bed is ', num2str(h_bed), ' m'])
% disp(num2str(t_total));
% disp(num2str(t_pres));
end
**Column 2 Sizing Function**

```matlab
function [V_bed_2, V_AC_2, t_total_2] = Column_Size_f_2(e_b, t_adsorp, t_pressurization, purity, P_des)

% Input the porosity of the bed, the time in seconds of adsorption,
% pressurization.

% Size Determination of columns
% ASSUMPTIONS
% 1. Instant equilibrium
% 2. 24/7 operation
% 3. 2:1 aspect ratio (h to D)
% 4. 10 minute cycle time
% 5. 5 minutes adsorbing, 5 minutes desorbing
% 6. Ideal gas
% 7. Density of AC assumed from paper
% 8. For modeling purposes, used input P of 1.5 bar and desorption P of 0.5
% bar for amount captured
% 9. No N2 or H2O adsorbed
% 10. Isothermal
% 11. Bed porosity of 0.5

% Process constants
MMCO2 = 44.01/1000; % kg Co2/mol
R = 8.314; % ideal gas constant for SI units
Rho_AC = 984; % density of activated carbon, kg/m^3
e_b = e_b; % bed porosity

% INPUTS
CO2_capture_tons = 100; % CO2 capture per day in tons

% Assume venting off of 0.25, capture 100% of remaining
CO2_capture_rate = 1; % Fraction of CO2 captured

Run_time_daily = 24; % hours of capture per day
Gas_in_fracCO2_2 = purity; % mole fraction CO2 in inlet flue gas stream
Inlet_P_2 = 1.3*10^5; % 1 bar inlet in Pa
Inlet_T = 303; % 30 Celsius in Kelvin for inlet
% t_ads_min = 5; % minutes of adsorption
% t_ads = t_adsorp; % seconds of adsorption
```
%Intermediates
CO2_molar_flow_daily = CO2_capture_kg/MMCO2; %daily moles of CO2 in (captured)
Op_time = Run_time_daily*3600; %seconds of operation daily
CO2_molar_flow_cap = CO2_molar_flow_daily/Op_time; %molar flow of CO2/s (captured)
Gas_molar_flows = CO2_molar_flow_cap/CO2_capture_rate; %total molar flow rate
of gas/s (total)
Volumetric_flow = CO2_molar_flow_daily*R*Inlet_T/Inlet_P_2; %volumetric flow rate of gas (total)
% t_ads = t_ads_min*60; %seconds of adsorption
%Capture of CO2 (based on 1.5 bar adsorption, 0.5 bar desorption)
P_ads_2 = 1.3; %bar
P_ads_kPa_2 = P_ads_2*100; %kPa
PPC_ads_kPa_2 = P_ads_kPa_2*Gas_in_fracCO2_2; %partial pressure CO2 in kPa
P_des_2 = P_des; %bar
P_des_kPa_2 = P_des_2*100; %kPa
PPC_des_kPa_2 = P_des_kPa_2*Gas_in_fracCO2_2; %partial pressure CO2 in kPa (assume pure
CO2)
%DOUBLE CHECK THIS DESORPTION THING
T_ads = Inlet_T-273; %Celsius
[sel_ads,AA_CO2_ads_2,AA_N2_ads_2] = selectivityIP5(T_ads, P_ads_kPa_2,purity); %programmed
in function with 15% CO2 and some input P in kPa
%purity_ads = AA_CO2_ads/(AA_CO2_ads+AA_N2_ads);
[sel_des,AA_CO2_des,AA_N2_des] = selectivityIP3(T_des, P_des_kPa, purity_ads); %programmed
with
Net_CO2_2 = AA_CO2_ads_2-AA_CO2_des_2; %net CO2 captured (mol/kg AC)
%Deliverables/Outputs
kg_AC_2 = t_ads*CO2_molar_flow_cap/Net_CO2_2; %Mass of AC needed for capture (kg)
V_AC_2 = kg_AC_2/Rho_AC; %volume of AC in m^3
V_bed_2 = V_AC_2/(1-e_b); %volume of bed in m^3
D_bed_2 = (V_bed_2*4/2/pi)^(1/3);
h_bed_2 = D_bed_2*2;
t_total_2 = t_ads+t_pressurization;
end
Column 1 Sizing Function with Bed Volumes Output

function [V_bed, V_AC, t_total] = Column_Size_f_input(e_b, t_adsorp, t_pressurization, T, P_ads, P_des)

% Input the porosity of the bed, the time in seconds of adsorption, pressurization.

% Size Determination of columns
% ASSUMPTIONS
% 1. Instant equilibrium
% 2. 24/7 operation
% 3. 2:1 aspect ratio (h to D)
% 4. 10 minute cycle time
% 5. 5 minutes adsorbing, 5 minutes desorbing
% 6. Ideal gas
% 7. Density of AC assumed from paper
% 8. For modeling purposes, used input P of 1.3 bar and desorption P of 0.6 bar for amount captured
% 9. No N2 or H2O adsorbed
% 10. Isothermal
% 11. Bed porosity of 0.5

% Process constants
MMCO2 = 44.01/1000; % kg Co2/mol
R = 8.314; % ideal gas constant for SI units
Rho_AC = 984; % density of activated carbon, kg/m^3
e_bed = e_b; % bed porosity

% INPUTS
CO2_capture_tons = 100; % CO2 capture per day in tons

% Assume venting off of 0.25, capture 100% of remaining
CO2_capture_rate = 1; % Fraction of CO2 captured

Run_time_daily = 24; % hours of capture per day
Gas_in_fracCO2 = 0.15; % mole fraction CO2 in inlet flue gas stream
Inlet_P = P_ads * 10^5; % 1 bar inlet in Pa
Inlet_T = T+273; %30 Celsius in Kelvin for inlet
% t_ads_min = 5; %minutes of adsorption
t_des_min = 5; %minutes of desorption

%Intermediates
CO2_capture_kg = CO2_capture_tons*1000; %CO2 capture per day in tons
CO2_molar_flow_daily = CO2_capture_kg/MMCO2; %daily moles of CO2 in (captured)
Op_time = Run_time_daily*3600; %seconds of operation daily
CO2_molar_flow_cap = CO2_molar_flow_daily/Op_time; %molar flow of CO2/s (captured)
CO2_molar_flow = CO2_molar_flow_cap/CO2_capture_rate; %molar flow of CO2/s (total)
Gas_molar_flow = CO2_molar_flow/Gas_in_fracCO2/CO2_capture_rate; %total molar flow rate of
gas/s (total)
Volumetric_gas = Gas_molar_flow*R*Inlet_T/Inlet_P; %volumetric flow rate of gas (total)
% t_ads = t_ads_min*60; %seconds of adsorption
t_ads = t_adsorp; %seconds of adsorption
% t_pres = t_pressurization; %seconds of pressurization
t_des = t_des_min*60; %seconds of desorption

%Capture of CO2 (based on 1.5 bar adsorption, 0.5 bar desorption)
P_ads = P_ads; %bar
P_ads_kPa = P_ads*100; %kPa
PPC_ads_kPa = P_ads_kPa*Gas_in_fracCO2; %partial pressure CO2 in kPa
P_des = P_des; %bar
P_des_kPa = P_des_kPa*100; %kPa
PPC_des_kPa = P_des_kPa*Gas_in_fracCO2; %partial pressure CO2 in kPa (assume pure CO2)
%DOUBLE CHECK THIS DESORPTION THING
T_ads = Inlet_T-273; %Celsius
T_des = Inlet_T-273; %Celsius
[sel_ads,AA_CO2_ads,AA_N2_ads] = selectivityIP4(T_ads, P_ads_kPa); %programmed in function with 15% CO2 and some input P in kPa
%purity_ads = AA_CO2_ads/(AA_CO2_ads+AA_N2_ads);
[sel_des,AA_CO2_des,AA_N2_des] = selectivityIP3(T_des, P_des_kPa, purity_ads); %programmed with
[sel_des,AA_CO2_des,AA_N2_des] = selectivityIP4(T_des, P_des_kPa); %programmed with
Net_CO2 = AA_CO2_ads-AA_CO2_des; %net CO2 captured (mol/kg AC)

%Deliverables/Outputs
kg_AC = t_ads*CO2_molar_flow_cap/Net_CO2; %Mass of AC needed for capture (kg)
V_AC = kg_AC/Rho_AC; %volume of AC in m^3
V_bed = V_AC/(1-e_bed); %volume of bed in m^3
D_bed = (V_bed*4/2/pi)^(1/3);
h_bed = D_bed*2;
t_total = t_adsorp+t_pressurization;
% disp(['The diameter of the bed is ', num2str(D_bed), ' m']);
% disp(['The height of the bed is ', num2str(h_bed), ' m']);
% disp([num2str(t_total)]);
% disp([num2str(t_pres)]);
end
Column 2 Sizing Function with Bed Volumes Output

function [V_bed_2, V_AC_2, t_total_2] = Column_Size_f_2_input(e_b, t_adsorp, t_pressurization, purity, T, P_ads, P_des)
%Input the porosity of the bed, the time in seconds of adsorption, pressurization.

% Size Determination of columns
% ASSUMPTIONS
% 1. Instant equilibrium
% 2. 24/7 operation
% 3. 2:1 aspect ratio (h to D)
% 4. 10 minute cycle time
% 5. 5 minutes adsorbing, 5 minutes desorbing
% 6. Ideal gas
% 7. Density of AC assumed from paper
% 8. For modeling purposes, used input P of 1.5 bar and desorption P of 0.5
% bar for amount captured
% 9. No N2 or H2O adsorbed
% 10. Isothermal
% 11. Bed porosity of 0.5

%Process constants
MMCO2 = 44.01/1000; %kg Co2/mol
R = 8.314; %ideal gas constant for SI units
Rho_AC = 984; %density of activated carbon, kg/m^3
e_b = e_b; %bed porosity

% INPUTS
CO2_capture_tons = 100; %CO2 capture per day in tons

%Assume venting off of 0.25, capture 100% of remaining
CO2_capture_rate = 1; %Fraction of CO2 captured

Run_time_daily = 24; %hours of capture per day
Gas_in_fracCO2_2 = purity; % mole fraction CO2 in inlet flue gas stream
Inlet_P_2 = P_ads*10^5; % 1 bar inlet in Pa
Inlet_T = T+273; % 30 Celsius in Kelvin for inlet
% t_ads_min = 5; % minutes of adsorption
% t_ads = t_ads_min; % seconds of adsorption
% t_pres_2 = t_pressurization; % seconds of pressurization
% t_des_min = 2; % minutes of desorption

% Intermediates
CO2_capture_kg = CO2_capture_tons*1000; % CO2 capture per day in tons
CO2_molar_flow_daily = CO2_capture_kg/MMCO2; % daily moles of CO2 in (captured)
Op_time = Run_time_daily*3600; % seconds of operation daily
CO2_molar_flow_cap = CO2_molar_flow_daily/Op_time; % molar flow of CO2/s (captured)
CO2_molar_flow = CO2_molar_flow_cap/CO2_capture_rate; % molar flow of CO2/s (total)
Gas_molar_flow = CO2_molar_flow/Gas_in_fracCO2_2/CO2_capture_rate; % total molar flow rate of gas/s (total)
Volumetric_gas = Gas_molar_flow*R*Inlet_T/Inlet_P_2; % volumetric flow rate of gas (total)
% t_ads = t_ads_min*60; % seconds of adsorption
% t_des = t_des_min*60; % seconds of desorption

% Capture of CO2 (based on 1.5 bar adsorption, 0.5 bar desorption)
P_ads_2 = P_ads; % bar
P_ads_kPa_2 = P_ads_2*100; % kPa
PPC_ads_kPa_2 = P_ads_kPa_2*Gas_in_fracCO2_2; % partial pressure CO2 in kPa
P_des_2 = P_des; % bar
P.des_kPa_2 = P_des_2*100; % kPa
PPC_des_kPa_2 = P_des_kPa_2*Gas_in_fracCO2_2; % partial pressure CO2 in kPa (assume pure CO2)
% DOUBLE CHECK THIS DESORPTION THING
T_ads = Inlet_T-273; % Celsius
T_des = Inlet_T-273; % Celsius
[sel_ads,AA_CO2_ads_2,AA_N2_ads_2] = selectivityIP5(T_ads, P_ads_kPa_2,purity); % programmed in function with 15% CO2 and some input P in kPa
%purity_ads = AA_CO2_ads/(AA_CO2_ads+AA_N2_ads);
%[sel_des,AA_CO2_des,AA_N2_des] = selectivityIP3(T_des, P_des_kPa, purity_ads); % programmed with
%[sel_des,AA_CO2_des_2,AA_N2_des_2] = selectivityIP5(T_des, P_des_kPa_2,purity); % programmed with
Net_CO2_2 = AA_CO2_ads_2-AA_CO2_des_2; % net CO2 captured (mol/kg AC)

% Deliverables/Outputs
kg_AC_2 = t_ads*CO2_molar_flow_cap/Net_CO2_2; % Mass of AC needed for capture (kg)
V_AC_2 = kg_AC_2/Rho_AC; % Volume of AC in m^3
V_bed_2 = V_AC_2/(1-e_b); % Volume of bed in m^3
D.bed_2 = (V.bed_2*4/2/pi)^(1/3);
h.bed_2 = D.bed_2*2;
t_total_2 = t_ads+t_pressurization;
% disp(['The diameter of the bed is ', num2str(D.bed), ', m']);
% disp(['The height of the bed is ', num2str(h.bed), ', m']);
% disp(num2str(t_total));
% disp(num2str(t_press));
end
function [V_bed, V_AC, t_total, kg_AC, D_bed, h_bed] = Column_Size_f_print(e_b, t_adsorp, t_pressurization)

% Input the porosity of the bed, the time in seconds of adsorption, pressurization.

% Size Determination of columns
% ASSUMPTIONS
% 1. Instant equilibrium
% 2. 24/7 operation
% 3. 2:1 aspect ratio (h to D)
% 4. 10 minute cycle time
% 5. 5 minutes adsorbing, 5 minutes desorbing
% 6. Ideal gas
% 7. Density of AC assumed from paper
% 8. For modeling purposes, used input P of 1.5 bar and desorption P of 0.5 bar for amount captured
% 9. No N2 or H2O adsorbed
% 10. Isothermal
% 11. Bed porosity of 0.5

% Process constants
MMCO2 = 44.01/1000; % kg Co2/mol
R = 8.314; % ideal gas constant for SI units
Rho_AC = 984; % density of activated carbon, kg/m^3
e_bed = e_b; % bed porosity

% INPUTS
CO2_capture_tons = 100; % CO2 capture per day in tons

% Assume venting off of 0.25, capture 100% of remaining
CO2_capture_rate = 1; %Fraction of CO2 captured

Run_time_daily = 24; %hours of capture per day
Gas_in_fracCO2 = 0.15; %mole fraction CO2 in inlet flue gas stream
Inlet_P = 1.3*10^5; % bar inlet in Pa
Inlet_T = 303; %30 Celsius in Kelvin for inlet
% t_ads_min = 5; %minutes of adsorption
t_des_min = 5; %minutes of desorption

%Intermediates
CO2_capture_kg = CO2_capture_tons*1000; %CO2 capture per day in tons
CO2_molar_flow_daily = CO2_capture_kg/MMCO2; %daily moles of CO2 in (captured)
Op_time = Run_time_daily*3600; %seconds of operation daily
CO2_molar_flow_cap = CO2_molar_flow_daily/Op_time; %molar flow of CO2/s (captured)
CO2_molar_flow = CO2_molar_flow_cap/CO2_capture_rate; %molar flow of CO2/s (total)
Gas_molar_flow = CO2_molar_flow/Gas_in_fracCO2/CO2_capture_rate; %total molar flow rate of gas/s (total)
Volumetric_gas = Gas_molar_flow*R*Inlet_T/Inlet_P; %volumetric flow rate of gas (total)
% t_ads = t_ads_min*60; %seconds of adsorption
x_ads = t_adsorp; %seconds of adsorption
x_pres = t_pressurization; %seconds of pressurization
x_des = t_des_min*60; %seconds of desorption

%Capture of CO2 (based on 1.5 bar adsorption, 0.5 bar desorption)
P_ads = 1.3; %bar
P_ads_kPa = P_ads*100; %kPa
PPC_ads_kPa = P_ads_kPa*Gas_in_fracCO2; %partial pressure CO2 in kPa
P_des = 0.6; %bar
P_des_kPa = P_des*100; %kPa
PPC_des_kPa = P_des_kPa*Gas_in_fracCO2; %partial pressure CO2 in kPa (assume pure CO2)

%DOUBLE CHECK THIS DESORPTION THING
T_ads = Inlet_T-273; %Celsius
T_des = Inlet_T-273; %Celsius
[sel_ads,AA_CO2_ads,AA_N2_ads] = selectivityIP4(T_ads, P_ads_kPa); %programmed in function with 15% CO2 and some input P in kPa
%purity_ads = AA_CO2_ads/(AA_CO2_ads+AA_N2_ads);
[sel_des,AA_CO2_des,AA_N2_des] = selectivityIP4(T_des, P_des_kPa, purity_ads); %programmed with
[sel_des,AA_CO2_des,AA_N2_des] = selectivityIP3(T_des, P_des_kPa); %programmed with
Net_CO2 = AA_CO2_ads-AA_CO2_des; %net CO2 captured (mol/kg AC)

%Deliverables/Outputs
kg_AC = t_ads*CO2_molar_flow_cap/Net_CO2; %Mass of AC needed for capture (kg)
V_AC = kg_AC/Rho_AC; %volume of AC in m^3
V_bed = V_AC/(1-e_bed); %volume of bed in m^3
D_bed = (V_bed*4/2/pi)^(1/3);
h_bed = D_bed*2;
T_total = t_adsorp+T_pressurization;
disp(['The diameter of the bed is ', num2str(D_bed), ' m']);
disp(['The height of the bed is ', num2str(h_bed), ' m']);
disp(['The total adsorption time of the bed is ', num2str(t_total), ' s']);
disp(['The total pressurization time of the bed is ', num2str(t_pres), ' s']);
end
Column 2 Sizing Function with Bed Variables Output with Display

function [V_bed_2, V_AC_2, t_total_2, kg_AC_2, D_bed_2, h_bed_2] = Column_Size_f_print_2(e_b, t_adsorp, t_pressurization, purity, P_des)
%Input the porosity of the bed, the time in seconds of adsorption, pressurization.

% Size Determination of columns
% ASSUMPTIONS
% 1. Instant equilibrium
% 2. 24/7 operation
% 3. 2:1 aspect ratio (h to D)
% 4. 10 minute cycle time
% 5. 5 minutes adsorbing, 5 minutes desorbing
% 6. Ideal gas
% 7. Density of AC assumed from paper
% 8. For modeling purposes, used input P of 1.5 bar and desorption P of 0.5 bar for amount captured
% 9. No N2 or H2O adsorbed
% 10. Isothermal
% 11. Bed porosity of 0.5

%Process constants
MMCO2 = 44.01/1000; %kg Co2/mol
R = 8.314; %ideal gas constant for SI units
Rho_AC = 984; %density of activated carbon, kg/m^3
e_b = e_b; %bed porosity

% INPUTS
CO2_capture_tons = 100; %CO2 capture per day in tons

%Assume venting off of 0.25, capture 100% of remaining
CO2_capture_rate = 1; %Fraction of CO2 captured

Run_time_daily = 24; %hours of capture per day
Gas_in_fracCO2_2 = purity; %mole fraction CO2 in inlet flue gas stream
Inlet_P_2 = 1.3*10^5; %1 bar inlet in Pa
Inlet_T = 303; %30 Celsius in Kelvin for inlet
% t_ads_min = 5; %minutes of adsorption
t_des_min = 2; %minutes of desorption

%Intermediates
CO2_capture_kg = CO2_capture_tons*1000; %CO2 capture per day in tons
CO2_molar_flow_daily = CO2_capture_kg/MMCO2; %daily moles of CO2 in (captured)
Op_time = Run_time_daily*3600; %seconds of operation daily
CO2_molar_flow_cap = CO2_molar_flow_daily/Op_time; %molar flow of CO2/s (captured)
CO2_molar_flow = CO2_molar_flow_cap/CO2_capture_rate; %molar flow of CO2/s (total)
Gas_molar_flow = CO2_molar_flow/Gas_in_fracCO2_2/CO2_capture_rate; %total molar flow rate of gas/s (total)
Volumetric_gas = Gas_molar_flow*R*Inlet_T/Inlet_P_2; %volumetric flow rate of gas (total)
% t_ads = t_ads_min*60; %seconds of adsorption
t_ads = t_adsorp; %seconds of adsorption
t_pres_2=t_pressurization; %seconds of pressurization
%Capture of CO2 (based on 1.5 bar adsorption, 0.5 bar desorption)
P_ads_2 = 1.3; %bar
P_ads_kPa_2 = P_ads_2*100; %kPa
PFC_ads_kPa_2 = P_ads_kPa_2*Gas_in_fracCO2_2; %partial pressure CO2 in kPa
P_des_2 = P_des; %bar
P_des_kPa_2 = P_des_2*100; %kPa
PFC_des_kPa_2 = P_des_kPa_2*Gas_in_fracCO2_2; %partial pressure CO2 in kPa (assume pure CO2)
%DOUBLE CHECK THIS DESORPTION THING
T_ads = Inlet_T-273; %Celsius
T_des = Inlet_T-273; %Celsius
[sel_ads,AA_CO2_ads_2,AA_N2_ads_2] = selectivityIP5(T_ads, P_ads_kPa_2,purity); %programmed in function with 15% CO2 and some input P in kPa
%purity_ads = AA_CO2_ads/(AA_CO2_ads+AA_N2_ads);
[sel_des,AA_CO2_des,AA_N2_des] = selectivityIP3(T_des, P_des_kPa, purity_ads); %programmed with
[sel_des,AA_CO2_des_2,AA_N2_des_2] = selectivityIP5(T_des, P_des_kPa_2,purity); %programmed with
Net_CO2_2 = AA_CO2_ads_2-AA_CO2_des_2; %net CO2 captured (mol/kg AC)

%Deliverables/Outputs
kg_AC_2 = t_ads*CO2_molar_flow_cap/Net_CO2_2; %Mass of AC needed for capture (kg)
V_AC_2 = kg_AC_2/Rho_AC; %volume of AC in m^3
V_bed_2 = V_AC_2/(1-e_b); %volume of bed in m^3
D_bed_2 = (V_bed_2*4/2/pi)^(1/3);
h_bed_2 = D_bed_2*2;
t_total_2 = t_adsorp+t_pressurization;
disp(['The diameter of the bed is ', num2str(D_bed_2), ' m']);
disp(['The height of the bed is ', num2str(h_bed_2), ' m']);
disp(['The total adsorption time of the bed is ', num2str(t_total_2), ' s']);
disp(['The total pressurization time of the bed is ', num2str(t_pres_2), ' s']);
end
Column 1 Sizing Function with Bed Variables Output with no Display

function [V_bed, V_AC, t_total, kg_AC, D_bed, h_bed] = Column_Size_f_print_input(e_b, t_adsorp, t_pressurization, T, P_ads, P_des)
%Input the porosity of the bed, the time in seconds of adsorption, pressurization.

% Size Determination of columns
% ASSUMPTIONS
% 1. Instant equilibrium
% 2. 24/7 operation
% 3. 2:1 aspect ratio (h to D)
% 4. 10 minute cycle time
% 5. 5 minutes adsorbing, 5 minutes desorbing
% 6. Ideal gas
% 7. Density of AC assumed from paper
% 8. For modeling purposes, used input P of 1.5 bar and desorption P of 0.5
% bar for amount captured
% 9. No N2 or H2O adsorbed
% 10. Isothermal
% 11. Bed porosity of 0.5

%Process constants
MMCO2 = 44.01/1000; %kg Co2/mol
R = 8.314; %ideal gas constant for SI units
Rho_AC = 984; %density of activated carbon, kg/m^3
e_bed = e_b; % bed porosity

% INPUTS
CO2_capture_tons = 100; % CO2 capture per day in tons
Assume venting off of 0.25, capture 100% of remaining
CO2_capture_rate = 1; % fraction of CO2 captured

Run_time_daily = 24; % hours of capture per day
Gas_in_fracCO2 = 0.15; % mole fraction CO2 in inlet flue gas stream
Inlet_P = P_ads*10^5; % 1 bar inlet in Pa
Inlet_T = T+273; % 30 Celsius in Kelvin for inlet
% t_ads_min = 5; % minutes of adsorption
t_des_min = 5; % minutes of desorption

% Intermediates
CO2_capture_kg = CO2_capture_tons*1000; % CO2 capture per day in tons
CO2_molar_flow_daily = CO2_capture_kg/MMCO2; % daily moles of CO2 in (captured)
Op_time = Run_time_daily*3600; % seconds of operation daily
CO2_molar_flow_cap = CO2_molar_flow_daily/Op_time; % molar flow of CO2/s (captured)
CO2_molar_flow = CO2_molar_flow_cap/CO2_capture_rate; % molar flow of CO2/s (total)
Gas_molar_flow = CO2_molar_flow/Gas_in_fracCO2/CO2_capture_rate; % total molar flow rate of gas/s (total)
Volumetric_gas = Gas_molar_flow*R*Inlet_T/Inlet_P; % volumetric flow rate of gas (total)
% t_ads = t_ads_min*60; % seconds of adsorption
% t_pres = t_pressurization; % seconds of pressurization
% t_des = t_des_min*60; % seconds of desorption

% Capture of CO2 (based on 1.5 bar adsorption, 0.5 bar desorption)
P_ads = P_ads; % bar
P_ads_kPa = P_ads*100; % kPa
PPC_ads_kPa = P_ads_kPa*Gas_in_fracCO2; % partial pressure CO2 in kPa
P_des = P_des; % bar
P_des_kPa = P_des*100; % kPa
PPC_des_kPa = P_des_kPa*Gas_in_fracCO2; % partial pressure CO2 in kPa (assume pure CO2)

% DOUBLE CHECK THIS DESORPTION THING
T_ads = Inlet_T-273; % Celsius
T_des = Inlet_T-273; % Celsius
[sel_ads, AA_CO2_ads, AA_N2_ads] = selectivityIP4(T_ads, P_ads_kPa); % programmed in function with 15% CO2 and some input P in kPa
purity_ads = AA_CO2_ads/(AA_CO2_ads+AA_N2_ads);

% [sel_des, AA_CO2_des, AA_N2_des] = selectivityIP3(T_des, P_des_kPa, purity_ads); % programmed with
% [sel_des, AA_CO2_des, AA_N2_des] = selectivityIP4(T_des, P_des_kPa); % programmed with
Net_CO2 = AA_CO2_ads-AA_CO2_des; % net CO2 captured (mol/kg AC)

% Deliverables/Outputs
kg_AC = t_ads*CO2_molar_flow_cap/Net_CO2; % Mass of AC needed for capture (kg)
V_AC = kg_AC/Rho_AC; % volume of AC in m^3
V_bed = V_AC/(1-e_bed); % volume of bed in m^3
D_bed = (V_bed*4/2/pi)^(1/3);

h_bed = D_bed*2;
t_total = t_ads+t_pressurization;
% disp(['The diameter of the bed is ', num2str(D_bed), ' m'])
% disp(['The height of the bed is ', num2str(h_bed), ' m'])
% disp(['The total adsorption time of the bed is ', num2str(t_total), ' s'])
% disp(['The total pressurization time of the bed is ', num2str(t_pres), ' s'])
Column 2 Sizing Function with Bed Variables Output with no Display

function [V_bed_2, V_AC_2, t_total_2, kg_AC_2, D_bed_2, h_bed_2] = Column_Size_f_print_2_input(e_b, t_adsorp, t_pressurization, purity, T, P_ads, P_des)
%Input the porosity of the bed, the time in seconds of adsorption, pressurization.

% Size Determination of columns
% ASSUMPTIONS
% 1. Instant equilibrium
% 2. 24/7 operation
% 3. 2:1 aspect ratio (h to D)
% 4. 10 minute cycle time
% 5. 5 minutes adsorbing, 5 minutes desorbing
% 6. Ideal gas
% 7. Density of AC assumed from paper
% 8. For modeling purposes, used input P of 1.5 bar and desorption P of 0.5 bar for amount captured
% 9. No N2 or H2O adsorbed
% 10. Isothermal
% 11. Bed porosity of 0.5
% Process constants
MMCO2 = 44.01/1000; % kg CO2/mol
R = 8.314; % ideal gas constant for SI units
Rho_AC = 984; % density of activated carbon, kg/m^3
e_b = e_b; % bed porosity

% INPUTS
CO2_capture_tons = 100; % CO2 capture per day in tons

% Assume venting off of 0.25, capture 100% of remaining
CO2_capture_rate = 1; % Fraction of CO2 captured

Run_time_daily = 24; % hours of capture per day
Gas_in_fracCO2_2 = purity; % mole fraction CO2 in inlet flue gas stream
Inlet_P_2 = P_ads*10^5; % 1 bar inlet in Pa
Inlet_T = T+273; % 30 Celsius in Kelvin for inlet
% t_ads_min = 5; % minutes of adsorption
% t_des_min = 2; % minutes of desorption

% Intermediates
CO2_capture_kg = CO2_capture_tons*1000; % CO2 capture per day in tons
CO2_molar_flow_daily = CO2_capture_kg/MMCO2; % daily moles of CO2 in (captured)
Op_time = Run_time_daily*3600; % seconds of operation daily
CO2_molar_flow_cap = CO2_molar_flow_daily/Op_time; % molar flow of CO2/s (captured)
CO2_molar_flow = CO2_molar_flow_cap/CO2_capture_rate; % molar flow of CO2/s (total)
Gas_molar_flow = CO2_molar_flow/Gas_in_fracCO2_2/CO2_capture_rate; % total molar flow rate of gas/s (total)
Volumetric_gas = Gas_molar_flow*R*Inlet_T/Inlet_P_2; % volumetric flow rate of gas (total)
% t_ads = t_ads_min*60; % seconds of adsorption
% t_des = t_des_min*60; % seconds of desorption

% Capture of CO2 (based on 1.5 bar adsorption, 0.5 bar desorption)
P_ads_2 = P_ads; % bar
PPC_ads_kPa_2 = P_ads_2*100; % kPa
P_des_2 = P_des; % bar
PPC_des_kPa_2 = P_des_2*100; % kPa

% DOUBLE CHECK THIS DESORPTION THING
T_ads = Inlet_T-273; % Celsius
T_des = Inlet_T-273; % Celsius
[sel_ads,AA_CO2_ads_2,AA_N2_ads_2] = selectivityIP5(T_ads, P_ads_kPa_2,purity); % programmed in function with 15% CO2 and some input P in kPa
% purity_ads = AA_CO2_ads/(AA_CO2_ads+AA_N2_ads);
% [sel_des,AA_CO2_des,AA_N2_des] = selectivityIP3(T_des, P_des_kPa, purity_ads); % programmed
% with
Net_CO2_2 = AA_CO2_ads_2-AA_CO2_des_2; % net CO2 captured (mol/kg AC)

% Deliverables/Outputs
kg_AC_2 = t_ads*CO2_molar_flow_cap/Net_CO2_2; % Mass of AC needed for capture (kg)
V_AC_2 = kg_AC_2/Rho_AC; % volume of AC in m^3
V_bed_2 = V_AC_2/(1-e_b); % volume of bed in m^3
D_bed_2 = (V_bed_2*4/2/pi)^(1/3);
h_bed_2 = D_bed_2*2;
t_total_2 = t_adsorp+t_pressurization;

% disp(['The diameter of the bed is ', num2str(D_bed_2), ' m'])
% disp(['The height of the bed is ', num2str(h_bed_2), ' m'])
% disp(['The total adsorption time of the bed is ', num2str(t_total_2), ' s'])
% disp(['The total pressurization time of the bed is ', num2str(t_pres_2), ' s'])
end

---

**Model Function**

```matlab
function [Volumetric_flow_1,Volumetric_flow_2,Volumetric_flow_3,D_bed_1,D_bed_2,
h_bed_1,h_bed_2,V_AC_1,V_AC_2] = model_function(T1,P_ads_1,P_des_1, T2,P_ads_2, P_des_2);

% simple equilibrium model

%% Constants
% MAKE SURE CONSTANTS LINE UP WITH SIZING MODEL
% Below is copy and pasted from Column_Size model (currently)

T_1 = T1; %degrees C

run Column_Size_Input_nodisp

Volumetric_flow_2_m3 = Volumetric_gas; %m3/s for 1.3 bar (into first column)
Volumetric_flow_1_m3 = Volumetric_gas*P_ads_1; %m3/s for 1.0 bar (into first blower)
[Volumetric_flow_1] = Volumetric_flow_1_m3*2118.88; %ft3/min
```
% Process constants
% MM CO2 = 44.01/1000; % kg Co2/mol
% R = 8.314; % ideal gas constant for SI units
% Rho AC = 984; % density of activated carbon, kg/m^3
% e_b = 0.5; % bed porosity
%
% Gas in frac CO2 = 0.15; % mole fraction CO2 in inlet flue gas stream
% Inlet P = 1.3*10^5; % 1.3 bar inlet in Pa
% Inlet T = 303; % 30 Celsius in Kelvin for inlet
%
% Gas molar flow
% Volumetric gas

%% Column 1 adsorption

% t_step = 0.1; % seconds
t_pres = 120; % seconds
t_initialization = 0:t_step:t_pres;
t_vector = 0:0.1:(t_ads);
v_step_total = t_step*Volumetric_gas; % volume of gas admitted per time step
n_step_total = t_step*Gas_molar_flow; % moles of gas admitted per time step

% Initialize variables
empty = zeros(1,length(t_vector));
empty_initialization = zeros(1,length(t_initialization));
P_initialization = empty_initialization;
N2_saturation = empty_initialization;
P_bed = empty;
moles_N2 = empty;
moles_CO2 = empty;
total_moles = moles_N2+moles_CO2;
Bed_frac_saturated = empty;

% Initial guess

[V_bed, V_AC, t_total] = Column_Size_f_input(0.5,200,100,T_1,P_ads_1,P_des_1);
V_bed_matrix = zeros(1,300);
t_pres_prev=zeros(1,11);
length(100:1:300);
t_total_matrix=zeros(201,10);
for k = 100:1:300;
    [V_bed, V_AC, t_total] = Column_Size_f_input(0.5,200,100,T_1,P_ads_1,P_des_1);
    for j = 1:10;
        t_pres_prev(1) = 100;
        % Pressure initialization
        % Initially assuming no pressure drop
        for i = 1:length(t_initialization);
            P_initialization(i) = n_step_total*i*R*Inlet_T/(V_bed - V_AC);
            if P_initialization(i) >= 130000;
                break
            end
        end
    end
    t_pres = i/t_step; % seconds
    t_pres_prev(j+1)=t_pres;
P_initialization = P_initialization(1:i);
\[
[V_{\text{bed}}, V_{\text{AC}}, t_{\text{total}}] = \text{Column\_Size\_f\_input}(0.5, \\
k, \{(t_{\text{pres}}+t_{\text{pres\_prev}}(j))/2, T_1, P_{\text{ads\_1}}, P_{\text{des\_1}}\}); \\
\text{t\_total\_matrix(k-99,j)=t\_total; if t\_total>=300 && t\_total<=305 break} \\
\text{end} \\
\text{end} \\
\text{if t\_total>=300 && t\_total<=305 break} \\
\text{end} \\
\text{end} \]

\[
t_{\text{pres}}=(t_{\text{pres}}+t_{\text{pres\_prev}}(j))/2; \\
[V_{\text{bed}}, V_{\text{AC\_1}}, t_{\text{total}}, kg_{\text{AC}}, D_{\text{bed}}, h_{\text{bed}}] = \text{Column\_Size\_f\_print\_input\_nodisp}(0.5, \\
k, t_{\text{pres}}, T_1, P_{\text{ads\_1}}, P_{\text{des\_1}}); \\
\]

% Approximation of bed pressure and number of moles during initialization 
% steps 
P_{\text{bed}(1,1:i)} = P_{\text{Initialization}}; 
\text{moles\_N2 = n\_step\_total*i*(1-Gas\_in\_frac\text{CO2});} 
\text{total\_moles = moles\_N2+moles\_CO2;}

% Amount CO2 adsorbed during initialization 
% ASSUMING 86% capture 
% without 86% capture, put rate into Column\_Size and use 
% CO2\_molar\_flow\_cap 
% Commented this out since it shouldn't be needed 
% CO2\_initialization = CO2\_molar\_flow\_cap*(t\_saturation+t\_pres); %moles CO2 
% Bed\_CO2\_capacity = kg\_AC*(Net\_CO2); %moles CO2 
% Bed\_distance\_saturated(1,i+t\_saturation/t\_step) = 
% CO2\_initialization/Bed\_CO2\_capacity*h\_bed; 

% Pseudo Steady-State Operation (after initialization) 
t\_saturation = Net\_CO2*kg\_AC/CO2\_molar\_flow\_cap; 
t\_total = t\_saturation+t\_pres; 

% Captured amount of CO2 and N2 
CO2\_ads = kg\_AC*AA\_CO2\_ads; %total moles of CO2 adsorbed 
N2\_ads = kg\_AC*AA\_N2\_ads; %total moles of CO2 adsorbed 

%% Column 1 Desorption 
% Desorption pressure: P\_des 
% Assumes lots of stuff, like 
% 1. Rapid depressurization (relatively) 
% 2. No equilibrium formation in the meantime during depressurization 
% 3. Gas removed only comes from AC effectively 
CO2\_working\_capacity = AA\_CO2\_ads - AA\_CO2\_des; 
CO2\_recovered = kg\_AC*(CO2\_working\_capacity); 
N2\_working\_capacity = AA\_N2\_ads - AA\_N2\_des; 
N2\_recovered = kg\_AC*(N2\_working\_capacity); 
Purity\_col1 = CO2\_recovered/(CO2\_recovered+N2\_recovered); 

% Desorption blower flow rates 
Volumetric\_flow\_2\_m3 = Volumetric\_flow\_1\_m3*Gas\_in\_frac\text{CO2}/Purity\_col1*1.0/P\_ads\_1; %m3/s 
into blower two (out of column 1) 
[Volumetric\_flow\_2] = Volumetric\_flow\_2\_m3*2118.88; %ft3/min
% This is the same flow rate into the third blower, but with a different
% pressure difference

%% Assign variables
[D_bed_1] = D_bed*3.28; %feet
[h_bed_1] = h_bed*3.28; %feet

%% Column 2
T_2 = T2; %degrees C
P_ads_2 = P_ads_2; %adsorption pressure in bar
P_des_2 = P_des_2; %desorption pressure in bar
Gas_in_fracCO2_2 = Purity_coll;
run Column_Size_2_input_nodisp
Volumetric_flow_into_2 = Volumetric_gas; %m3/s

t_step = 0.1; %seconds
t_pres = 120; %seconds
t_initialization = 0:t_step:t_pres;
t_vector = 0:0.1:(t_ads);
v_step_total_2 = t_step*Volumetric_gas; %volume of gas admitted per time step
n_step_total_2 = t_step*Gas_molar_flow; %moles of gas admitted per time step

%Initialize variables
empty = zeros(1,length(t_vector));
empty_initialization = zeros(1,length(t_initialization));
P_initialization = empty_initialization;
N2_saturation = empty_initialization;
P_bed = empty;
moles_N2 = empty;
moles_CO2 = empty;
total_moles = moles_N2+moles_CO2;
Bed_frac_saturated = empty;

%Initial guess
[V_bed_2, V_AC_2, t_total_2] = Column_Size_f_2_input(0.5,10,110,Purity_coll1,T_2,P_ads_2,P_des_2);
V_bed_matrix = zeros(1,300);
t_pres_prev=zeros(1,11);
length(10:1:120);
t_total_matrix=zeros(length(10:1:120),10);
for k = 10:1:120;
    [V_bed_2, V_AC_2, t_total_2] = Column_Size_f_2_input(0.5,10,110,Purity_coll1,T_2,P_ads_2,P_des_2);
    for j = 1:10;
        t_pres_prev(1) = 20;
        % Pressure initialization
        % Initially assuming no pressure drop
        for i = 1:length(t_initialization);
            P_initialization(i) = n_step_total_2*i*R*Inlet_T/(V_bed_2 - V_AC_2);
            if P_initialization(i) >= 130000;
                break
            end
        end
    end
end
end

t_pres_2 = i/t_step; %seconds
t_pres_prev(j+1)=t_pres_2 ;
P_initialization = P_initialization(1:i);

[V_bed_2, V_AC_2, t_total_2] = Column_Size_f_2_input(0.5,
k,(t_pres_2+t_pres_prev(j))/2,Purity_col1,T_2,P_ads_2,P_des_2);
t_total_matrix(k-9,j)=t_total_2;
if t_total_2>=120 && t_total_2<=125
  break
end
if t_total_2>=120 && t_total_2<=125
  break
end

t_pres_2=(t_pres_2+t_pres_prev(j))/2;
[V_bed_2, V_AC_2, t_total_2,kg_AC_2,D_bed_2,h_bed_2] =
Column_Size_f_print_2_input_nodisp(0.3, k,t_pres_2,Purity_col1,T_2,P_ads_2,P_des_2);

% Approximation of bed pressure and number of moles during initialization
% steps
P_bed(1,1:i) = P_initialization;
moles_N2_2 = n_step_total*i*(1-Gas_in_fracCO2_2);
total_moles = moles_N2_2+moles_CO2;

%Amount CO2 adsorbed during initialization
% ASSUMING 86% capture
% without 86% capture, put rate into Column_Size and use
% CO2_molar_flow_cap
%Commented this out since it shouldn't be needed

% CO2_initialization = CO2_molar_flow_cap*(t_saturation+t_pres); %moles CO2
% Bed_CO2_capacity = kg_AC*(Net_CO2); %moles CO2
% Bed_distance_saturated(1,i+t_saturation/t_step) =
CO2_initialization/Bed_CO2_capacity*h_bed;

% Pseudo Steady-State Operation (after initialization)
t_saturation_2 = Net_CO2_2*kg_AC_2/CO2_molar_flow_cap;
t_total_2 = t_saturation_2+t_pres_2;

%Captured amount of CO2 and N2
CO2_ads_2 = kg_AC_2*AA_CO2_ads_2; %total moles of CO2 adsorbed
N2_ads_2 = kg_AC_2*AA_N2_ads_2; %total moles of CO2 adsorbed

% Column 2 Desorption
% Desorption pressure: P_des
% Assumes lots of stuff, like
% 1. Rapid depressurization (relatively)
% 2. No equilibrium formation in the meantime during depressurization
% 3. Gas removed only comes from AC effectively
CO2_working_capacity_2 = AA_CO2_ads_2 - AA_CO2_des_2;
CO2_recovered_2 = kg_AC_2*(CO2_working_capacity_2);
N2_working_capacity_2 = AA_N2_ads_2 - AA_N2_des_2;
N2_recovered_2 = kg_AC_2*(N2_working_capacity_2);
Purity_col2 = CO2_recovered_2/(CO2_recovered_2+N2_recovered_2);
%disp(['The purity from column 2 is ' num2str(Purity_col2)]);

%% Volumetric Flow 3
Volumetric_flow_3_m3 = Volumetric_flow_2_m3*Purity_col1/Purity_col2*P_ads_1/P_ads_2; %m3/s
into blower two (out of column 1)
[Volumetric_flow_3] = Volumetric_flow_3_m3*2118.88; %ft3/min
%% Assign variables
[D_bed_2] = D_bed_2*3.28; %feet
[h_bed_2] = h_bed_2*3.28; %feet
End

---

**Purity Determination Function**

function [Purity_col2] = purity_function(T1,P_ads_1,P_des_1, T2,P_ads_2, P_des_2);

% simple equilibrium model

%% Constants
% MAKE SURE CONSTANTS LINE UP WITH SIZING MODEL
% Below is copy and pasted from Column_Size model (currently)
\[ T_1 = T_1; \] % degrees C
\[ P_{ads_1} = P_{ads_1}; \] % adsorption pressure in bar
\[ P_{des_1} = P_{des_1}; \] % desorption pressure in bar

run Column_Size_Input_nodisp

\begin{align*}
\text{Volumetric\_flow\_2\_m}\_3 &= \text{Volumetric\_gas}; \quad \text{\% m3/s for 1.3 bar (into first column)} \\
\text{Volumetric\_flow\_1\_m}\_3 &= \text{Volumetric\_gas}\cdot1/P_{ads_1}; \quad \text{\% m3/s for 1.0 bar (into first blower)} \\
[V\_\text{Volumetric\_flow\_1}] &= \text{Volumetric\_flow\_1\_m}\_3\cdot2118.88; \quad \text{\% ft3/min}
\end{align*}

% Process constants
\begin{align*}
\text{MMCO2} &= 44.01/1000; \quad \text{\% kg Co2/mol} \\
\text{R} &= 8.314; \quad \text{\% ideal gas constant for SI units} \\
\text{Rho\_AC} &= 984; \quad \text{\% density of activated carbon, kg/m}^3 \\
\text{e}\_b &= 0.5; \quad \text{\% bed porosity} \\
\text{Gas\_in\_fracCO2} &= 0.15; \quad \text{\% mole fraction CO2 in inlet flue gas stream} \\
\text{Inlet\_P} &= 1.3\cdot10^5; \quad \text{\% 1.3 bar inlet in Pa} \\
\text{Inlet\_T} &= 303; \quad \text{\% 30 Celsius in Kelvin for inlet}
\end{align*}

% Gas molar flow
% Volumetric_gas

%% Column 1 adsorption
\begin{align*}
t\_step &= 0.1; \quad \text{\% seconds} \\
t\_pres &= 120; \quad \text{\% seconds} \\
t\_initialization &= 0:t\_step:t\_pres; \\
t\_vector &= 0:0.1:(t\_ads); \\
v\_step\_total &= t\_step\cdot\text{Volumetric\_gas}; \quad \text{\% volume of gas admitted per time step} \\
n\_step\_total &= t\_step\cdot\text{Gas\_molar\_flow}; \quad \text{\% moles of gas admitted per time step}
\end{align*}

% Initialize variables
\begin{align*}
\text{empty} &= \text{zeros}(1,\text{length}(t\_vector)); \\
\text{empty\_initialization} &= \text{zeros}(1,\text{length}(t\_initialization));
\end{align*}

\begin{align*}
\text{P\_initialization} &= \text{empty\_initialization}; \\
\text{N2\_saturation} &= \text{empty\_initialization}; \\
\text{P\_Bed} &= \text{empty}; \\
\text{moles\_N2} &= \text{empty}; \\
\text{moles\_CO2} &= \text{empty}; \\
\text{total moles} &= \text{moles\_N2}+\text{moles\_CO2}; \\
\text{Bed\_frac\_saturated} &= \text{empty};
\end{align*}

% Initial guess
\begin{align*}
[V\_\text{Bed}, V\_\text{AC}, t\_\text{total}] &= \text{Column\_Size\_f\_input}(0.5,200,100,T\_1,P\_ads\_1,P\_des\_1); \\
\text{V\_Bed\_matrix} &= \text{Zeros}(1,300); \\
\text{t\_pres\_prev} &= \text{zeros}(1,11); \\
\text{length}(100:1:300); \\
\text{t\_total\_matrix} &= \text{zeros}(201,10); \\
\text{for} \ k &= 100:1:300; \\
[V\_\text{Bed}, V\_\text{AC}, t\_\text{total}] &= \text{Column\_Size\_f\_input}(0.5,200,100,T\_1,P\_ads\_1,P\_des\_1); \\
\text{for} \ j &= 1:10; \\
\text{t\_pres\_prev}(1) &= 100; \\
\text{Pressure\_initialization}; \\
\text{% Initially assuming no pressure drop} \\
\text{for} \ i &= 1:\text{length}(t\_initialization);
P_initialization(i) = n_step_total*i*R*Inlet_T/(V_bed - V_AC);
if P_initialization(i) >= 130000;
    break
end

t_pres = i/t_step; %seconds
t_pres_prev(j+1)=t_pres;
P_initialization = P_initialization(1:i);

[V_bed, V_AC, t_total] = Column_Size_f_input(0.5, k, (t_pres+t_pres_prev(j))/2, T_1, P_ads_1, P_des_1);
t_total_matrix(k-99,j)=t_total;
if t_total>=300 && t_total<=305
    break
end
if t_total>=300 && t_total<=305
    break
end
t_pres=(t_pres+t_pres_prev(j))/2;
[V_bed, V_AC, t_total, kg_AC, D_bed, h_bed] = Column_Size_f_print_input_nodisp(0.5, k, t_pres, T_1, P_ads_1, P_des_1);

% Approximation of bed pressure and number of moles during initialization
% steps
P_bed(1,1:i) = P_initialization;
moles_N2 = n_step_total*i*(1-Gas_in_fracCO2);
total_moles = moles_N2+moles_CO2;
%Amount CO2 adsorbed during initialization
% ASSUMING 86% capture
% without 86% capture, put rate into Column_Size and use
% CO2_molar_flow_cap

%Commented this out since it shouldn't be needed
% CO2_initialization = CO2_molar_flow_cap*(t_saturation+t_pres); %moles CO2
% Bed_CO2_capacity = kg_AC*(Net_CO2); %moles CO2
% Bed_distance_saturated(1,i+t_saturation/t_step) =
% CO2_initialization/Bed_CO2_capacity*h_bed;

% Pseudo Steady-State Operation (after initialization)
t_saturation = Net_CO2*kg_AC/CO2_molar_flow_cap;
t_total = t_saturation+t_pres;

%Captured amount of CO2 and N2
CO2_ads = kg_AC*AA_CO2_ads; %total moles of CO2 adsorbed
N2_ads = kg_AC*AA_N2_ads; %total moles of CO2 adsorbed

% Column 1 Desorption
% Desorption pressure: P_des
% Assumes lots of stuff, like
% 1. Rapid depressurization (relatively)
% 2. No equilibrium formation in the meantime during depressurization
% 3. Gas removed only comes from AC effectively
\[ \text{CO}_2\text{ working capacity} = \text{AA}_\text{CO}_2\text{ ads} - \text{AA}_\text{CO}_2\text{ des}; \]
\[ \text{CO}_2\text{ recovered} = \text{kg}_\text{AC}(\text{CO}_2\text{ working capacity}); \]
\[ \text{N}_2\text{ working capacity} = \text{AA}_\text{N}_2\text{ ads} - \text{AA}_\text{N}_2\text{ des}; \]
\[ \text{N}_2\text{ recovered} = \text{kg}_\text{AC}(\text{N}_2\text{ working capacity}); \]
\[ \text{Purity}_\text{col1} = \frac{\text{CO}_2\text{ recovered}}{\text{CO}_2\text{ recovered} + \text{N}_2\text{ recovered}}; \]

% Desorption blower flow rates
\[ \text{Volumetric flow}_2\text{ m}^3 = \text{Volumetric flow}_1\text{ m}^3 \times \text{Gas in frac CO}_2 \times \frac{\text{Purity}_\text{col1}}{1.0}; \] % m^3/s into blower two (out of column 1)
\[ [\text{Volumetric flow}_2] = \text{Volumetric flow}_2\text{ m}^3 \times 2118.88; \] % ft^3/min
% This is the same flow rate into the third blower, but with a different % pressure difference

%% Assign variables
[D_bed_1] = D_bed*3.28; % feet
[h_bed_1] = h_bed*3.28; % feet

%% Column 2
T_2 = T2; % degrees C
P_ads_2 = P_ads_2; % adsorption pressure in bar
P_des_2 = P_des_2; % desorption pressure in bar
Gas_in_fracCO2_2 = Purity_col1;

run Column_Size_2_input_nodisp

Volumetric_flow_into_2 = Volumetric_gas; % m^3/s

\[ t\text{ step} = 0.1; \] % seconds
\[ t\text{ pres} = 120; \] % seconds
\[ t\text{ initialization} = 0:0.1:(t\text{ ads}); \]
\[ \text{t vector} = 0:0.1:(t\text{ ads}); \]
\[ \text{v step total 2} = t\text{ step}\times\text{Volumetric gas}; \] % volume of gas admitted per time step
\[ \text{n step total 2} = t\text{ step}\times\text{Gas molar flow}; \] % moles of gas admitted per time step

% Initialize variables
empty = zeros(1,length(t_vector));
empty_initialization = zeros(1,length(t_initialization));

P_initialization = empty_initialization;
N2_saturation = empty_initialization;
P_bed = empty;
moles_N2 = empty;
moles_CO2 = empty;
total_moles = moles_N2+moles_CO2;
Bed_frac_saturated = empty;

% Initial guess
[V_bed_2, V_AC_2, t_total_2] =
Column_Size_2_input(0.5,10,110,Purity_col1,T_2,P_ads_2,P_des_2);
V_bed_matrix = zeros(1,300);
t_pres_prev=zeros(1,11);
length(10:1:120);
t_total_matrix=zeros(length(10:1:120),10);
for k = 10:1:120;

\[ [V_{\text{bed}2}, V_{\text{AC}2}, t_{\text{total}2}] = \text{Column\_Size\_f\_2\_input}(0.5, 10, 110, \text{Purity\_col1}, T_2, P_{\text{ads}2}, P_{\text{des}2}); \]

\begin{verbatim}
for j = 1:10;
    t_pres_prev(1) = 20;
    \% Pressure initialization
    \% Initially assuming no pressure drop
    for i = 1:length(t_initialization);
        P_initialization(i) = n_step_total_2*i*R*Inlet_T/(V_{\text{bed}2} - V_{\text{AC}2});
        if P_initialization(i) >= 130000;
            break
        end
    end
    t_pres_2 = i/t_step; \%seconds
    t_pres_prev(j+1)=t_pres_2;
    P_initialization = P_initialization(1:i);
    [V_{\text{bed}2}, V_{\text{AC}2}, t_{\text{total}2}] = Column\_Size\_f\_2\_input(0.5, k, (t_pres_2+t_pres_prev(j))/2, Purity\_col1, T_2, P_{\text{ads}2}, P_{\text{des}2});
    t_total_matrix(k-9,j)=t_{\text{total}2};
    if t_{\text{total}2}>=120 && t_{\text{total}2}<=125
        break
    end
end
if t_{\text{total}2}>=120 && t_{\text{total}2}<=125
    break
end
t_pres_2=(t_pres_2+t_pres_prev(j))/2;
[V_{\text{bed}2}, V_{\text{AC}2}, t_{\text{total}2}, kg\_AC_2, D_{\text{bed}2}, h_{\text{bed}2}] = \\
\text{Column\_Size\_f\_print\_2\_input\_nodisp}(0.3, k, t_{\text{pres}_2}, \text{Purity\_col1}, T_2, P_{\text{ads}2}, P_{\text{des}2});
\end{verbatim}

\% Approximation of bed pressure and number of moles during initialization
\% steps
P_{\text{bed}}(1,1:i) = P_{\text{initialization}};
moles_{\text{N2}_2} = n_{\text{step}_{\text{total}}}*i*(1-G_{\text{in\_fracCO2}_2});
total\_moles = moles_{\text{N2}_2} + moles_{\text{CO2}_2};
\%Amount CO2 adsorbed during initialization
\% ASSUMING 86\% capture
\% without 86\% capture, put rate into Column\_Size and use
\% CO2\_molar\_flow\_cap
\%Commented this out since it shouldn't be needed
\% CO2_{\text{initialization}} = CO2\_molar\_flow\_cap*(t_{\text{saturation}+t_{\text{pres}}}); \%moles CO2
\% Bed\_CO2\_capacity = kg\_AC\,*\,(Net\_CO2); \%moles^{CO2}_2
\% Bed\_distance\_saturated(1,i+t_{\text{saturation}}/t_{\text{step}}) =
CO2_{\text{initialization}}/Bed\_CO2\_capacity\,*h_{\text{bed}};

\% Pseudo Steady-State Operation (after initialization)
t_{\text{saturation}_2} = Net\_CO2_2*kg\_AC_2/CO2\_molar\_flow\_cap;
t_{\text{total}_2} = t_{\text{saturation}_2}+t_{\text{pres}_2};
\%Captured amount of CO2 and N2
CO2_{\text{ads}_2} = kg\_AC_2\,*AA\_CO2\_ads_2; \%total moles of CO2 adsorbed
N2_{\text{ads}_2} = kg\_AC_2\,*AA\_N2\_ads_2; \%total moles of CO2 adsorbed
%% Column 2 Desorption
% Desorption pressure: P_des
% Assumes lots of stuff, like
% 1. Rapid depressurization (relatively)
% 2. No equilibrium formation in the meantime during depressurization
% 3. Gas removed only comes from AC effectively
CO2_working_capacity_2 = AA_CO2_ads_2 - AA_CO2_des_2;
CO2_recovered_2 = kg_AC_2*(CO2_working_capacity_2);
N2_working_capacity_2 = AA_N2_ads_2 - AA_N2_des_2;
N2_recovered_2 = kg_AC_2*(N2_working_capacity_2);
Purity_col2 = CO2_recovered_2/(CO2_recovered_2+N2_recovered_2);
%disp('The purity from column 2 is ' num2str(Purity_col2));

%% Volumetric Flow 3
Volumetric_flow_3_m3 = Volumetric_flow_2_m3*Purity_col1/Purity_col2*P_ads_1/P_ads_2; %m3/s into blower two (out of column 1)
[Volumetric_flow_3] = Volumetric_flow_3_m3*2118.88; %ft3/min

%% Assign variables
[D_bed_2] = D_bed_2*3.28; %feet
[h_bed_2] = h_bed_2*3.28; %feet

End
Model Sweep

clear
tic
T=19:0.5:21;
adsP1=1.4:0.025:1.6;
adsP2=1:0.025:1.4;
desP1=0.5:0.025:0.7;
desP2=0.5:0.025:0.7;

a=length(T);
b=length(adsP1);
c=length(adsP2);
d=length(desP1);
e=length(desP2);
a*b*c*d*e

Q1=zeros(a,b,c,d,e);
Q2=zeros(a,b,c,d,e);
Q3=zeros(a,b,c,d,e);
D1=zeros(a,b,c,d,e);
D2=zeros(a,b,c,d,e);
h1=zeros(a,b,c,d,e);
h2=zeros(a,b,c,d,e);
VAC1=zeros(a,b,c,d,e);
VAC2=zeros(a,b,c,d,e);

Timp=zeros(a*b*c*e*d,1);
adsP1imp=zeros(a*b*c*e*d,1);
adsP2imp=zeros(a*b*c*e*d,1);
desP1imp=zeros(a*b*c*e*d,1);
desP2imp=zeros(a*b*c*e*d,1);
Q1imp=zeros(a*b*c*e*d,1);
Q2imp=zeros(a*b*c*e*d,1);
Q3imp=zeros(a*b*c*e*d,1);
D1imp=zeros(a*b*c*e*d,1);
D2imp=zeros(a*b*c*e*d,1);
h1imp=zeros(a*b*c*e*d,1);
h2imp=zeros(a*b*c*e*d,1);
VAC1imp=zeros(a*b*c*e*d,1);
VAC2imp=zeros(a*b*c*e*d,1);

for i=1:a;
    for j=1:b;
        for k=1:c;
            for l=1:d;
                for m=1:e;
                    A=T(i);
                    B=adsP1(j);
                    C=adsP2(k);
                    D=desP1(l);
                    E=desP2(m);

                    [Q1(i,j,k,l,m),
                    Q2(i,j,k,l,m),Q3(i,j,k,l,m),D1(i,j,k,l,m),D2(i,j,k,l,m),h1(i,j,k,l,m),h2(i,j,k,l,m),VAC1(i,j,k,l,m),VAC2(i,j,k,l,m)]=model_function(A,B,D, A,C,E);
counter=1;
for i=1:a;
  for j=1:b;
    for k=1:c;
      for l=1:d;
        for m=1:e;
          Q1imp(counter)=Q1(i,j,k,l,m);
          Q2imp(counter)=Q2(i,j,k,l,m);
          Q3imp(counter)=Q3(i,j,k,l,m);
          h1imp(counter)=h1(i,j,k,l,m);
          h2imp(counter)=h2(i,j,k,l,m);
          D1imp(counter)=D1(i,j,k,l,m);
          D2imp(counter)=D2(i,j,k,l,m);
          VAC1imp(counter)=VAC1(i,j,k,l,m);
          VAC2imp(counter)=VAC2(i,j,k,l,m);
          Timp(counter)=T(i);
          adsP1imp(counter)=adsP1(j);
          adsP2imp(counter)=adsP2(k);
          desP1imp(counter)=desP1(l);
          desP2imp(counter)=desP2(m);
        end
      end
    end
  end
end

VAC1imp=VAC1imp*35.3147;
VAC2imp=VAC2imp*35.3147;
adsP1imp=adsP1imp*14.5;
adsP2imp=adsP2imp*14.5;
desP1imp=desP1imp*14.5;
desP2imp=desP2imp*14.5;

length1=a*b*c*d*e;
length2=num2str(length1);
Trange=strcat('B1:B',length2);
adsP1range=strcat('D1:D',length2);
adsP2range=strcat('F1:F',length2);
desP1range=strcat('H1:H',length2);
desP2range=strcat('J1:J',length2);
Q1range=strcat('L1:L',length2);
Q2range=strcat('N1:N',length2);
Q3range=strcat('P1:P',length2);
h1range=strcat('R1:R',length2);
h2range=strcat('T1:T',length2);
D1range=strcat('V1:V',length2);
D2range=strcat('X1:X',length2);
TCrange=strcat('AF1:AF',length2);
CCO2range=strcat('AB1:AB',length2);
ROIrange=strcat('AD1:AD',length2);
netErange=strcat('AF1:AF',length2);
VAC1range=strcat('AI1:AI',length2);
VAC2range=strcat('AK1:AK',length2);

filename='ProfitabilityAnalysis.xlsx';
	xlswrite(filename,Timp,'Costs',Trange);	xlswrite(filename,adsP1imp,'Costs',adsP1range);	xlswrite(filename,adsP2imp,'Costs',adsP2range);	xlswrite(filename,desP1imp,'Costs',desP1range);	xlswrite(filename,desP2imp,'Costs',desP2range);	xlswrite(filename,Q1imp,'Costs',Q1range);	xlswrite(filename,Q2imp,'Costs',Q2range);	xlswrite(filename,Q3imp,'Costs',Q3range);	xlswrite(filename,D1imp,'Costs',D1range);	xlswrite(filename,D2imp,'Costs',D2range);	xlswrite(filename,h1imp,'Costs',h1range);	xlswrite(filename,h2imp,'Costs',h2range);	xlswrite(filename,length1,'Costs','A2');	xlswrite(filename,VAC1imp,'Costs',VAC1range);	xlswrite(filename,VAC2imp,'Costs',VAC2range);

toc
Costing Script

TC=xlsread('Costing-Spreadsheet (1).xlsx','TC');
CCO2=xlsread('Costing-Spreadsheet (1).xlsx','CCO2');

    v=T(i);
    n=length(adsP);
    m=repmat(v,1,n);

figure
hold on

for i=1:length(T)
    plot(adsP,CCO2(i,:),'LineWidth',2);
end
legend('show','location','northeast')
legend('26','26.5','27','27.5','28')
xlabel('Adsorption Pressure (bar)')
ylabel('$/Tonne CO2')
hold off

figure
hold on

for i=1:length(adsP)
    plot(T,CCO2(:,i),'LineWidth',2);
end
legend('show','location','northwest')
legend('1','1.1','1.2','1.3','1.4','1.5')
xlabel('Temperature (C)')
ylabel('$/Tonne CO2')
Cost Organization Script

% Costs sorting/indexing script

%Inputs
%Index dimension 1
%EXAMPLES FOLLOW IN EACH SECTION

TC=xlsread(filename,'Costs',TCrange);
CC02=xlsread(filename,'Costs',CC02range);
ROI=xlsread(filename,'Costs',ROIrange);
netE=xlsread(filename,'Costs',netErang);

Length_adsP1 = length(adsP1);
Length_adsP2 = length(adsP2);
Length_desP1 = length(desP1);
Length_desP2 = length(desP2);
Length_T = length(T);

% adsPlimp=adsPlimp/14.5;
% adsP2imp=adsP2imp/14.5;
% desPlimp=desPlimp/14.5;
% desP2imp=desP2imp/14.5;

%Initialize results matrices
TC_r = zeros(Length_T,Length_adsP1,Length_adsP2,Length_desP1,Length_desP2);
CC02_r = zeros(Length_T,Length_adsP1,Length_adsP2,Length_desP1,Length_desP2);
ROI_r = TC_r;
netE_r = TC_r;

%Code to place the results where they belong
% for i=1:length(Timp);
% for j=1:length(T);
% if Timp(i) == T(j);
%   a=j;
%   end
% end
% for j=1:length(adsP1);
% if adsPlimp(i) == adsP1(j);
%   b=j;
%   end
% end
% for j=1:length(adsP2);
% if adsP2imp(i) == adsP2(j);
%   c=j;
%   end
% end
% for j=1:length(desP1);
% if desPlimp(i) == desP1(j);
%   d=j;
%   end
% end
end
for j=1:length(desP2);
    if desP2imp(i) == desP2(j);
        e=j;
    end
end
TC_r(a,b,c,d,e) = TC(i);
CCO2_r(a,b,c,d,e) = CCO2(i);
end

minimum=min(CCO2)
coord=find(CCO2==minimum)
Tmin=Timp(coord)
adsP1min=adsP1imp(coord)
adsP2min=adsP2imp(coord)
desP1min=desP1imp(coord)
desP2min=desP2imp(coord)
purity=purity_function(Tmin,adsP1min,desP1min,Tmin,adsP2min,desP2min)

% co2total=[];
% figure
% hold on
% for i = 1:Length_T;
%     for j=1:Length_T;
%         co2total=[co2total,CCO2_r(i,1,1,1,j)];
%     end
%     plot(desP2,co2total)
% end
% legend('show')
Appendix C: VBA Code

The following is the code used to assist costing in the spreadsheets that used the costing methods from Seider et al.

Sub Costing()
    Application.ScreenUpdating = False
    Application.DisplayStatusBar = False
    Set wsN = ThisWorkbook.Sheets("Notes")
    Set wsC = ThisWorkbook.Sheets("Costs")
    Set wsPM = ThisWorkbook.Sheets("ProfitabilityMeasures")
    a = wsC.Cells(2, 1).Value

    For i = 1 To a
        wsN.Cells(15, 11).Value = wsC.Cells(i, 2).Value
        wsN.Cells(7, 6).Value = wsC.Cells(i, 4).Value
        wsN.Cells(7, 12).Value = wsC.Cells(i, 6).Value
        wsN.Cells(3, 4).Value = wsC.Cells(i, 12).Value
        wsN.Cells(3, 5).Value = wsC.Cells(i, 14).Value
        wsN.Cells(3, 6).Value = wsC.Cells(i, 16).Value
        wsN.Cells(11, 8).Value = wsC.Cells(i, 22).Value
        wsN.Cells(11, 11).Value = wsC.Cells(i, 24).Value
        wsN.Cells(18, 7).Value = wsC.Cells(i, 35).Value
        wsN.Cells(18, 8).Value = wsC.Cells(i, 37).Value

        Application.Calculation = xlCalculationAutomatic
        wsC.Cells(i, 30).Value = wsPM.Cells(16, 5).Value
        wsC.Cells(i, 32).Value = wsPM.Cells(14, 5).Value
        wsC.Cells(i, 26).Value = wsN.Cells(23, 2).Value
        wsC.Cells(i, 28).Value = wsN.Cells(25, 7).Value
    Next i
    Application.ScreenUpdating = True
End Sub
Appendix D: Material Safety Data Sheets

D.1. Material Safety Data Sheet 3: Activated Carbon

“CLEANING THE WORLD WITH ACTIVATED CARBON”

SAFETY DATA SHEET

Section 1 - Identity

Identity (As Used on Label and List): GC Activated Carbon (Including, but not limited to GC C-40, GC 4 x 8B, GC 4 x 8S, GC 6 x 12, GC 6 x 12S, GC 8 x 30, GC 8 x 30AW, GC 8 x 30S, GC 8 x 30SAW, GC 12 x 40, GC 12 x 40AW, GC 12x40SAW, GC 20 x 50, GC 20 x 50S, GC Powdered, GC WDC activated carbons)

Manufacturers Name: General Carbon Corporation
33 Paterson Street
Paterson, NJ 07501
Tel: (973)523-2223
www.generalcarbon.com
Date Prepared: February 16, 2017

Section 2 - Hazardous Identification

2.1 GHS-US Classification

<table>
<thead>
<tr>
<th>Eye Irritation</th>
<th>2B H320</th>
</tr>
</thead>
<tbody>
<tr>
<td>STOT</td>
<td>SE 3 H335</td>
</tr>
</tbody>
</table>

Hazards not otherwise classified: Combustible dust. May form combustible dust concentrations in air. All powdered activated carbons are classified as weakly explosive (Dust explosion class St1): Given the necessary conditions of a strong ignition source, right concentrations of airborne carbon dust, adequate oxygen levels, and confinement, the potential for a deflagration event exists. A combustible dust hazard assessment and employee training should be carried out. See sections 7 and 9 for further information on combustible dust precautions.
2.2 Label Elements

Hazard Pictograms
Signal word (GHS-US): Warning
Hazard Statements:
H320- Causes eye irritation
H335- May cause respiratory irritation
Precautionary statements (GHS-US):
P261- Avoid breathing dust
P264- Wash thoroughly after handling
P271- Use in well-ventilated area
P280- Wear protective gloves/clothing/eye & face protect
2.3 Other Hazards
No additional information available

2.4 Unknown acute toxicity (GHS-US) No data available

Section 3: Composition/information on ingredients
3.1 Substances
Not applicable
3.2 Mixture
<table>
<thead>
<tr>
<th>Name</th>
<th>CAS #</th>
<th>%</th>
<th>GHS_US classification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>7440-44-0</td>
<td>100</td>
<td>Not classified</td>
</tr>
</tbody>
</table>

Section 4 – First Aid Measures
4.1 Description of first aid measures
First aid after inhalation
Remove person to fresh air. If not breathing, administer CPR or artificial respiration. Get immediate medical attention.
First aid after skin contact
If skin reddening or irritation develops, seek medical attention
First aid after eye contact
Immediately flush eyes with plenty of water for at least 15 minutes. If irritation persists, get medical attention.
First aid after ingestion
If the material is swallowed, get immediate medical attention or advice. DO NOT induce vomiting unless directed to do so by medical personnel.

4.2 Most important symptoms and effects, both acute and delayed
Symptoms/injuries after inhalation
May cause respiratory irritation
Symptoms/injuries after skin contact
May cause skin irritation
Symptoms/injuries after eye contact
Causes serious eye damage
Symptoms/injuries after ingestion
May be harmful if swallowed

4.3 Indication of any immediate medical attention and special treatment needed
No additional information available.

Section 5: Firefighting measures
5.1 Extinguishing media
Suitable extinguishing media
If involved with fire, flood with plenty of water
Unsuitable extinguishing media
None

5.2 Special hazards arising from substance or mixture
Fire hazard
None known
Explosion hazard
None known
Reactivity
Contact with strong oxidizers such as ozone, liquid oxygen, chlorine, etc. may result in fire.
5.3 Advice for firefighters

Protection during firefighting

Firefighters should wear full protective gear.
Section 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

General measures

Avoid contact with the skin and eyes

6.1.1 For non-emergency personnel

No additional information available

6.1.2 For emergency responders

No additional information available

6.2 Environmental precautions

None

6.3 Methods and material for containment and cleaning up

For containment

If possible, stop flow of product

Methods for cleaning up

Shovel or sweep up and put in closed container for disposal

6.4 Reference to other sections

No additional information available

Section 7: Handling and storage

7.1 Precautions for safe handling

Avoid contact with eyes. Wet activated carbon removes oxygen from air causing severe hazard to workers inside carbon vessels or confined spaces

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Protect containers from physical damage. Store in dry, cool, well-ventilated area. Store away from strong oxidizers, strong acids, ignition sources, combustible materials, and heat. An adequate air gap between packages is recommended to reduce propagation in the case of fire.

Handling: A hazard assessment should be carried out. As with all finely divided materials, ground all transfer, blending, and dust collecting equipment to prevent static discharge. Remove all strong ignition sources from material handling, transfer, and processing areas where dust may be present or accumulate. Practice good housekeeping. Excessive accumulations of dust or dusty conditions can create the potential of secondary explosions. Inspection of hidden surfaces for dust accumulation should be made routinely. If possible, eliminate the pathways for dust to accumulate in hidden areas. Fine carbon dust may penetrate electrical equipment and cause electrical shorts. Where dusting is unavoidable, dust-proof boxes and regular electrical line maintenance are recommended. Refer to NFPA standards 654 for guidance. Caution employees—no smoking in carbon storage and handling areas. Carbon is difficult to ignite, however, cutting and welding operations should be carried out using hot work permit systems where precautions are taken not to ignite carbon, which may smolder undetected.

7.3 Specific end use(s)

No additional information available
Section 8: Exposure controls/ personal protection

8.1 Control parameters
No additional information available

8.2 Exposure controls
Appropriate engineering controls: Local exhaust and general ventilation must be adequate to meet exposure standards
Hand Protection: None required under normal product handling conditions
Eye Protection: Safety glasses
Skin and body protection: Wear suitable working clothes
Respiratory protection: If airborne concentrations are above the applicable exposure limits, use NIOSH approved respiratory protection

Section 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state: Solid
Appearance: Particulate
Color: Black
Odor: No data available
Odor threshold: No data available
Ph: No data available
Relative evaporation rate: No data available
Melting point: No data available
Freezing point: No data available
Boiling point: No data available
Flash point: No data available
Self ignition temperature: No data available
Decomposition temperature: No data available
Flammability (solid, gas): No data available
Vapor Pressure: No data available
Relative Vapor density @ 20 deg C: No data available
Relative Density: 28-33 lb/ cubic foot
Solubility: No data available
Log Pow: No data available
Log Kow: No data available
Viscosity, kinematic: No data available
Viscosity, dynamic: No data available
Explosive properties: No data available
Oxidizing properties: No data available
Explosive limits: No data available

Combustible dust: These products may contain combustible dusts. May form combustible dust concentrations in air. All powdered activated carbons are weakly explosive. No specific information on these carbons are available.

Typical combustible dust data for a variety of activated carbons: $K_{st}$ values reported between 43-113 (various sources).

Dust explosion class St1 ($K_{st}$ values < 200 are Class St1-weakly explosive). MEC (minimum explosible concentration) in air: 50 and 60 g/m³ (two reports) Volatile content (by weight): < 8% ASTM D3175-11 (Watercarb)

MIT (minimum ignition temperature) values reported between 400-680°C (752-1256°F) (four reports)
Maximum Absolute Explosion pressure values reported between 6.0-8.6 bar (four reports)
9.2 Other information
No additional information available

Section 10: Stability and reactivity

10.1 Reactivity
Contact with strong oxidizers such as ozone, liquid oxygen, chlorine, etc. may result in fire

10.2 Chemical stability
Stable under normal conditions

10.3 Possibility of hazardous reactions
Will not occur

10.4 Conditions to avoid
None

10.5 Incompatible materials
Strong oxidizing and reducing agents such as ozone, liquid oxygen or chlorine.

10.6 Hazardous decomposition products
Carbon monoxide may be generated in the event of a fire.

Section 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity: Not classified
Carbon (7440-44-0)
LD50 oral rat: >10000 mg/kg
Skin corrosion/irritation: Not classified
Serious eye damage/irritation: Causes eye irritation
Respiratory or skin sensitization: Not classified
Germ cell mutagenicity: Not classified
Carcinogenicity: Not classified
Reproductive toxicity: Not classified
Specific target organ toxicity: May cause respiratory irritation (single exposure)
Specific target organ toxicity: Not classified (repeated exposure)
Aspiration hazard: Not classified

Section 12: Ecological Information

12.1 Toxicity
No additional information available

12.2 Persistence and degradability
No additional information available

12.3 Bioaccumulative potential
No additional information available

12.4 Mobility in soil
No additional information available
12.5 Other adverse effects
Section 13: Disposal concerns
13.1 Waste treatment methods
Waste Disposal recommendations: Dispose of contents/container in accordance with local/regional/international regulations

Section 14: Transportation information
In accordance with DOT/ADR/RID/ADNR/IMDG/ICAO/IATA

14.1 UN Number
Not applicable. See Note 1 below.

14.2 UN proper shipping name
Not applicable

Note 1: Under the UN classification for activated carbon, all activated carbons have been identified as a class 4.2 product. However, this product has been tested according to the United Nations Transport of Dangerous Goods test protocol for a “self-heating substance” (United Nations Transportation of Dangerous Goods, Manual of Tests and Criteria, Part III, Section 33.3.1.6 - Test N.4 - Test Method for Self Heating Substances) and it has been specifically determined that this product does not meet the definition of a self heating substance (class 4.2) or any other hazard class, and therefore should not be listed as a hazardous material. This information is applicable only for the Activated Carbon Product identified in this document.

Section 15: Regulatory information
15.1 US Federal regulations
Carbon (7440-44-0)
Listed on the United States TSCA inventory

15.3 US State regulations
No additional information available

Section 16: Other information
Full text of H-phrases:

Eye Irrit. 2B: Serious eye damage/eye irritation Category 2B
STOT SE 3: Specific target organ toxicity (single exposure) Category 3
H335: May cause respiratory irritation
NFPA health hazard: 1 - Exposure could cause irritation but only minor residual injury even if no treatment is given.

NFPA fire hazard: 1 - Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur (e.g., mineral oil). Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F).

NFPA reactivity: 0 - Normally stable, even under fire exposure conditions, and are not reactive with water.

***The information contained herein is accurate to the best of our knowledge. General Carbon Corporation makes no warranty with respect hereto said information and disclaims all liability from reliance there in.***
# SAFETY DATA SHEET

## Section 1. Identification

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>GHS product identifier</td>
<td>Nitrogen</td>
</tr>
<tr>
<td>Chemical name</td>
<td>nitrogen</td>
</tr>
<tr>
<td>Other means of identification</td>
<td>nitrogen (dot); nitrogen gas; Nitrogen NF, Nitrogen FG</td>
</tr>
<tr>
<td>Product use</td>
<td>Synthetic/Analytical chemistry.</td>
</tr>
<tr>
<td>Synonym</td>
<td>nitrogen (dot); nitrogen gas; Nitrogen NF, Nitrogen FG</td>
</tr>
<tr>
<td>SDS #</td>
<td>001040</td>
</tr>
<tr>
<td>Supplier's details</td>
<td>Airgas USA, LLC and its affiliates</td>
</tr>
<tr>
<td></td>
<td>259 North Radnor-Chester Road</td>
</tr>
<tr>
<td></td>
<td>Suite 100</td>
</tr>
<tr>
<td></td>
<td>Radnor, PA 19087-5283</td>
</tr>
<tr>
<td></td>
<td>1-610-687-5253</td>
</tr>
<tr>
<td>24-hour telephone</td>
<td>1-866-734-3438</td>
</tr>
</tbody>
</table>

## Section 2. Hazards identification

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>OSHA/HCS status</td>
<td>This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).</td>
</tr>
<tr>
<td>Classification of the substance or mixture</td>
<td>GASES UNDER PRESSURE - Compressed gas</td>
</tr>
</tbody>
</table>

### GHS label elements

- **Signal word**: Warning
- **Hazard statements**: Contains gas under pressure; may explode if heated. May displace oxygen and cause rapid suffocation.

### Precautionary statements

- **General**: Read and follow all Safety Data Sheets (SDS’S) before use. Read label before use. Keep out of reach of children. If medical advice is needed, have product container or label at hand. Close valve after each use and when empty. Use equipment rated for cylinder pressure. Do not open valve until connected to equipment prepared for use. Use a back flow preventative device in the piping. Use only equipment of compatible materials of construction.

- **Prevention**: Not applicable.

- **Response**: Not applicable.

- **Storage**: Protect from sunlight when ambient temperature exceeds 52°C/125°F. Store in a well-ventilated place.

- **Disposal**: Not applicable.

- **Hazards not otherwise classified**: In addition to any other important health or physical hazards, this product may displace oxygen and cause rapid suffocation.
Section 3. Composition/information on ingredients

Substance/mixture : Substance
Chemical name : nitrogen
Other means of identification : nitrogen (dot); nitrogen gas; Nitrogen NF, Nitrogen FG

CAS number/other identifiers

<table>
<thead>
<tr>
<th>Ingredient name</th>
<th>%</th>
<th>CAS number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>100</td>
<td>7727-37-9</td>
</tr>
</tbody>
</table>

Any concentration shown as a range is to protect confidentiality or is due to batch variation.

There are no additional ingredients present which, within the current knowledge of the supplier and in the concentrations applicable, are classified as hazardous to health or the environment and hence require reporting in this section.

Occupational exposure limits, if available, are listed in Section 8.

Section 4. First aid measures

Description of necessary first aid measures

Eye contact : Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Continue to rinse for at least 10 minutes. Get medical attention if irritation occurs.

Inhalation : Remove victim to fresh air and keep at rest in a position comfortable for breathing. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Get medical attention if adverse health effects persist or are severe. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband. In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.

Skin contact : Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. Get medical attention if symptoms occur. Wash clothing before reuse. Clean shoes thoroughly before reuse.

Ingestion : As this product is a gas, refer to the inhalation section.

Most important symptoms/effects, acute and delayed

Potential acute health effects

Eye contact : Contact with rapidly expanding gas may cause burns or frostbite.
Inhalation : No known significant effects or critical hazards.
Skin contact : Contact with rapidly expanding gas may cause burns or frostbite.
Frostbite : Try to warm up the frozen tissues and seek medical attention.
Ingestion : As this product is a gas, refer to the inhalation section.

Over-exposure signs/symptoms

Eye contact : No specific data.
Inhalation : No specific data.
Skin contact : No specific data.
Ingestion : No specific data.

Indication of immediate medical attention and special treatment needed, if necessary

Notes to physician : In case of inhalation of decomposition products in a fire, symptoms may be delayed.
The exposed person may need to be kept under medical surveillance for 48 hours.

Section 3. Composition/information on ingredients
Section 4. First aid measures

Specific treatments : No specific treatment.
Protection of first-aiders : No action shall be taken involving any personal risk or without suitable training. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

See toxicological information (Section 11)

Section 5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media : Use an extinguishing agent suitable for the surrounding fire.
Unsuitable extinguishing media : None known.

Specific hazards arising from the chemical

Hazardous thermal decomposition products : Contains gas under pressure. In a fire or if heated, a pressure increase will occur and the container may burst or explode.

Special protective actions for fire-fighters : Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Contact supplier immediately for specialist advice. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool.

Special protective equipment for fire-fighters : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

For non-emergency personnel : No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Avoid breathing gas. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.

For emergency responders : If specialised clothing is required to deal with the spillage, take note of any information in Section 8 on suitable and unsuitable materials. See also the information in "For non-emergency personnel".

Environmental precautions : Ensure emergency procedures to deal with accidental gas releases are in place to avoid contamination of the environment. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

Methods and materials for containment and cleaning up

Small spill : Immediately contact emergency personnel. Stop leak if without risk.
Large spill : Immediately contact emergency personnel. Stop leak if without risk. Note: see Section 1 for emergency contact information and Section 13 for waste disposal.

Section 7. Handling and storage

Precautions for safe handling Protective measures : Put on appropriate personal protective equipment (see Section 8). Contains gas under pressure. Avoid contact with eyes, skin and clothing. Avoid breathing gas. Empty containers retain product residue and can be hazardous. Do not puncture or incinerate...
Section 4. First aid measures

Nitrogen container. Use equipment rated for cylinder pressure.

Close valve after each use and when empty. Protect cylinders from physical damage; do not drag, roll, slide, or drop.
Section 7. Handling and storage

Advice on general occupational hygiene: Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Remove contaminated clothing and protective equipment before entering eating areas. See also Section 8 for additional information on hygiene measures.

Conditions for safe storage, including any incompatibilities: Store in accordance with local regulations. Store in a segregated and approved area. Store away from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see Section 10). Keep container tightly closed and sealed until ready for use. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F).

Section 8. Exposure controls/personal protection

Control parameters Occupational exposure limits

<table>
<thead>
<tr>
<th>Ingredient name</th>
<th>Exposure limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>Oxygen Depletion [Asphyxiant]</td>
</tr>
</tbody>
</table>

Appropriate engineering controls: Good general ventilation should be sufficient to control worker exposure to airborne contaminants.

Environmental exposure controls: Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

Individual protection measures Hygiene measures: Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.

Eye/face protection: Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists, gases or dusts. If contact is possible, the following protection should be worn, unless the assessment indicates a higher degree of protection: safety glasses with sideshields.

Skin protection
Hand protection: Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. Considering the parameters specified by the glove manufacturer, check during use that the gloves are still retaining their protective properties. It should be noted that the time to breakthrough for any glove material may be different for different glove manufacturers. In the case of mixtures, consisting of several substances, the protection time of the gloves cannot be accurately estimated.

Body protection: Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Other skin protection: Appropriate footwear and any additional skin protection measures should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Respiratory protection: Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.
### Section 9. Physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Appearance Physical state</strong></td>
<td>Gas. [Compressed gas.]</td>
</tr>
<tr>
<td><strong>Color</strong></td>
<td>Colorless.</td>
</tr>
<tr>
<td><strong>Molecular weight</strong></td>
<td>28.02 g/mole</td>
</tr>
<tr>
<td><strong>Molecular formula</strong></td>
<td>N2</td>
</tr>
<tr>
<td><strong>Boiling/condensation point</strong></td>
<td>-196°C (-320.8°F)</td>
</tr>
<tr>
<td><strong>Melting/freezing point</strong></td>
<td>-210.01°C (-346°F)</td>
</tr>
<tr>
<td><strong>Critical temperature</strong></td>
<td>-146.95°C (-232.5°F)</td>
</tr>
<tr>
<td><strong>Odor</strong></td>
<td>Odorless.</td>
</tr>
<tr>
<td><strong>Odor threshold</strong></td>
<td>Not available.</td>
</tr>
<tr>
<td><strong>pH</strong></td>
<td>Not available.</td>
</tr>
<tr>
<td><strong>Flash point</strong></td>
<td>Not available.</td>
</tr>
<tr>
<td><strong>Burning time</strong></td>
<td>Not applicable.</td>
</tr>
<tr>
<td><strong>Burning rate</strong></td>
<td>Not applicable.</td>
</tr>
<tr>
<td><strong>Evaporation rate</strong></td>
<td>Not available.</td>
</tr>
<tr>
<td><strong>Flammability (solid, gas)</strong></td>
<td>Not available.</td>
</tr>
<tr>
<td><strong>Lower and upper explosive (flammable) limits</strong></td>
<td>Not available.</td>
</tr>
<tr>
<td><strong>Vapor pressure</strong></td>
<td>Not available.</td>
</tr>
<tr>
<td><strong>Vapor density</strong></td>
<td>0.967 (Air = 1) Liquid Density@BP: 50.46 lb/ft³ (808.3 kg/m³)</td>
</tr>
<tr>
<td><strong>Specific Volume (ft³/lb)</strong></td>
<td>13.8889</td>
</tr>
<tr>
<td><strong>Gas Density (lb/ft³)</strong></td>
<td>0.072</td>
</tr>
<tr>
<td><strong>Relative density</strong></td>
<td>Not applicable.</td>
</tr>
<tr>
<td><strong>Solubility in water</strong></td>
<td>Not available.</td>
</tr>
<tr>
<td><strong>Partition coefficient: n-octanol/water</strong></td>
<td>0.67</td>
</tr>
<tr>
<td><strong>Auto-ignition temperature</strong></td>
<td>Not available.</td>
</tr>
<tr>
<td><strong>Decomposition temperature</strong></td>
<td>Not available.</td>
</tr>
<tr>
<td><strong>SADT</strong></td>
<td>Not available.</td>
</tr>
<tr>
<td><strong>Viscosity</strong></td>
<td>Not applicable.</td>
</tr>
</tbody>
</table>

### Section 10. Stability and reactivity

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Reactivity</strong></td>
<td>No specific test data related to reactivity available for this product or its ingredients.</td>
</tr>
<tr>
<td><strong>Chemical stability</strong></td>
<td>The product is stable.</td>
</tr>
<tr>
<td><strong>Possibility of hazardous reactions</strong></td>
<td>Under normal conditions of storage and use, hazardous reactions will not occur.</td>
</tr>
<tr>
<td><strong>Conditions to avoid</strong></td>
<td>No specific data.</td>
</tr>
</tbody>
</table>
Section 10. Stability and reactivity

Irritation/Corrosion
Not available.

Sensitization
Not available.

Mutagenicity
Not available.

Carcinogenicity
Not available.

Reproductive toxicity
Not available.

Teratogenicity
Not available.

Specific target organ toxicity (single exposure)
Not available.

Specific target organ toxicity (repeated exposure)
Not available.

Aspiration hazard
Not available.

Information on the likely routes of exposure
Not available.

Potential acute health effects

Eye contact: Contact with rapidly expanding gas may cause burns or frostbite.
Inhalation: No known significant effects or critical hazards.
Skin contact: Contact with rapidly expanding gas may cause burns or frostbite.
Ingestion: As this product is a gas, refer to the inhalation section.

Symptoms related to the physical, chemical and toxicological characteristics

Eye contact: No specific data.
Inhalation: No specific data.
Skin contact: No specific data.
Ingestion: No specific data.

Delayed and immediate effects and also chronic effects from short and long term exposure

Short term exposure

Potential immediate effects: Not available.
Potential delayed effects: Not available.

Long term exposure

Potential immediate effects: Not available.
Potential delayed effects: Not available.
Section 10. Stability and reactivity

Potential chronic health effects

Not available
**Section 11. Toxicological information**

- **Mutagenicity**: No known significant effects or critical hazards.
- **Teratogenicity**: No known significant effects or critical hazards.
- **Developmental effects**: No known significant effects or critical hazards.
- **Fertility effects**: No known significant effects or critical hazards.

**Numerical measures of toxicity**

**Acute toxicity estimates**

Not available.

**Section 12. Ecological information**

**Toxicity**

Not available.

**Persistence and degradability**

Not available.

**Bioaccumulative potential**

<table>
<thead>
<tr>
<th>Product/ingredient name</th>
<th>LogPow</th>
<th>BCF</th>
<th>Potential</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nitrogen</td>
<td>0.67</td>
<td>-</td>
<td>low</td>
</tr>
</tbody>
</table>

**Mobility in soil**

**Soil/water partition coefficient (Koc)**

Not available.

**Other adverse effects**

No known significant effects or critical hazards.

**Section 13. Disposal considerations**

**Disposal methods**

The generation of waste should be avoided or minimized wherever possible. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Waste should not be disposed of untreated to the sewer unless fully compliant with the requirements of all authorities with jurisdiction. Empty Airgas-owned pressure vessels should be returned to Airgas. Waste packaging should be recycled. Incineration or landfill should only be considered when recycling is not feasible. This material and its container must be disposed of in a safe way. Empty containers or liners may retain some product residues. Do not puncture or incinerate container.

**Section 14. Transport information**

<table>
<thead>
<tr>
<th>UN number</th>
<th>DOT</th>
<th>TDG</th>
<th>Mexico</th>
<th>IMDG</th>
<th>IATA</th>
</tr>
</thead>
<tbody>
<tr>
<td>UN1066</td>
<td>NITROGEN, COMPRESSED</td>
<td>NITROGEN, COMPRESSED</td>
<td>NITROGEN, COMPRESSED</td>
<td>NITROGEN, COMPRESSED</td>
<td>NITROGEN, COMPRESSED</td>
</tr>
</tbody>
</table>

Date of issue: 5/26/2016  Date of previous issue: 8/7/2015  Version: 0.02
Nitrogen

Section 14. Transport information

| Packing group | - | - | - | - | - | - |
| Additional information | Limited quantity Yes. Packaging instruction | Passenger aircraft Quantity limitation: 75 kg Cargo aircraft Quantity limitation: 150 kg | Product classified as per the following sections of the Transportation of Dangerous Goods Regulations: 2.13-2.17 (Class 2). Explosive Limit and Limited Quantity Index 0.125 Passenger Carrying Road or Rail Index 75 | - | - | Passenger and Cargo Aircraft Quantity limitation: 75 kg Cargo Aircraft Only Quantity limitation: 150 kg |

“Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product.”

Special precautions for user: Transport within user's premises: always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code: Not available.

Section 15. Regulatory information

U.S. Federal regulations: TSCA 8(a) CDR Exempt/Partial exemption: This material is listed or exempted. United States inventory (TSCA 8b): This material is listed or exempted.

Clean Air Act Section 112 (b) Hazardous Air Pollutants (HAPs): Not listed Clean Air Act Section 602 Class I Substances: Not listed Clean Air Act Section 602 Class II Substances: Not listed DEA List I Chemicals (Precursor Chemicals): Not listed DEA List II Chemicals (Essential Chemicals): Not listed SARA 302/304: Not listed
Composition/information on ingredients

No products were found.

SARA 304 RQ : Not applicable.

SARA 311/312
Classification : Sudden release of pressure

Composition/information on ingredients

<table>
<thead>
<tr>
<th>Name</th>
<th>%</th>
<th>Fire hazard</th>
<th>Sudden release of pressure</th>
<th>Reactive</th>
<th>Immediate (acute) health hazard</th>
<th>Delayed (chronic) health hazard</th>
</tr>
</thead>
</table>

SECTION: 1. Product and company identification

1.1. Product identifier
Product form : Substance
Name : Carbon dioxide
CAS No : 124-38-9
Formula : CO2
Other means of identification : Medipure® Carbon Dioxide, Extendapak® EX-2, Refrigerant gas R744, carbonic anhydride, carbonic acid gas

1.2. Relevant identified uses of the substance or mixture and uses advised against
Use of the substance/mixture : Industrial use. Use as directed.

1.3. Details of the supplier of the safety data sheet
Praxair, Inc.
10 Riverview Drive
Danbury, CT 06810-6268
- USA
T 1-800-772-9247 (1-800-PRAXAIR) - F 1-716-879-2146
www.praxair.com

1.4. Emergency telephone number
Emergency number : Onsite Emergency: 1-800-645-4633

CHEMTREC, 24hr/day 7days/week
— Within USA: 1-800-424-9300, Outside USA: 001-703-527-3887
(collect calls accepted, Contract 17729)

SECTION 2: Hazard identification

2.1. Classification of the substance or mixture
GHS-US classification
Liquefied gas  H280

2.2. Label elements
GHS-US labeling
Hazard pictograms (GHS-US) : 

Signal word (GHS-US) : WARNING
2.3. Other hazards

Other hazards not contributing to the classification:

- Asphyxiant in high concentrations
- Contact with liquid may cause cold burns/frostbite

**WARNING:** Concentration levels of carbon dioxide above about 1 percent are dangerous. Praxair recommends continuous monitoring with alarms to indicate unsafe conditions before and during potential personnel exposure. Use appropriate monitoring devices to ensure a safe oxygen level (minimum of 19.5 percent) and a safe carbon dioxide level.

2.4. Unknown acute toxicity (GHS US)

No data available

### SECTION 3: Composition/Information on ingredients

#### 3.1. Substance

- **Name:** Carbon dioxide
- **CAS No:** 124-38-9

<table>
<thead>
<tr>
<th>Name</th>
<th>Product identifier</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon dioxide</td>
<td>(CAS No) 124-38-9</td>
<td>99.5%</td>
</tr>
</tbody>
</table>

#### 3.2. Mixture

Not applicable

### SECTION 4: First aid measures

#### 4.1. Description of first aid measures

- **First-aid measures after inhalation:** Remove to fresh air and keep at rest in a position comfortable for breathing. If not breathing, give artificial respiration, with supplemental oxygen given by qualified personnel. If breathing is difficult, qualified personnel should give oxygen. Call a physician.

- **First-aid measures after skin contact:** MAY CAUSE FROSTBITE. For exposure to liquid, cold vapor, or solid carbon dioxide (dry ice), immediately warm frostbite area with warm water not to exceed 41°C (105°F). Water temperature should be tolerable to normal skin. Maintain skin warming for at least 15 minutes or until normal coloring and sensation have returned to the affected area. In case of massive exposure, remove clothing while showering with warm water. Seek medical evaluation and treatment as soon as possible.

- **First-aid measures after eye contact:** Immediately flush eyes thoroughly with water for at least 15 minutes. Hold the eyelids open and away from the eyeballs to ensure that all surfaces are flushed thoroughly. Contact an ophthalmologist immediately.

- **First-aid measures after ingestion:** Ingestion is not considered a potential route of exposure.

#### 4.2. Most important symptoms and effects, both acute and delayed

No additional information available

#### 4.3. Indication of any immediate medical attention and special treatment needed

None.

### SECTION 5: Firefighting measures

#### 5.1. Extinguishing media

- Suitable extinguishing media: Use extinguishing media appropriate for surrounding fire.

#### 5.2. Special hazards arising from the substance or mixture

- **Explosion hazard:** Heat of fire can build pressure in container and cause it to rupture. Containers are equipped with a pressure relief device. (Exceptions may exist where authorized by DOT.) No part of the container should be subjected to a temperature higher than 125°F (52°C).
- **Reactivity:** No reactivity hazard other than the effects described in sub-sections below.
**SECTION 6: Accidental release measures**

### 6.1. Personal precautions, protective equipment and emergency procedures

**General measures**

WARNING! Liquid and gas under pressure. Rapid release of gaseous carbon dioxide through a pressure relief device (PRD) or valve can result in the formation of dry ice, which is very cold and can cause frostbite.

#### 6.1.1. For non-emergency personnel

No additional information

#### 6.1.2. For emergency responders

No additional information available

#### 6.2. Environmental precautions

Try to stop release.

#### 6.3. Methods and material for containment and cleaning up

For containment

Prevent waste from contaminating the surrounding environment. Discard any product, residue, disposable container, or liner in an environmentally acceptable manner, in full compliance with federal, provincial, and local regulations. If necessary, call your local supplier for assistance.

#### 6.4. Reference to other sections

See also sections 8 and 13.

---

**SECTION 7: Handling and storage**

### 7.1. Precautions for safe handling
Precautions for safe handling:

Avoid breathing gas

Do not get in eyes, on skin, or on clothing

This gas is heavier than air and in an enclosed space tends to accumulate near the floor, displacing air and pushing it upward. This creates an oxygen-deficient atmosphere near the floor. Ventilate space before entry. Verify sufficient oxygen concentration.

**WARNING:** Concentration levels of carbon dioxide above about 1 percent are dangerous. Praxair recommends continuous monitoring with alarms to indicate unsafe conditions before and during potential personnel exposure. Use appropriate monitoring devices to ensure a safe oxygen level (minimum of 19.5 percent) and a safe carbon dioxide level.

Wear leather safety gloves and safety shoes when handling cylinders. Protect cylinders from physical damage; do not drag, roll, slide or drop. While moving cylinder, always keep in place removable valve cover. Never attempt to lift a cylinder by its cap; the cap is intended solely to protect the valve. When moving cylinders, even for short distances, use a cart (trolley, hand truck, etc.) designed to transport cylinders. Never insert an object (e.g., wrench, screwdriver, pry bar) into cap openings; doing so may damage the valve and cause a leak. Use an adjustable strap wrench to remove over-tight or rusted caps. Slowly open the valve. If the valve is hard to open, discontinue use and contact your supplier. Close the container valve after each use; keep closed even when empty. Never apply flame or localized heat directly to any part of the container. High temperatures may damage the container and could cause the pressure relief device to fail prematurely, venting the container contents. For other precautions in using this product, see section 16.
7.2. Conditions for safe storage, including any incompatibilities

Storage conditions: Store in a cool, well-ventilated place. Store and use with adequate ventilation. Store only where temperature will not exceed 125°F (52°C). Firmly secure containers upright to keep them from falling or being knocked over. Install valve protection cap, if provided, firmly in place by hand. Store full and empty containers separately. Use a first-in, first-out inventory system to prevent storing full containers for long periods.

This gas is heavier than air and in an enclosed space tends to accumulate near the floor, displacing air and pushing it upward. This creates an oxygen-deficient atmosphere near the floor. Ventilate space before entry. Verify sufficient oxygen concentration.

7.3. Specific end use(s)

None.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

<table>
<thead>
<tr>
<th>Carbon dioxide (124-38-9)</th>
<th>ACGIH TLV-TWA (ppm)</th>
<th>5000 ppm</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACGIH</td>
<td>ACGIH TLV-STEL (ppm)</td>
<td>30000 ppm</td>
</tr>
<tr>
<td>USA OSHA</td>
<td>OSHA PEL (TWA) (mg/m³)</td>
<td>9000 mg/m³</td>
</tr>
<tr>
<td>USA OSHA</td>
<td>OSHA PEL (TWA) (ppm)</td>
<td>5000 ppm</td>
</tr>
<tr>
<td>USA IDLH</td>
<td>US IDLH (ppm)</td>
<td>40000 ppm</td>
</tr>
<tr>
<td>ACGIH</td>
<td>Not established</td>
<td></td>
</tr>
<tr>
<td>USA OSHA</td>
<td>Not established</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Carbon dioxide (124-38-9)</th>
<th>ACGIH TLV-TWA (ppm)</th>
<th>5000 ppm</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACGIH</td>
<td>ACGIH TLV-STEL (ppm)</td>
<td>30000 ppm</td>
</tr>
<tr>
<td>USA OSHA</td>
<td>OSHA PEL (TWA) (mg/m³)</td>
<td>9000 mg/m³</td>
</tr>
<tr>
<td>USA OSHA</td>
<td>OSHA PEL (TWA) (ppm)</td>
<td>5000 ppm</td>
</tr>
</tbody>
</table>

8.2. Exposure controls

Appropriate engineering controls: Use a local exhaust system with sufficient flow velocity to maintain an adequate supply of air in the worker's breathing zone. Mechanical (general): General exhaust ventilation may be acceptable if it can maintain an adequate supply of air. WARNING: Concentration levels of carbon dioxide above about 1 percent are dangerous. Praxair recommends continuous monitoring with alarms to indicate unsafe conditions before and during potential personnel exposure. Use appropriate monitoring devices to ensure a safe oxygen level (minimum of 19.5 percent) and a safe carbon dioxide level.


Eye protection: Wear safety glasses when handling cylinders; vapor-proof goggles and a face shield during cylinder changeout or whenever contact with product is possible. Select eye protection in accordance with OSHA 29 CFR 1910.133.

Skin and body protection: As needed for welding, wear hand, head, and body protection to help prevent injury from radiation and sparks. (See ANSI Z49.1.) At a minimum, this includes welder’s gloves and protective goggles, and may include arm protectors, aprons, hats, and shoulder protection as well as substantial clothing.

Respiratory protection: When workplace conditions warrant respirator use, follow a respiratory protection program that meets OSHA 29 CFR 1910.134, ANSI Z88.2, or MSHA 30 CFR 72.710 (where applicable). Use an air-supplied or air-purifying cartridge if the action level is exceeded. Ensure that the respirator has the appropriate protection factor for the exposure level. If cartridge type respirators are used, the cartridge must be appropriate for the chemical exposure. For emergencies or instances with unknown exposure levels, use a self-contained breathing apparatus (SCBA).

Thermal hazard protection: Wear cold insulating gloves when transfilling or breaking transfer connections.
### SECTION 9: Physical and chemical properties

#### 9.1. Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physical state</td>
<td>Gas</td>
</tr>
<tr>
<td>Appearance</td>
<td>Colorless gas</td>
</tr>
<tr>
<td>Molecular mass</td>
<td>44 g/mol</td>
</tr>
<tr>
<td>Color</td>
<td>Colorless</td>
</tr>
<tr>
<td>Odor</td>
<td>Odorless</td>
</tr>
<tr>
<td>Odor threshold</td>
<td>No data available</td>
</tr>
<tr>
<td>pH</td>
<td>3.7 (carbonic acid)</td>
</tr>
<tr>
<td>Relative evaporation rate (butyl acetate=1)</td>
<td>No data available</td>
</tr>
<tr>
<td>Relative evaporation rate (ether=1)</td>
<td>Not applicable</td>
</tr>
<tr>
<td>Melting point</td>
<td>No data available</td>
</tr>
<tr>
<td>Freezing point</td>
<td>No data available</td>
</tr>
<tr>
<td>Boiling point</td>
<td>-78.5 °C (-109.3°F)</td>
</tr>
<tr>
<td>Flash point</td>
<td>No data available</td>
</tr>
<tr>
<td>Critical temperature</td>
<td>31 °C (87.7°F)</td>
</tr>
<tr>
<td>Auto-ignition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>Decomposition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
<td>No data available</td>
</tr>
<tr>
<td>Vapor pressure</td>
<td>57.3 bar (831 psig)</td>
</tr>
<tr>
<td>Critical pressure</td>
<td>73.7 bar (1069 psig)</td>
</tr>
<tr>
<td>Relative vapor density at 20 °C</td>
<td>762</td>
</tr>
<tr>
<td>Relative density</td>
<td>1.22</td>
</tr>
<tr>
<td>Relative gas density</td>
<td>1.52</td>
</tr>
<tr>
<td>Solubility</td>
<td>Water: 2000 mg/l Completely soluble</td>
</tr>
<tr>
<td>Log Pow</td>
<td>0.83</td>
</tr>
<tr>
<td>Log Kow</td>
<td>Not applicable</td>
</tr>
<tr>
<td>Viscosity, kinematic</td>
<td>Not applicable</td>
</tr>
<tr>
<td>Viscosity, dynamic</td>
<td>Not applicable</td>
</tr>
<tr>
<td>Explosive properties</td>
<td>Not applicable</td>
</tr>
<tr>
<td>Oxidizing properties</td>
<td>None</td>
</tr>
<tr>
<td>Explosion limits</td>
<td>No data available</td>
</tr>
</tbody>
</table>

#### 9.2. Other information

- **Gas group**: Liquefied gas
- **Additional information**: Gas/vapor heavier than air. May accumulate in confined spaces, particularly at or below ground level

### SECTION 10: Stability and reactivity

#### 10.1. Reactivity

No reactivity hazard other than the effects described in sub-sections below.

#### 10.2. Chemical stability

Stable under normal conditions.

#### 10.3. Possibility of hazardous reactions

None.

#### 10.4. Conditions to avoid

None under recommended storage and handling conditions (see section 7).

#### 10.5. Incompatible materials
### 10.6. Hazardous decomposition products

Electrical discharges and high temperatures decompose carbon dioxide into carbon monoxide and oxygen. The welding process may generate hazardous fumes and gases.

### SECTION 11: Toxicological information

#### 11.1. Information on toxicological effects

<table>
<thead>
<tr>
<th>Effect</th>
<th>Classification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acute toxicity</td>
<td>Not classified</td>
</tr>
<tr>
<td>Skin corrosion/irritation</td>
<td>Not classified</td>
</tr>
<tr>
<td>Serious eye damage/irritation</td>
<td>Not classified</td>
</tr>
<tr>
<td>Respiratory or skin sensitization</td>
<td>Not classified</td>
</tr>
<tr>
<td>Germ cell mutagenicity</td>
<td>Not classified</td>
</tr>
<tr>
<td>Carcinogenicity</td>
<td>Not classified</td>
</tr>
<tr>
<td>Reproductive toxicity</td>
<td>Not classified</td>
</tr>
<tr>
<td>Specific target organ toxicity (single exposure)</td>
<td>Not classified</td>
</tr>
<tr>
<td>Specific target organ toxicity (repeated exposure)</td>
<td>Not classified</td>
</tr>
<tr>
<td>Aspiration hazard</td>
<td>Not classified</td>
</tr>
</tbody>
</table>

#### 11.2. Toxicity

<table>
<thead>
<tr>
<th>Substance</th>
<th>Classification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon dioxide (124-38-9)</td>
<td>No ecological damage caused by this product.</td>
</tr>
</tbody>
</table>

#### 12.1. Persistence and degradability

<table>
<thead>
<tr>
<th>Substance</th>
<th>Classification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon dioxide (124-38-9)</td>
<td>No ecological damage caused by this product.</td>
</tr>
</tbody>
</table>

#### 12.3. Bioaccumulative potential

<table>
<thead>
<tr>
<th>Substance</th>
<th>Classification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon dioxide (124-38-9)</td>
<td>(no bioaccumulation)</td>
</tr>
<tr>
<td>Log Pow</td>
<td>0.83</td>
</tr>
<tr>
<td>Log Kow</td>
<td>Not applicable.</td>
</tr>
<tr>
<td>Bioaccumulative potential</td>
<td>No ecological damage caused by this product.</td>
</tr>
</tbody>
</table>

#### 12.4. Mobility in soil

<table>
<thead>
<tr>
<th>Substance</th>
<th>Classification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon dioxide (124-38-9)</td>
<td>No ecological damage caused by this product.</td>
</tr>
</tbody>
</table>
### 12.5. Other adverse effects

<table>
<thead>
<tr>
<th>Effect</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Effect on ozone layer</td>
<td>None</td>
</tr>
<tr>
<td>Global warming potential [CO2=1]</td>
<td>1</td>
</tr>
<tr>
<td>Effect on the global warming</td>
<td>When discharged in large quantities may contribute to the greenhouse effect</td>
</tr>
</tbody>
</table>

### SECTION 13: Disposal considerations

**13.1. Waste treatment methods**

- Waste treatment methods: May be vented to atmosphere in a well ventilated place. Discharge to atmosphere in large quantities should be avoided. Do not discharge into any place where its accumulation could be dangerous. Contact supplier if guidance is required.

- Waste disposal recommendations: Do not attempt to dispose of residual or unused quantities. Return container to supplier.

### SECTION 14: Transport information

#### In accordance with DOT

- Transport document description: UN1013 Carbon dioxide, 2.2
- UN-No. (DOT): UN1013
- Proper Shipping Name (DOT): Carbon dioxide
- Class (DOT): 2.2 - Class 2.2 - Non-flammable compressed gas 49 CFR 173.115
- Hazard labels (DOT): 2.2 - Non-flammable gas

#### Additional information

- Emergency Response Guide (ERG) Number: 120
- Other information: No supplementary information available.
- Special transport precautions driver's: Avoid transport on vehicles where the load space is not separated from the driver's compartment. Ensure vehicle driver is aware of the potential hazards of the load and knows what to do in the event of an accident or an emergency. Before transporting product containers:
  - Ensure there is adequate ventilation.
  - Ensure that containers are firmly secured.
  - Ensure cylinder valve is closed and not leaking.
  - Ensure valve outlet cap nut or plug (where provided) is correctly fitted.
  - Ensure valve protection device (where provided) is correctly fitted.

#### Transport by sea

- UN-No. (IMDG): 1013
- Proper Shipping Name (IMDG): CARBON DIOXIDE
- Class (IMDG): 2 - Gases
- MFAG-No: 120

#### Air transport

- UN-No. (IATA): 1013
- Proper Shipping Name (IATA): Carbon dioxide
- Class (IATA): 2
- Civil Aeronautics Law: Gases under pressure/Gases nonflammable nontoxic under pressure

### SECTION 15: Regulatory information
## 15.2. International regulations

**CANADA**

<table>
<thead>
<tr>
<th>Carbon dioxide (124-38-9)</th>
<th>Listed on the Canadian DSL (Domestic Substances List)</th>
</tr>
</thead>
</table>

**EU-Regulations**

<table>
<thead>
<tr>
<th>Carbon dioxide (124-38-9)</th>
<th>Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)</th>
</tr>
</thead>
</table>

## 15.2.2. National regulations

<table>
<thead>
<tr>
<th>Carbon dioxide (124-38-9)</th>
<th>Listed on the AICS (Australian Inventory of Chemical Substances)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)</td>
</tr>
<tr>
<td></td>
<td>Listed on the Japanese ENCS (Existing &amp; New Chemical Substances) inventory</td>
</tr>
<tr>
<td></td>
<td>Listed on the Korean ECL (Existing Chemicals List)</td>
</tr>
<tr>
<td></td>
<td>Listed on NZIoC (New Zealand Inventory of Chemicals)</td>
</tr>
<tr>
<td></td>
<td>Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)</td>
</tr>
<tr>
<td></td>
<td>Listed on the Canadian IDL (Ingredient Disclosure List)</td>
</tr>
<tr>
<td></td>
<td>Listed on INSQ (Mexican National Inventory of Chemical Substances)</td>
</tr>
<tr>
<td></td>
<td>Listed on CICR (Turkish Inventory and Control of Chemicals)</td>
</tr>
</tbody>
</table>

## 15.3. US State regulations

### Carbon dioxide (124-38-9)

<table>
<thead>
<tr>
<th>U.S. - California - Proposition 65 - Carcinogens List</th>
<th>No</th>
</tr>
</thead>
<tbody>
<tr>
<td>U.S. - California - Proposition 65 - Developmental Toxicity</td>
<td>No</td>
</tr>
<tr>
<td>U.S. - California - Proposition 65 - Reproductive Toxicity - Female</td>
<td>No</td>
</tr>
<tr>
<td>U.S. - California - Proposition 65 - Reproductive Toxicity - Male</td>
<td>No</td>
</tr>
</tbody>
</table>

**State or local regulations**

<table>
<thead>
<tr>
<th>U.S. - Massachusetts - Right To Know List</th>
</tr>
</thead>
<tbody>
<tr>
<td>U.S. - New Jersey - Right to Know Hazardous Substance List</td>
</tr>
<tr>
<td>U.S. - Pennsylvania - RTK (Right to Know) List</td>
</tr>
</tbody>
</table>

### Carbon dioxide (124-38-9)

<table>
<thead>
<tr>
<th>U.S. - California - Proposition 65 - Carcinogens List</th>
<th>U.S. - California - Proposition 65 - Developmental Toxicity</th>
<th>U.S. - California - Proposition 65 - Reproductive Toxicity - Female</th>
<th>U.S. - California - Proposition 65 - Reproductive Toxicity - Male</th>
<th>Non-significant risk level (NSRL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
</tbody>
</table>

### Carbon dioxide (124-38-9)

<table>
<thead>
<tr>
<th>U.S. - Massachusetts - Right To Know List</th>
</tr>
</thead>
<tbody>
<tr>
<td>U.S. - New Jersey - Right to Know Hazardous Substance List</td>
</tr>
<tr>
<td>U.S. - Pennsylvania - RTK (Right to Know) List</td>
</tr>
</tbody>
</table>
State regulations Massachusetts: This material is listed.
New York: This material is not listed.
New Jersey: This material is listed.
Pennsylvania: This material is listed.

International regulations

International lists National inventory
Australia: This material is listed or exempted.
Canada: This material is listed or exempted.
China: This material is listed or exempted.
Europe: This material is listed or exempted.
Japan: Not determined.
Malaysia: Not determined.
New Zealand: This material is listed or exempted.
Philippines: This material is listed or exempted.
Republic of Korea: This material is listed or exempted.
Taiwan: This material is listed or exempted.

Canada

WHMIS (Canada): Class A: Compressed gas.
CEPA Toxic substances: This material is not listed.
Canadian ARET: This material is not listed.
Canadian NPRI: This material is not listed.
Alberta Designated Substances: This material is not listed.
Ontario Designated Substances: This material is not listed.
Quebec Designated Substances: This material is not listed.

Section 16. Other information

Hazardous Label requirements: Class A: Compressed gas.

Hazardous Material Information System (U.S.A.)

Caution: HMIS® ratings are based on a 0-4 rating scale, with 0 representing minimal hazards or risks, and 4 representing significant hazards or risks. Although HMIS® ratings are not required on SDSs under 29 CFR 1910.1200, the preparer may choose to provide them. HMIS® ratings are to be used with a fully implemented HMIS® program. HMIS® is a registered mark of the National Paint & Coatings Association (NPCA). HMIS® materials may be purchased exclusively from J. J. Keller (800) 327-6868.

The customer is responsible for determining the PPE code for this material. National Fire Protection Association (U.S.A.)

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Copyright ©2001, National Fire Protection Association, Quincy, MA 02269. This warning system is intended to be interpreted and applied only by properly trained individuals to identify fire, health and reactivity hazards of chemicals. The user is referred to certain limited number of chemicals with recommended classifications in NFPA 49 and NFPA 325, which would be used as a guideline only. Whether the chemicals are classified by NFPA or not, anyone using the 704 systems to classify chemicals does so at their own risk.

**Procedure used to derive the classification**

<table>
<thead>
<tr>
<th>Classification</th>
<th>Justification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Press. Gas Comp. Gas, H280</td>
<td>Expert judgment</td>
</tr>
</tbody>
</table>

**History**

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
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<tbody>
<tr>
<td>Date of printing</td>
<td>: 5/26/2016</td>
</tr>
<tr>
<td>Date of issue/Date of revision</td>
<td>: 5/26/2016</td>
</tr>
<tr>
<td>Date of previous issue</td>
<td>: 8/7/2015</td>
</tr>
<tr>
<td>Version</td>
<td>: 0.02</td>
</tr>
</tbody>
</table>
Key to abbreviations

ATE = Acute Toxicity Estimate
BCF = Bioconcentration Factor
GHS = Globally Harmonized System of Classification and Labelling of Chemicals
IATA = International Air Transport Association
IBC = Intermediate Bulk Container
IMDG = International Maritime Dangerous Goods
LogPow = logarithm of the octanol/water partition coefficient
UN = United Nations

References

Not available.

Indicates information that has changed from previously issued version. Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.
SECTION 16: Other information

Other information:

- When you mix two or more chemicals, you can create additional, unexpected hazards. Obtain and evaluate the safety information for each component before you produce the mixture. Consult an industrial hygienist or other trained person when you evaluate the end product. Before using any plastics, confirm their compatibility with this product.

Fumes and gases produced during welding and cutting processes can be dangerous to your health and may cause serious lung disease. KEEP YOUR HEAD OUT OF FUMES. DO NOT BREATHE FUMES AND GASES. Use enough ventilation, local exhaust, or both to keep fumes and gases from your breathing zone and the general area. Short-term overexposure to fumes may cause dizziness, nausea, and dryness or irritation of the nose, throat, and eyes; or may cause other similar discomfort. Contaminants in the air may add to the hazard of fumes and gases. One such contaminant, chlorinated hydrocarbon vapors from cleaning and degreasing activities, poses a special risk. DO NOT USE ELECTRIC ARCS IN THE PRESENCE OF CHLORINATED HYDROCARBON VAPORS—HIGHLY TOXIC PHOSGENE MAY BE PRODUCED. Metal coatings such as paint, plating, or galvanizing may generate harmful fumes when heated. Residues from cleaning materials may also be harmful. AVOID ARC OPERATIONS ON PARTS WITH PHOSPHATE RESIDUES (ANTI-RUST, CLEANING PREPARATIONS)—HIGHLY TOXIC PHOSPHINE MAY BE PRODUCED.

The opinions expressed herein are those of qualified experts within Praxair, Inc. We believe that the information contained herein is current as of the date of this Safety Data Sheet. Since the use of this information and the conditions of use are not within the control of Praxair, Inc, it is the user's obligation to determine the conditions of safe use of the product.

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Praxair asks users of this product to study this SDS and become aware of the product hazards and safety information. To promote safe use of this product, a user should (1) notify employees, agents, and contractors of the information in this SDS and of any other known product hazards and safety information, (2) furnish this information to each purchaser of the product, and (3) ask each purchaser to notify its employees and customers of the product hazards and safety information.

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NFPA health hazard: 2 - Intense or continued exposure could cause temporary incapacitation or possible residual injury unless prompt medical attention is given.

NFPA fire hazard: 0 - Materials that will not burn.

NFPA reactivity: 0 - Normally stable, even under fire exposure conditions, and are not reactive with water.

NFPA specific hazard: SA - This denotes gases which are simple asphyxiants.
HMIS III Rating