Solvent Selection and Recycling for Carbon Absorption in a Pulverized Coal Power Plant

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Simulated Annealing is used to optimize the solvent selection and recycling conditions for a carbon dioxide absorber in a pulverized coal power plant. The project uses Aspen Plus V7.1 to model a pulverized coal power plant and the carbon capture system. Simulated Annealing is introduced via the CAPE OPEN feature in Aspen Plus to find the best combination to absorb the most carbon dioxide while using the least amount of power for carbon absorption. With this optimal configuration, retrofitting carbon absorption into current power plants will cause a smaller drop in efficiency than that of the current practice. This project will lead to improved sustainability for fossil fuel power plants, by reducing the amount of emissions from fossil fuel power plants without a significant reduction in efficiency.

Introduction

Sustainability has become a focus of our efforts in the United States. The goal is to not use all of the natural resources and pollute the world before future generations have a chance to see it. One of the goals of the sustainability projects is to capture carbon dioxide emissions or to eliminate them altogether from power plants, cars, etc. With the present technology, we cannot eliminate all of the carbon emissions and still meet the energy demand for the population. Coal fired power plants produce and release tons upon tons of carbon dioxide into the atmosphere daily. In order to become more sustainable, these emissions need to be reduced, and with the present technology, it is possible to capture the carbon dioxide from the flue gas. However, this comes with costs to efficiency. The focus of this study therefore is on optimizing the performance of the absorption of carbon dioxide from the flue gas of a pulverized coal power plant.

PC Power Plant

Three mains types of fossil fuel power plants exist today: integrated gasification combined cycle (IGCC), pulverized coal (PC), and natural gas combined cycle (NGCC). Each of these processes varies in their efficiency and plant/operating costs. Before introducing a carbon dioxide absorber, NGCC is the most efficient and maintains the lowest startup and operating costs. IGCC and PC are roughly equal in terms of efficiency and plant cost, but on average, the IGCC plants are slightly more efficient and cost less that PC plants. However, when a carbon dioxide absorber is introduced into each of the types of plants, the efficiencies decrease and cost increase.

Studies show that the efficiency dropped by 5 to 12 percent in each plant type upon introducing the absorber system, but the PC plant had the largest drop in efficiency. The costs increased by 20 to 40 % for each plant when the absorber was introduced. The cost component included the initial cost of the equipment as well as the \cot of operation.¹ The absorber was optimized to remove at least 90 percent of the carbon dioxide from the flue gas of the power plants.

PC power plants are the focus of this article, which may seem strange, as they are the lowest efficiency and highest cost to produce and operate. So, why study carbon absorption in them? The answer is that the vast majority of power plants in operation today are pulverized coal plants. Thus, it is ideal to find a way to retrofit the old plants with a carbon dioxide absorption system. This would improve the sustainability of the current plants, while avoiding the need to build new ones.

FIG. 1: Graphical representation of the carbon absorption section of a PC power plant produced by Aspen Plus. Material streams are shown solid. The main components are the two absorbers, which are

aligned vertically on the left side, and the four strippers, which are aligned vertically in the center of the graphic. These components absorb carbon dioxide using solvent, and regenerate that solvent respectively.

PC plants can operate as two different types depending on the type of steam utilized: sub-critical steam or supercritical steam. When carbon capture components are included in the plant design, the supercritical plants cost slightly less and are slightly more efficient than the sub-critical PC plants.¹ Thus, the choice of exploring supercritical steam PC plants was made for the purpose of this study. The design of a PC plant consists of three main parts: the boiler, the steam cycle, and the flue gas treatment. Coal is first pulverized and then fed into a boiler, where it is combusted producing carbon dioxide among other gases. The heat generated by this combustion reaction is transferred to a cycling water reactor, which heats water to supercritical steam to turn a turbine, thus generating power. The flue gas from the boiler is treated before being released to the atmosphere in order to remove sulfur, mercury, and any other harmful gases.

Carbon Capture

Carbon can be removed from processes in four main ways including: pre-combustion, oxyfuel, industrial processes, and post combustion.² Each of these types removes carbon at different parts of the plant's cycle or through different conditions within the process. These methods are generally used in combustion processes involving carbon such as coal-fired power plants because the carbon source is non-mobile and relatively concentrated in a single stream; thus, they are not appropriate when the carbon source is small or mobile, such as a car.

In pre-combustion processes, the fuel, which is normally some coal derivative, is partially oxidized to form carbon monoxide and hydrogen. Then steam is added to the carbon monoxide to convert it into carbon dioxide. Thus, the fuel is converted into pure carbon dioxide and hydrogen before the combustion process. At this point, the carbon dioxide is removed using solvents, and the hydrogen is combusted in the boiler producing only water as the byproduct.

In oxyfuel processes, the fuel is burned in almost pure oxygen. This generates a much higher boiler temperature, which causes the flue gas to be comprised of carbon dioxide, water, and some excess oxygen. The flue gas can be easily cooled to remove the water vapor by condensation, producing an essentially pure carbon dioxide stream, which can easily be collected. The downside to this method is that the materials used in the boiler must be specially designed to withstand the more extreme operating conditions.

In industrial processes, the carbon is removed by various means. Membranes can be used to remove carbon dioxide selectively from a gaseous stream; however, they require a slower moving stream than is typically found in power plants. Another method is cryogenic cooling, which physically removes the carbon species. This method required a large amount of energy. These methods, while effective in certain conditions, are not appropriate for a PC power plant.

Finally, in post-combustion $CO₂$ absorption, carbon dioxide is separated from the flue gas. The power plant would operate as normal, but have one additional component at the end of the process for removing the carbon dioxide before exiting as stack gas. This method is the easiest to implement into an existing power plant. Generally, the carbon absorption is done with chemical solvents to pull unwanted molecules from the flue gas similar to how other unwanted molecules (nitrous oxides, sulfur oxides, mercury, etc.) are currently removed. The solvent used depends heavily on the concentration of the flue gas components, but theoretically, a solvent could be used for any fuel if the waste concentrations are known. Each of these methods varies in their implementation and operational costs. The efficiency of the plant will also decrease upon implementing one of these systems. This means that each one should be fully considered before implementing one into the plant. However, the focus of this study is on the retrofitting of a carbon dioxide system to current plants. The post-combustion process is ideal for this purpose, thus it is used in the modeling efforts for the project.

Post-combustion processes use solvents to absorb the carbon dioxide, but that can be done in two different ways: physical or reactive. Physical absorption is used when the species to be separated exists in a relatively high concentration in the flue gas. It typically uses water to dissolve the gas from the process stream, and then pressure is reduced to remove the gas from the solvent to recycle it. Reactive absorption uses a chemical reaction between the carbon dioxide and the solvent to pull carbon from the flue gas. This method works best with relatively low partial pressures of the species to be separated, which is the case with carbon dioxide in a PC power plant. Reactive absorption³ is the only type considered in this study, thus only solvents capable of reacting with carbon dioxide on some level are considered. The solvents themselves will be diluted with water to test several different concentrations of solvent.

Optimization

The goal of optimizing the carbon dioxide absorption is a very complex problem. There are several different variables in the model. Each of these affects the absorption and costs in different ways. Some of these variables include the operation conditions in the absorber (temperature, pressure, etc.), the solvent(s), the concentration of solvent and water, and even the height of the separation column itself. The work of this project is focused on solvent selection as well as solvent cycling. These two focuses lead to a complex problem, which is impossible to solve by hand. This creates a need for a computer program or method to assist with the calculations.

Gradient-based methods (based on the first derivative)

FIG. 2: It is ideal for energy requirement for the absorption section to be at a minimum. For this data, the reflux ratio was set to 1, the feed plate to 2, and the concentration of solvent (MEA) was set to 0.3 for all data points. Clearly, as the number of trays is increased, the energy requirement decreases. The flowsheet incorporated a design specification of 95% absorption of carbon dioxide.

are effective for well-behaved functions with a single minimum or maximum.⁴ However, this problem introduces many minimums into the function, which would cause a derivative based method to become "stuck" in a local minimum, and not find the global, or best, minimum value. In order to combat this, a method called Simulated Annealing is utilized. This method is probabilistic in nature.

Simulated Annealing is based on the annealing of metals, which causes the molecules to arrange themselves in the optimum configuration to increase strength.⁴ The method generates a starting value. Then it generates a move and compares the two. If the move has a lower value (or higher if a maximum is sought), it is accepted and replaces the starting value. If the move is higher however, it is accepted by a probability, which decreases the longer the program is run. This means there is a chance that even if the program finds a non-global minimum, it can escape the "well."⁴

Simulated Annealing is ideal for this case because the program will intelligently sift through the different combinations of variables to find the global optimum for the complex function presented, which will be the best settings to maximize carbon absorption and minimize the costs.⁵ The Aspen Plus V7.1 program is used to model the PC power plant entirely. Utilizing the CAPE OPEN capability in Aspen Plus, other functions can be introduced. This capability will provide a means to use Simulated Annealing and Aspen Plus together to find the solution.⁶

Discussion

The first objective for the project was to establish how some of the variables affect the carbon captured and the power requirements of the power plant. This was done by manually varying a variable and running the flowsheet. The variables explored in this way were the number of trays in the strippers (which is where the solvent is regenerated), the concentration of solvent in the recycle stream, and the reflux ratio in the strippers. The results of these tests are presented later. Before the results, it is important to gain an understanding of the Aspen Plus flowsheet used for the project.

Description of the Aspen Model

Similar to a PC power plant, the Aspen Plus model can be split into three distinct parts: the boiler, the steam cycle, and the carbon absorbers. The focus of this article is on the carbon absorption section, but the other parts are included for completeness. For a detailed description of the power plant components, modeled using Aspen Plus, consult Bhown, A S $,7$ where stream compositions as well as block descriptions can be found.

Boiler

The boiler is modeled using a coal stream and three different air streams feeding into a mixer. This mixer breaks down each of the streams into their elemental components. This is needed because coal is reported to industries as an elemental breakdown, not in terms of molecules. Thus, there is no way to model the combustion reaction using coal molecules. The stream then flows into the boiler, allowing a combustion reaction that produces heat, which is transferred to the steam cycle.

FIG. 3: The carbon curve is located above the legend, while the power is located below in the figure. It is ideal for absorption to be a maximum, while power is at a minimum. For this data, the reflux ratio was set to 1, the feed plate to 2, and the number of trays was set to 20 for all data points. Notice the power consumption for 0 solvent is 0, which is expected because that is the power required to regenerate the solvent. The optimum concentration at these conditions appears to be between

0.3 and 0.5 by mass of MEA.

The boiler also has a second component, which removes the fly ash, then other particulates. In real boilers, this is done at the same time as the combustion, but Aspen Plus requires it to be done in separate processes. Following the boiler, there are several components used to remove mercury, sulfur, and nitrous products from the flue gas.

Steam Cycle

The steam cycle is modeled by utilizing the heat produced by the boiler section to heat water to super critical conditions. That steam is then used to turn ten turbines: three high pressure, two mid pressure, and five low pressure. The final steam product is condensed and recycled to the heat exchanger from the boiler for reheating. The steam section of the PC power plant is the most visually complex part of the Aspen Plus chart, which makes it difficult to graphically display. There are several work streams utilized to combine the power generated from the turbines in a single block, which calculates the total power produced.

Carbon Absorption

In order to develop the dependence curves for different variables, the flow sheet must be fully run at each new condition. The variables tested in this way were the solvent concentration, the number of trays in the strippers, and the reflux ratio in the strippers. After running the chart several pieces of data were collected while preparing the chart for the next run including the condenser and reboiler duty in each stripper as well as the amount of carbon removed from the absorber.

Procedure

In order to develop the dependence curves for different variables, the flow sheet must be fully run at each new condition. The variables tested in this way were the solvent concentration, the number of trays in the strippers, and the reflux ratio in the strippers. After running the chart several pieces of data were collected while preparing the chart for the next run including the condenser and reboiler duty in each stripper as well as the amount of carbon removed from the absorber.

Results

Each of the figures, excluding Figure 1, have been prepared using data collected by running Aspen Plus simulations. There were four variables considered, and the data was collected while varying one of four variables and keeping the other three constant. The four variables

FIG. 4: For this data, the number of trays was set to 20, feed plate at 2, and the concentration of solvent (MEA) was set to 0.3 for all data points. The optimum in this case appears to be around a reflux ratio of 1. The flowsheet incorporated a design specification of

95% absorption of carbon dioxide.

FIG. 5: For this data, the number of trays was set to 20, the reflux ratio to 1, and the concentration of solvent (MEA) was set to 0.3 for all data points. This shows the effect of the feed plate to the strippers on the thermal power requirement.

considered were the number of trays in the strippers, the concentration of solvent into the absorber, the feed plate (or inlet location) for the strippers, and the reflux ratio in the strippers. All of the simulations also incorporate a design specification to absorb as close to 95% of the carbon dioxide as possible. For this reason, the carbon capture percentage is not shown on most figures because the change is minimal in those cases.

In each of the figures, the energy requirement is reported as the summation of the heating and cooling requirements of each column. By examining the figures, one can gain an appreciation of how strongly the considered variable affects the efficiency of the design. Figure 2 considers the number of trays in each stripper. As the number of trays increases, the power requirements of the column are decreased. Figure 4 looks roughly inverted from Figure 2, which is because increasing the reflux ratio, decreases the minimum number of trays needed. As such the reflux ratio and the number of trays are highly intertwined.

Figure 3 represents the effect of the concentration of

solvent being fed into the stripping section. This is the only variable that also shows the percent absorbance of carbon dioxide. This is because the concentration was the only variable that could not always meet the design requirement of 95% absorption of carbon dioxide. The concentration of MEA in the solvent stream has the strongest effect on the overall performance of the absorbance section. It is important to feed in enough solvent to perform the absorption to the design specification, but if too much solvent is fed in (measured by concentration), the power requirement increases rapidly. The ideal concentration of solvent appears to be between 30% and 50% mass percent.

The final considered variable was the placement of the flue gas feed; the results of which are shown in Figure 5. It became more efficient, the lower the feed was placed. This makes sense because the liquid should be fed at the top of the absorber, while the gas should be fed at the bottom for the most efficient absorption. An important thought is that each of these figures can be produced at many combinations of the other three variables, thus the figures only begin to show the complexity of the optimization problem. Clearly, an optimization method is required for this purpose, and Simulated Annealing has been chosen.

Ongoing and Future Work

At this point, the flowsheet is being prepared for Simulated Annealing. This will provide the optimal configuration of the four considered variables. Additionally, a second solvent called DEA is being introduced into the flowsheet. Data will be generated for how the efficiency changes with different mixes of DEA with MEA as well as different concentrations of DEA as the only solvent. Finally, Simulated Annealing will be used again to determine the optimum configuration for the mixture of solvents.

Conclusions and Recommendations

The optimization of carbon dioxide absorbers in a PC power plant involves many different variables. These include the type of solvent(s) used, the concentration of

the solvent(s), the number of trays in the strippers, the reflux ratio in each stripper, and many more. This problem cannot be optimized by hand. Rather, it requires the technique Simulated Annealing, which is a probabilistic method. This allows the method to escape local minima and find the global minima, unlike gradient based methods.

It is clear from the results section that the amount of carbon dioxide and the power requirements for solvent regeneration depend on the selection for reflux ratio, solvent concentration, feed plate location, and number of trays. It is also theorized that there will be a dependence on many more such selections such a second solvent. The optimal selection for each variable would lead to the highest absorption and the lowest requirement of power for solvent regeneration. Simulated Annealing will intelligently sift through the many combinations and find the best choices for the variables. This method is introduced into Aspen Plus using the CAPE OPEN capabilities.

Once the optimal configuration is discovered, it can be used to reduce the impact of retrofitting carbon absorption into power plants. Power plants each have a lower efficiency when operated with carbon absorption than without it. The optimal solution for the carbon absorption section would cause the lowest drop in efficiency. This project has been working on optimizing the carbon absorption in a PC power plant because the majority of power plants in operation are of this type. This type of absorption has been selected as a way to retrofit the current plants with carbon absorption to make them more sustainable. If we are to avoid the ill effects of releasing massive amounts of carbon dioxide into the atmosphere, it is important to introduce this technology into all current and future fossil fuel plants.

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