A modular framework for the analysis and optimization of power generation systems with CCS

David C. Miller*,a, John C. Eslicka, Andrew Leea, Juan E. Morinellya

*aU.S. Department of Energy, National Energy Technology Laboratory, 3610 Collins Ferry Rd, Morgantown, WV 26505, USA

Abstract

A significant number of efforts are underway to develop and assess technologies that will lead to technically and economically viable routes to reduce the CO2 emissions of fossil energy systems, particularly coal-fired power plants. Developing technologies to reduce emissions from these sources is essential for controlling atmospheric levels of CO2 because of the widespread reliance on coal as an inexpensive and abundant energy source. Two major systems-level design challenges exist. The first is how to design new plants that incorporate CCS technology. The second is how to retrofit existing plants to capture CO2. Both design challenges can benefit from an optimization approach, which considers the application of multiple potential technologies and analyzes ways in which the whole plant-wide system can be integrated to increase overall efficiency. This paper will present a modular framework for the analysis and optimization of power generation systems with CCS that helps to meet these design challenges.

In order to more completely understand the economic and operational tradeoffs associated with the various potential carbon capture technologies, and how they can be applied to new and existing plants, a unified, systemic framework has been developed to provide a common basis for evaluation. Given the complexity of the design problem and the fact that new technologies are continually being developed, this framework is modular in nature and incorporates algorithms for the selection, integration and optimization of carbon capture technologies for both new and existing plants. In addition to the framework itself, this paper discusses simulation modules representing various capture technologies and power plant components. The framework provides the means to link the various modules together in order to provide a holistic, system perspective of plant wide operations. Results of analyses and optimization scenarios performed with the framework are also presented.

© 2011 Published by Elsevier Ltd. Open access under CC BY-NC-ND license.

Keywords: CO2; carbon capture; fossil energy; process integration; process modeling; optimization;

* Corresponding author. Tel.: +1-304-285-6550; fax: +1-304-285-4403.
E-mail address: david.miller@netl.doe.gov
1. Introduction

Two major types of carbon capture systems are generally considered for application to power generation systems. Post-combustion systems are intended for application to new or existing pulverized coal (PC), combustion-based power plants. In these systems, CO₂ is typically separated from low pressure flue gas just prior to the stack using absorption, adsorption or membranes. The separation is challenging because the CO₂ is very dilute due to the presence of nitrogen in the air used for combustion. The current baseline technology is chemical absorption into an aqueous amine solution. Pre-combustion systems are typically considered for application to new Integrated Gasification Combined Cycle (IGCC) plants. They typically include a high pressure shift reactor to convert syngas to a mixture of hydrogen and CO₂, which can then be separated. Since most IGCC plants use pure oxygen, the CO₂ is not diluted with nitrogen, simplifying separation. In addition, since the resulting CO₂ stream is already at elevated pressure, the subsequent compression for sequestration is less costly. The current baseline technology is physical absorption via the Selexol process.

Alternative approaches for combustion-based PC plants include oxy-combustion and chemical looping combustion. Both of these approaches eliminate nitrogen from the combustion gas, raising the partial pressure of CO₂ which makes the separation easier. In an oxy-combustion system, oxygen is separated from air and fed to a conventional type of boiler. In a chemical looping system, solid metal particles are circulated between two reactors. In the first reactor, the metal is oxidized in air; in the second, the metal is reduced in the presence of fuel releasing the oxygen to participate in a combustion reaction with the fuel. To varying degrees, these technologies can be applied to existing plants as well as new plants. Oxy-combustion can make use of existing boilers so long as the oxygen concentration is diluted by recycling flue gas or captured CO₂. However, chemical looping would require replacement of the boiler, necessitating a major retrofit. The potential advantage of these approaches is that the combustion gas would have a significantly higher concentration of CO₂ reducing the difficulty of isolating the CO₂ for sequestration.

Given the wide range of power plant designs and technologies available for carbon capture, there is a distinct need for a unified, systemic framework to provide a common basis for evaluation of different combinations of technologies. In response to this, the U.S. Department of Energy’s National Energy Technology Laboratory (NETL) is developing a modular framework for power plants and carbon capture technologies. This project aims to provide a framework within which a wide range of combinations of technologies can be studied and optimized. With the significant investment in research into carbon capture, and the number of potential capture technologies, the framework being developed is modular in nature, to allow for new models to be easily developed and integrated into the framework as new technologies become available.

In order to effectively choose the best option for capturing carbon dioxide from flue gas streams, it is first necessary to assess and optimize the potential alternatives for achieving the desired carbon dioxide removal. However, in addition to the obvious trade-off between CO₂ removal and capital and operating costs, there are additional factors that impact plant performance that must be taken into account. These include additional auxiliary power demands due to the operation of the CO₂ capture units and compression of the captured CO₂, as well as parasitic losses of energy due to the temperature and pressure requirements of the carbon capture units. These effects can have a significant effect on the overall efficiency and performance of a power plant and could affect the choice of carbon capture technology to be employed under a given set of circumstances; thus, they need to be considered during the optimization process. This requires the use of multi-objective optimization techniques in order to assess the behaviour of the system, and to determine the “best” solution to the given problem.

To date, much assessment of potential carbon capture technologies has been done on a stand-alone basis, without considering the effects of integrating the carbon capture unit within an actual power plant. However, the addition of a carbon capture unit will have a significant effect on the overall performance of the plant, through changes to operating conditions, parasitic losses, additional auxiliary power demand and increases in operational costs. In all, the addition of carbon capture units to power plants will have a significant impact beyond the recovery of CO₂, affecting the output and cost per megawatt of electricity. Thus, it is important to perform studies and optimizations on the plant level, rather than just the carbon capture unit. This also allows for better analysis of heat integration and other effects, potentially reducing the loss of efficiency incurred by the addition of carbon capture units.
2. Modular Framework

The modular framework currently being developed at NETL is designed to allow easy integration and optimization of a wide range of modules representing the various parts of a power plant. The modular framework consists of an overarching framework that allows the connection of modules representing individual components or processes of the overall power plant. Individual modules connect to the framework via a common interface, allowing any combination of modules to be assessed. The modules themselves maybe developed in any software environment that can interact with the connection interface. Once a potential power plant design has been constructed by connecting the desired modules within the framework, the entire design can be optimized by manipulating the decision variables within the system and monitoring the outputs. Figure 1 shows an example of the NETL Modular Framework for Design and Optimization linking an existing PC power plant, CO₂ capture unit and compression train.

Figure 1. An example of the modular framework.

Currently, the commercial software modeFRONTIER® (ESTECO s.r.l.) [1] is used to provide the framework for connecting the modules and to perform the multi-objective optimizations of the system. modeFRONTIER allows for the integration of models developed in number of different software environments in a simple graphical interface. modeFRONTIER includes a range of different optimization algorithms for different situations, including single and multi-objective methods for discrete and continuous variables. Optimizers include implementations of genetic algorithms, simulated annealing, game theory and particle swarms, as well as a number of simpler algorithms. A wide range of data visualization tools are also included to aid data analysis, with features such as response surface methodologies and multi-criteria decision making tools.
The individual modules representing each of the components of the system have been developed using Aspen Plus® and Aspen Custom Modeler® (ACM) (Aspen Technology, Inc.). Aspen Plus is a well established process modeling environment, and contains models for a wide range of common unit operations found in industry. Aspen Custom Modeler allows for the development of additional unit operations to be employed in Aspen Plus simulations, either to represent processes not included in Aspen Plus, or to provide more detailed models for existing Aspen Plus unit operations. This is especially important for processes with slow kinetics (such as many solid adsorbents) where equilibrium is not achieved within the system, thus requiring a model that considers the reaction kinetics and material residence times.

The interface between Aspen Plus and modeFRONTIER is currently achieved using Visual Basic and Microsoft Excel. Each component of the power plant and carbon capture process is implemented as an Aspen Plus simulation, which is then linked to an Excel workbook to create a module. The entire power plant is then constructed in modeFRONTIER by connecting the Excel workbooks together in the desired combination. Different combinations of technologies and equipment can be examined by simply adding and removing different modules as desired. Additionally, by using Excel as an intermediary, it is possible to perform additional calculation outside of the Aspen Plus environment if desired, such as estimating capital costs.

Future goals of the project are to use the modular framework to develop reduced order models for the different modules coupled with derivative free optimization techniques to reduce the computational requirements for the optimization. These models will be used to search for the general location of the optima, whilst the more detailed models will be used for fine tuning of the system parameters. Work is also underway to enable superstructure-based process synthesis to facilitate the consideration of multiple process configurations in finding the optimum.

3. Power Plant and CCS Modules

Among the goals of the modular framework project at NETL is to develop a comprehensive library of modules for coal-based power plants and carbon capture technologies. To date, efforts have been focused primarily on developing models for a baseline sub-critical pulverized coal power plant and various carbon capture technologies, including aqueous amine absorption, solid sorbents and membrane separators. A brief outline of the modules developed thus far is given below.

Power Plant Modules

Fossil fuel power plants provide a large portion of the world's electricity output and come in a wide range of sizes and types. Existing types of fossil fuel power plants include coal-fired power plants operating at sub-critical, super-critical and even ultra-critical conditions, as well as natural gas combined cycle, oil-fired, oxy-fired and IGCC units.

A baseline model has been developed in Aspen Plus for a subcritical pulverized coal power plant generating a net output of approximately 550MW. The steam cycle used in the model contains a high pressure turbine stage, two intermediate pressure turbine stages and four low pressure turbine stages, with a steam flow rate of 3,670,000 lb/hr at normal operating conditions. In order to be able to better account for the effect of steam extraction, detailed designs of the boiler feed water heaters and condenser were conducted using Aspen’s Exchanger Design and Rating tool. In addition, the steam turbines include correlations to account for the effect of lower steam flow rates in the final stages.

The module also includes models for the boiler and flue gas desulfurization (FGD) unit. A submodel of the cooling tower allows evaporative water to be estimated. Coupled with the detailed condenser model, the effect of different cooling water temperatures on overall plant efficiency can also be evaluated. The model includes numerous correlations for process efficiency losses, such as steam leakage through the turbine seals. The plant model has been validated against a similar operating plant. More details on the sub-critical power plant model will be published in the near future. An analogous model for a super-critical PC power plant is under development.
**Amine Scrubbing Module**

Currently, the main commercial technology for capturing CO₂ from flue gas is by absorption using aqueous amine solutions. Amine scrubbing is a well-established technology, and a number of commercial technologies are available. Amine scrubbing processes use aqueous solutions of various amines to absorb CO₂ from the flue gas, before being regenerated via a temperature swing in a desorption column. A significant drawback to amine scrubbing is that they have a significant energy demand due to the large amounts of water used within the system. Amine solutions are corrosive, requiring the amines to be heavily diluted with water, resulting in significant energy demands to achieve desorption.

Aspen Plus was used to model an amine scrubbing system for the modular framework. The absorber and regenerator were modeled as columns using staged equilibrium calculations. The solvent used in the current module is a 30wt% aqueous solution of monoethanolamine (MEA). Flue gas from the FGD unit of the power plant module is first fed to a cooler and flash drum to reduce the gas temperature and to remove any condensate. The gas then enters the bottom of absorber column, where it is contacted counter-currently with the amine solution. A scrubbing section was added to the top of the absorption column to remove any amine that leaves the column, before the scrubbed gas is vented to the stack. The rich amine solution leaves the bottom of the absorption column.

The rich amine solution then enters a heat exchanger where it is preheated using hot regenerated amine solution from the regenerator. It is then fed to the regenerator, which is a column with a condenser and a reboiler. The reboiler uses steam from the power plant’s steam cycle. The regenerated amine solution is the returned to the hot side of the preheater, followed by a further heat exchanger to reduce the solution temperature before being returned to the absorber. Additional water is required to operate the condenser, absorber cooler and flue gas cooler, as well as make-up water for the amine solution.

**Solid Sorbents Modules**

One potential alternative to liquid solvent currently being investigated for the purposes of CCS is solid sorbents. Similar to liquid solvents, solid sorbents can be used to adsorb CO₂ from a gas stream and can be regenerated at higher temperatures. The main advantage of solid sorbents is that they generally require less energy to regenerate than liquid solvents, due to significantly lower heat capacities.

A number of different technologies exist for contacting gasses and solids that are applicable to carbon capture from flue gas. Common units are fluidized beds (both bubbling and fast fluidization), fixed beds and moving beds. Thus far, a model for bubbling fluidized beds has been developed in ACM for the modular framework that can be used to model both adsorbers and regenerators. The bubbling fluidized bed model is based on the model proposed by Kunii and Levenspiel [2], which depends on the behavior and characteristics of the bubbles within the bed. The model assumes that the fluidized bed consists of three phase: bubbles of gas rising through the bed, clouds of gas and solids associated with each bubble and an emulsion of gas and solids at minimum fluidization conditions.

The initial size and growth of the bubbles is predicted using the correlation of Mori and Wen [3], and the bubble velocity is described by the equations of Hilligardt and Werther [4]. Heat and mass transfer occurs between the contacting phases within the bed and is related to the size and velocity of the gas bubbles via the work of Sit and Grace [5]. Chemical reactions can occur between gas and solids wherever they are in contact, and the rate of reaction is defined by the equilibrium and kinetics of the reaction.

The bubbling fluidized bed model is entirely predictive, requiring only system inputs such as flue gas and sorbent compositions and feed rates in order to solve. The model is able to predict the CO₂ removal, reactor geometry and number of units required to process a given flue gas stream. In addition to the module for bubbling fluidized bed reactors, modules are also being developed for fast-fluidized conditions, as well as fixed and moving bed reactors.
The introduction of membrane technologies in power generation processes has gained interest in the recent literature as a viable option to mitigate CO₂ emissions. Gas permeation systems have been successfully applied to industrial processes such as acid gas removal from natural gas since the early 1980s [6]. However, post-combustion CO₂ capture using gas permeation is currently at a research and development stage.

The parasitic energy load of a carbon capture membrane process arises from the required compression or vacuum necessary to create the pressure difference across the selective layer to achieve the desired separation. A membrane system is advantageous because it does not require large amounts of water or solvents, and its non-moving, modular components are easy to operate and maintain. A recent simulation study by Merkel and collaborators states that a capture cost of $23/ton CO₂ can be achieved with a two-step counter-current sweep process [7]. In this process the flue gas is passed through the first membrane unit, where a vacuum pump is used to create a pressure drop across the membrane to improve separation. The partially cleaned flue gas is then passed to a second membrane unit, which uses atmospheric air as a sweep gas to improve recovery. The clean flue gas from this unit is vented to the stack, whilst the sweep gas and recovered CO₂ is used as feed air for the coal combustion. The gas stream recovered from the first membrane unit contains all the recovered CO₂ and is sent for compression and sequestration.

In order to evaluate the performance of membrane processes under the modular framework, rigorous hollow fiber gas permeation modules have been developed in ACM. The modules can be simulated with or without a sweep streams and are capable of predicting the associated permeate pressure drop. A detailed transport mechanism across the porous support for asymmetric membranes is included in the model. Simplified spiral wound simulation modules are also under development.

CO₂ Compression

An often neglected aspect of carbon capture processes is the pressurization of the final CO₂ stream to 2000+ psia. This process uses considerable energy (approximately 0.1 MW per MWnet of plant output). As such, it is important to optimize and potentially integrate this process with other portions of the overall power plant. Currently, a simple model for the compression of the captured CO₂ to a final pressure of 2020 psia has also been developed for use in the modular framework. The model consists of five compressions stages with intermediate intercoolers to remove moisture from the gas stream and to reduce the power requirements of the compressors by cooling the gas. The compression module also contains correlations to estimate the cost of the compressors and heat exchangers, and it allows for optimization of a number of design and operating parameters.

4. Results

As an example of the use of the modular framework, a study was performed to optimize the performance of a 550 MWnet sub-critical power plant with amine scrubbing using monoethanolamine and CO₂ compression in terms of capital cost and efficiency. The modular framework was used to connect the three modules together. Steam is extracted from the power plant to provide the heat for the reboiler of the absorber. The electrical requirements for blowers, pumps and compressors reduce the net power output of the plant.

modeFRONTIER was used to perform a multi objective optimization of the system, in order to minimize the Net Unit Heat Rate (NUHR) and estimated capital cost per MWnet whilst removing 90% of the CO₂ from the flue gas stream. The decision variables used in the optimization are shown in Table 1 and represent the key variables in the amine scrubbing and compression modules. Reflux ratio and distillate to feed ratio in the regenerator indirectly control the lean loading in the solvent. The Non-dominated Sorting Genetic Algorithm II (NSGA-II) [9] implemented in modeFRONTIER was used to perform the multi objective optimization and to locate the Pareto front. 25 initial designs were generated using the Uniform Latin Hypercube method for the optimization and the algorithm run for 30 generations.
Table 1. Decision variables for system optimization.

<table>
<thead>
<tr>
<th>Description</th>
<th>Lower Bound</th>
<th>Upper Bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature of the flue gas cooler (°F)</td>
<td>100</td>
<td>125</td>
</tr>
<tr>
<td>Temperature of the absorbent cooler (°F)</td>
<td>100</td>
<td>150</td>
</tr>
<tr>
<td>Number of Absorber Stages</td>
<td>10</td>
<td>20</td>
</tr>
<tr>
<td>Number of Stripper Stages</td>
<td>7</td>
<td>14</td>
</tr>
<tr>
<td>Stripper Feed Stage</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>Molar Reflux Ratio</td>
<td>0.25</td>
<td>0.8</td>
</tr>
<tr>
<td>Molar Distillate to Feed Ratio</td>
<td>0.03</td>
<td>0.08</td>
</tr>
<tr>
<td>Compressor Intercooler Temperature (°F)</td>
<td>90</td>
<td>150</td>
</tr>
</tbody>
</table>

Figure 2 show the optimization results for the two objective functions. Normalized capital costs are presented in this paper because space limitations do not allow for a complete description of the details and assumptions used in our calculations. Such details will be presented in a subsequent journal article. The best designs are along the Pareto front (indicated by the black curve) which illustrates that decreasing one objective will increase the other. These results demonstrate how adjusting the parameters of the carbon capture and compression processes and their integration into the overall power plant can have a significant effect on the cost and performance of the plant as a whole. For this study, the estimated capital cost for installing the carbon capture equipment varies by nearly 30% across the whole design space (not shown) and over 10% near the Pareto front, indicating the potential improvements that can be obtained using optimal designs. The optimization also reveals potential reduction in the NUHR (related to operating costs), demonstrating the value of performing multi objective optimizations of potential designs. This value could be further increased by considering additional carbon capture technologies, which could offer significantly different tradeoffs. By carefully studying these results and considering the specific requirements of a given project, the modular framework has the potential to significantly improve the final design selected for a carbon capture project.

Figure 2. Optimization of relative capital cost per net MW of electrical power produced versus Net Unit Heat Rate.
5. Conclusions

The NETL modular framework for the evaluation and optimization of power plants and carbon capture technologies provides a unified, systematic means of analyzing and comparing different combinations of technologies in order to determine optimal plant configurations for achieving cost-effective and efficient removal of carbon dioxide from power plant flue gases. Modules of several types of power plants and carbon capture technologies have been developed to demonstrate the capability of the system. From the results to date, the value of the system is demonstrated in the increased understanding of the interaction among conflicting objectives. In particular, it is clear that single designs are inadequate to understand the true potential of a given technology. The bulk of the design points in Figure 2 are not Pareto designs, meaning that they can be improved on the basis of both objectives. Thus, when comparing competing technologies for carbon capture, they should ideally be compared on the basis of optimized designs based on common criteria.

As new carbon capture technologies are developed, the framework’s modular design will allow new simulation modules to be developed and integrated. Since the framework allows for a wide range of different conditions and technologies to be analyzed on common basis, it will serve as a useful tool for the unbiased comparison of different alternatives.

References

1. ESTECO. modeFRONTIER, Trieste, Italy: ESTECO; 2010