The Role of Process Synthesis in the Systematic Design of Energy Efficient Fossil Fuel Power Plants with CO₂ Capture

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CO₂ capture and storage has a potential of reducing CO₂ emissions from large point sources such as fossil fuel power plants. CO₂ capture is associated with substantial capital expenditures, operational expenditures dominated by high energy use and potential operational restrictions on the underlying industrial processes. The main focus of significant research efforts worldwide is thus to reduce investment costs and improve efficiency of capture technologies. The systematic methodologies developed in our group at SINTEF/NTNU for design of energy efficient fossil fuel power plants with CO₂ capture are presented and show the importance of utilizing process synthesis in the design of such plants. These methods range from targeting minimum capture work for different CO₂ capture processes, optimization methods for process design of pre- and post-combustion capture processes, developing surrogate models for optimization.

1. Introduction

Fossil fuels, such as coal and natural gas, have been the primary source for power generation since the beginning of the twentieth century and are expected to form a significant portion of future energy portfolio. In a carbon constrained energy scenario, CO₂ capture and storage (CCS) has a potential of reducing CO₂ emissions from large point sources such as fossil fuel power plants. CO₂ capture is associated with substantial capital expenditures, operational expenditures dominated by high energy use and potential operational restrictions on the underlying industrial processes. The main focus of significant research efforts worldwide is thus to reduce investment costs and improve efficiency of capture technologies. Power plants have been built and improved using well established designs based on engineering thermodynamics, engineering judgement and operational experience. This has been mainly due to the simple configuration of these units compared to chemical processing plants. Efficiency improvements in fossil fuel based power plants are also to a large extent achieved through breakthroughs in materials of construction of the boiler, gas turbine or steam cycle components. Traditionally, there have been no significant efforts to utilize systematic methods to improve the efficiency of power plants apart from exergy analysis of these units to identify sources of efficiency loss. However the inclusion of CO₂ capture in fossil fuel power plants adds increased complexity in these units. They are characterized by a large number of design parameters that can be varied in order to achieve an energy efficient configuration. Engineering judgment based heuristics and sensitivity studies have been the main focus in developing "optimal" designs. In this context process synthesis and process integration have a significant role to play in the design of carbon capture systems integrated with power plants. Glaser et al. (2009) showed that savings in energy and cost can only be partly attributed to decisions made at the unit level while the significant portion of savings arise from optimal interaction between process units.

Process synthesis is the systematic generation of alternative process flowsheets and selection of a design whose configuration and parameters optimize a given objective function (Smith, 2005). Process integration is similar to process synthesis with an emphasis on energy efficiency and sustainability. Process integration is defined to be the systematic and general methods for designing integrated production systems, ranging from individual processes to total sites, with special emphasis on the efficient use of...
energy and reducing environmental effects (Gundersen, 2002). Process synthesis methods and tools have been evolving in response to challenges faced by the chemical process industry. The three broad classes of process synthesis methods are briefly described below:

- **Heuristics**: Heuristic rules and assumptions based on experience and engineering judgment have been used in all aspects of engineering. Heuristics are required to solve many of the problems industry poses as they can be used to reduce the solution space.
- **Thermodynamics**: Thermodynamic methods have been used to identify design targets before the design process. Insight obtained while developing concepts and procedures for targeting is used in the design phase by providing guidelines for the design. In addition, knowledge about target values can be used to check the quality of the design.
- **Optimization**: The first step in this method is to create a superstructure that embeds all feasible process options and interconnections that are possible optimal candidates. The design problem is formulated as a mathematical model with an objective function and a set of constraints.

It is worthwhile keeping in mind that heuristics, thermodynamic methods and optimization are rarely used as stand-alone methodologies in an industrial design process. It is common to define the synthesis problem as an optimization model and use thermodynamics and heuristics to reduce the solution space and hence numerical complexity.

There have been recent efforts to develop methodologies for optimal synthesis of power plants with CO$_2$ capture. Agarwal et al. (2010a, 2010b) present methods for integration of pressure swing adsorption process in post- and pre-combustion capture routes respectively. There is significant scope for methodologies for utilizing process synthesis methods to increase the efficiency of power plants with CO$_2$ capture. This paper provides an overview of three systematic process integration methodologies developed by SINTEF Energy Research and NTNU for design of energy efficient fossil fuel power plants with CO$_2$ capture. The first methodology presented falls under the thermodynamic method category of process synthesis while the other two fall under the optimization method category.

### 2. Thermodynamic benchmarking of CO$_2$ capture processes using minimum work targets

Identifying ways to increase the efficiency of power plants with CO$_2$ capture is important to ensure economic viability of the process. While there have been significant developments in the various capture processes in the three routes for CO$_2$ capture, there is no consistent and systematic approach to compare the processes and identify scope for further improvement.

An important aspect of Process Integration is establishing targets prior to design. The target efficiency for such processes will be a process scheme that requires the thermodynamically lowest possible energy input to produce the specified energy output. The resulting efficiency is the "ideal" efficiency which is the thermodynamic maximum attainable for such a process. This efficiency can never be achieved in practice as it requires perfectly reversible processes, but provides a thermodynamic target for process design.

The first law efficiency attainable by employing state-of-the-art technology can be thought of as a technology limited efficiency, and the difference between the thermodynamic limited and technology limited efficiencies quantifies the theoretical improvement potential and is a benchmark for the process. Additionally, the source(s) of this difference in efficiency can point to possible future direction for technology development (Anantharaman et al., 2012c).

#### 2.1 Methodology and results

The ultimate goal of the methodology is to increase the understanding of power plants with CO$_2$ capture, to identify the most promising capture technologies and to pinpoint what technology improvements should be most beneficial to pursue. The first step in the methodology is establishing minimum work targets to evaluate the maximum efficiency limited by thermodynamics. This limit is achieved by defining an ideal (reversible) process. A set of non-idealities in the form of technological limitations are added systematically in series to go from the thermodynamics limited to the technology limited cases. The difference between the thermodynamics limited and technology limited efficiencies can thus be attributed to the different sets of irreversibilities and quantified. This is represented visually in Figure 1.

The minimum capture work target is evaluated without defining any details of the configurations of the unit operations involved. The conceptual design of such processes is done by considering the reversible process unit defined by a set of inputs and outputs. Since ideal reversible processes are considered, the calculations are independent of the different possible process layouts and specifications for any capture route. More specifically, this approach means that for instance in post-combustion capture, no consideration of solvent or capture unit performance is included. Details on defining ideal CO$_2$ capture processes is given in Anantharaman et al. (2011, 2012c).
The thermodynamic minimum penalty for ideal processes calculated for different fuels for the three different capture routes, as shown in Figure 2. The methodology was applied to benchmark ideal CO₂ capture process routes with four fuels of differing HC ratio. The efficiency penalties are in the range 1.8-3.6 % points. The capture penalties for "real" power processes are quoted to be in the range of 8–15 % points in literature. This indicates that there should be room for technology improvements, while keeping in mind that regardless of technology development some irreversibilities will always be unavoidable.

Figure 1: Representation of systematic targeting and benchmarking of CO₂ capture processes

Figure 2: Efficiency penalty (in % points) for the three capture routes with fuels of different HC ratio

3. Energy integration in an NGCC plant with post-combustion CO₂ capture

Natural gas combined cycles (NGCC) is expected to play an important role in a future power system with a high share of renewables due to their relatively rapid load-changing capability. Within the field of post-combustion capture, the use of amine-based solvents have received the most attention and is beginning to reach commercial-scale implementation, e.g. at the Boundary Dam project in Canada. While there has been considerable attention devoted to different process configurations of the amine-based capture unit for decreasing energy penalty, there has been no significant effort towards a systematic method to optimally integrate a post-combustion MEA capture unit with an NGCC. The work presented by Anantharaman and Berstad (2012b) is the first effort to design optimal design of NGCC with post-combustion amine-based capture unit and is described in the following sub-section.

3.1 Methodology and results
The three main aspects of the plant that affect the overall process efficiency are heating, cooling and electric power. In other words the magnitude of the quantities at the interface between the power island, CO₂ capture unit and CO₂ compression train and how they interact with each other determines the overall
process efficiency (see Figure 3). Rather than evaluate these interactions manually to find the `best` plant configuration, this work presents a simulation-optimization methodology for process synthesis.

Figure 3: Interaction between different units in an NGCC with post-combustion CO₂ capture

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The results obtained show that direct integration of the reboiler in the CO₂ capture unit with the heat recovery steam generator (HRSG) results in an efficiency improvement of 0.4% points compared to the standard way of integration at IP/LP crossover. The number of pressure levels in the steam cycle goes from a 3 pressure level cycle in the base case to a 1 pressure level cycle.

A study of the part load operation of the NGCC with and without CO₂ capture using the integration option derived by using the methodology described above and is compared to the standard IP/LP crossover steam extraction case (Jordal et al., 2012). The results show that both options exhibit similar operational performance at full and part-load. The process option with direct integration of 40% of the reboiler into the HRSG results in a single pressure level steam cycle and the heat transfer area can be reduced with 38%.

4. Design of optimal Integrated Reforming Combined Cycle with CO₂ capture

Integrated Reforming Combined Cycle (IRCC) is a promising route for combined power generation and hydrogen production with CO₂ capture from natural gas. The design of an IRCC involves many parameters that interact in complex relationships resulting in several potential integration possibilities between the reforming, water gas shift, CO₂ capture units and the power cycle. Heat integration and design of the steam cycle forms a crucial aspect of the process design and these depend on the operating parameters of the process. Some of the parameters to be optimized in the reforming and water gas shift process are: (1) reformer operating pressure, (2) natural gas feed temperature to reformer, (3) reformer steam to carbon ratio, (4) HTS feed temperature and (5) LTS feed temperature. (Anantharaman et al. 2012a).
4.1 Methodology and results

The first step in process design is to a superstructure to embed potential unit operations in the process and all relevant interconnections among them. To reduce the complexity of incorporating reforming and water gas shift reactions in an optimization framework, surrogate models are used for these process units. Surrogate models are multivariable general purpose mapping models to be used in an optimization framework. The surrogate model of the reforming and water gas shift process is developed using a regular Latin hypercube sampling (LHS) and polynomial regression. Figure 5 shows a pictorial representation of the optimization methodology and implementation. A novel Mixed Integer Linear Programming (MILP)
model for simultaneous optimization and heat integration of chemical processes is used for target for maximum work and thus steam pressure levels and flows. The steam path superstructure shown in Figure 4 is used in this work also. This is used in detail heat exchanger network synthesis using the Sequential Framework for heat exchanger network synthesis (Anantharaman et al, 2010). The Mixed Integer Non-Linear Program (MINLP) formulation of the IRCC is modeled in GAMS using BARON as the solver. Details on model formulation are found in Johnsen (2011). Optimization of the process results in novel process configurations that have an efficiency of 49.4% with CO₂ capture. One of the novel aspects of the optimized process configuration is that only 1 pressure level steam cycle is selected, rather than the normal practise of assuming a 3 pressure level steam cycle.

5. Conclusions

Fossil fuel power plants with CO₂ capture are characterized by a large number of design parameters that can be varied in order to achieve an energy efficient configuration. Engineering judgment based heuristics and sensitivity studies have been the main focus in developing "optimal" designs. In this context process synthesis has a significant role to play in the design of carbon capture systems integrated with power plants. Three systematic process integration methodologies developed for design of energy efficient fossil fuel power plants with CO₂ capture were presented and showed the potential of utilizing process integration techniques in the design of fuel fired power plants with CO₂ capture. Further work will involve developing suitable methodologies applicable to the wide range of CO2 capture technologies available. An issue that has received little attention is the design of such plants incorporating details of the capture units and part-load performance characteristics. It is widely accepted that fossil fuel power plants with CO₂ capture are expected to change roles from being base-load power plants to load-following units. Thus incorporating part-load performance in design is important to ensure "good" operational characteristics at relevant load conditions.

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