Systems Analysis of Advanced Power Plant Carbon Capture Technologies

Investigators

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Abstract

This project is developing a flexible but powerful systems analysis modeling capability that relates the multiple design and performance parameters of fossil fuel electric power generation systems to the process parameters and material properties that influence the overall performance and cost of carbon capture technologies applied to reduce atmospheric emissions of CO_2. The team has developed preliminary performance and cost models for evaluating new materials used for carbon capture. These models will be incorporated in the Integrated Environmental Control Model (IECM) framework developed by Carnegie Mellon University to provide a common platform for conducting comparative analyses of emergent capture technology options for different types of power plants. We will employ the enhanced IECM for advanced carbon capture options to examine their environmental impacts and to determine the primary technical targets necessary to meet cost goals for power plants with carbon capture and storage. The expanded IECM will be used to help identify the most promising new options and R&D goals for advanced capture technologies.

Introduction

To mitigate climate change, carbon capture and storage (CCS) is a key technology option for deeply cutting carbon dioxide (CO_2) emissions from fossil fuel power plants [1]. Adding today's amine-based CCS to pulverized coal (PC) power plants for 90% CO_2 capture would increase the plant cost of generating electricity by roughly 70% to 80% and incur an energy penalty of about 25% to 40% [2]. Thus, there is a strong research focus on developing advanced capture processes having lower energy penalties and lower overall cost than current systems. Given a wide range of activities and approaches to advanced carbon capture, there is a strong need for a system-level analysis to provide "a common ground" to evaluate emergent carbon capture technologies.

Background

The systems model will employ and substantially expand the Integrated Environmental Control Model (IECM) framework developed by Carnegie Mellon University [3]. This model, rooted in fundamental mass and energy balance principles, can be used to conduct comparative analyses of emergent capture technology options for different types of power plants, including rigorous treatment and analysis of uncertainties, which are especially prevalent in emerging technologies.

A core element of this project is the development of models to characterize several emerging CO_2 capture processes being developed with GCEP funds by other university research teams. These involve the use of materials including ionic liquids (ILs) for pre-combustion capture (University of Notre Dame), and metal organic frameworks (MOFs) (Northwestern University) and activated carbon (Stanford University) for post-combustion capture. In this project we propose to substantially expand the IECM to explicitly include models of these advanced CO_2 capture processes, plus the capability to include a life cycle analysis of substances used for CO_2 capture.

Results to Date
The team evaluated ILs, MOFs, and activated carbon used for CO_2 capture. The team has assessed the status of available data on material properties and process in consultation with other GCEP researchers and developed technical and economic models for capture systems. All the models are currently coded in the MATLAB environment.

Results for Absorption Processes
This section reports our research results to date on ILs, which employ physical or chemical absorption processes to capture CO_2 from a mixed gas stream at IGCC plants.

Development of a Multistage Equilibrium Model for Gas Absorption
Absorption of CO_2 using ILs is considered as a steady-state vapor-liquid process consisting of a number of stages. Equilibrium is assumed to take place between vapor and liquid streams leaving each stage. A multi-stage equilibrium model is established to simulate the absorption process. The multi-stage process model takes into account the mass balance (M), equilibrium (E), summation (S), and enthalpy balance (H).

M*ass balance for each component at each stage (j)*:
$$L_{j-1}x_{i,j-1} - L_j x_{i,j} + V_{j+1}y_{i,j+1} - V_j y_{i,j} = 0$$

E*quilibrium for each component at each stage (j)*:
For physical absorption processes, the vapor-liquid equilibrium (VLE) is described in terms of a K-value as:

$$y_{i,j} = K_{i,j} \cdot x_{i,j} = \left(\frac{\emptyset_{i,j}^L}{\emptyset_{i,j}^V} \right) \cdot x_{i,j}$$

The K-value relates the vapor and liquid mole fractions and provides the basis for modeling the phase equilibrium based upon equations of state (EOS). The fugacity coefficient based on a generic Redlich-Kwong (RK) type of cubic EOS with binary interaction parameters is described as [4-5]:

$$\ln\emptyset_i = \ln\frac{RT}{P(V-b)} + \left(\frac{\partial nb}{\partial n_i}\right)\left(\frac{1}{V-b} - \frac{a}{RTb(V+b)}\right) + \frac{a}{RTb}\left(\frac{\left(\frac{\partial na}{\partial n_i}\right)}{a} - \frac{\left(\frac{\partial nb}{\partial n_i}\right)}{b} + 1\right)\ln\frac{V}{V+b}$$

For chemical absorption processes, a Langmuir-type absorption model that incorporates both the stoichiometric reaction and physical uptake is used to describe the equilibrium [6]. Total CO_2 uptake on the basis of mole ratio is predicted in terms of CO_2 pressure, Henry's law constant, and reaction equilibrium constant as [6]:

$$X_{co2,j} = \frac{n_{CO2}}{n_{IL_o}} = \frac{P_{CO2,j}/Hn_j}{1 - P_{CO2,j}/Hn_j} + \frac{k_{1,j}P_{CO2,j}C_3}{1+k_{1,j}P_{CO2,j}}$$

Summation based on mole fractions for each stage (j):

$$\sum y_{i,j} = 1$$

$$\sum x_{i,j} = 1$$

Enthalpy balance for each stage (j):

$$L_{j-1}h_{j-1} - L_j h_j + V_{j+1}H_{j+1} - V_j H_j + \Delta H - Q = 0$$

There is no reaction heat term for physical absorption. For chemical absorption, the energy requirements (ΔH) for solvent regeneration include the solvent heating and enthalpy of reaction plus heat of water vaporization if the water vapor is considered.

Development of Engineering-Economic Models

This study employs the costing method and nomenclature of the Electric Power Research Institute's Technical Assessment Guide [7]. The performance model discussed above are linked to engineering-economic models that estimate the capital cost, annual operating and maintenance (O&M) costs, and total annual levelized cost of electricity (LCOE) for an IL-based CCS system.

The total capital requirement (TCR) of a CO_2 capture system includes the direct process facilities (PFC) cost plus a number of indirect cost categories. The direct cost components include the absorbers, flash drums, solvent circulation pumps, sump tanks, heat exchangers, process stream compressors, CO_2 product compressors, and hydraulic power recovery turbines. The estimation approach developed by Chen (2005) for Selxol-based CO_2 capture systems is adopted to estimate the individual component costs [8]. The indirect costs such as the general facilities cost (GFC) and engineering and home office fees are estimated empirically as a percentage of PFC. The process contingency depends on the status of technology development and is estimated as a percentage of PFC, whereas the project contingency depends on the project design level and is estimated as a percentage of the sum of PFC, GFC and process contingency. Other indirect cost categories considered include interest charges, royalty fees, preproduction cost, and inventory capital cost.

Variable O&M costs include IL makeup, power use, and CO_2 transport &storage if applicable, while fixed O&M costs include operating labor, maintenance costs, and administrative and support labor costs. Variable O&M costs are estimated as the product of the quantity used times the unit price. Operating labor is estimated in terms of hourly labor rate, personnel per shift, and number of shifts. Total maintenance cost is estimated empirically as a percentage of total plant cost, while administrative and support labor is estimated as a percentage of operating plus maintenance labor.

Pre-combustion CO$_2$ Capture System Using ILs as a Physical Solvent

The systems analysis for a pre-combustion capture process started with physical absorption for CO$_2$ capture. The ionic liquid, 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([hmim][Tf$_2$N]), is selected for capturing CO$_2$ from the shifted fuel gas mixture mainly because of its stability, low viscosity, and low water solubility [9]. Figures 1(a) and (b) show the solubility of CO$_2$ and H$_2$ in a binary system, respectively. The vapor-liquid equilibrium model based on the RK EOS is further adjusted by incorporating additional binary interaction parameters of CO$_2$ and H$_2$ and then applied to predict the simultaneous solubility of CO$_2$ and H$_2$ in a tertiary system.

(a)   (b)
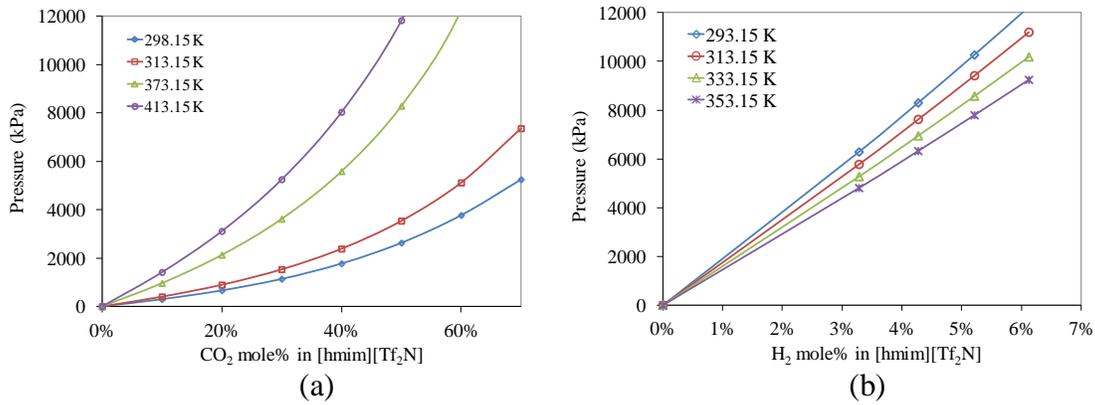
Figure 1. PT-*x* phase diagram of CO$_2$ and H$_2$ in [hmim][Tf$_2$N]
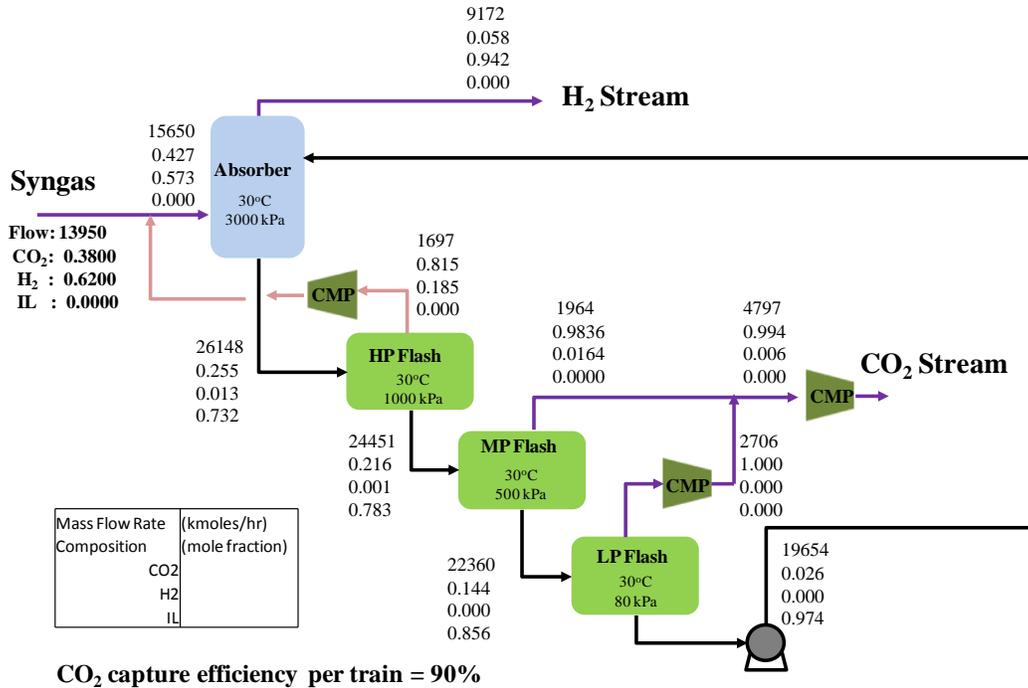
Figure 2. A Pre-combustion CO$_2$ Capture System Using [hmim][Tf$_2$N]

The phase equilibrium correlations of CO_2 and H_2 in [hmim][Tf$_2$N] based on the RK EOS are integrated in the newly developed multi-stage process model for the gas absorption that uses [hmim][Tf$_2$N] as the solvent for pre-combustion CO_2 capture. Figure 2 shows the capture process configuration adopted for the analysis: CO_2 is absorbed by [hmim][Tf$_2$N] in a packed column, and the CO_2-rich solvent stream out of the absorber is regenerated in pressure-swing flash drums arranged in series.

Table 1 Major Technical and Economic Parameters and Assumptions

Category	Parameter	Unit	Value
Performance	Syngas flow rate	kmol/hr	27900
	Syngas pressure	kPa	3000
	Syngas temperature	^{o}C	30
	CO_2 concentration	%	38
	CO_2 removal efficiency	%	90
	Number of trains	#	2
	Capacity factor	%	75
	Absorber pressure	kPa	3000
	High pressure in flash drum	kPa	1000
	Middle pressure in flash drum	kPa	500
	Low pressure in flash drum	kPa	80
	Lean-solvent temperature	^{o}C	30
	Temperature in HP/MP/LP flash drums	^{o}C	30
	Solvent loss rate	kg IL/t CO_2	0.23
	Compressor efficiency	%	80
	Pump efficiency	%	75
	Power recovery turbine efficiency	%	75
	CO_2 product pressure	MPa	15.3
Cost	Fixed charge factor	fraction	0.113
	Discount rate	%	7.09
	Construction time	yr	3
	General facilities capital	% PFC	10
	Engineering & overhead fees	% PFC	7
	Process contingency cost	% PFC	30
	Project contingency cost	% PFC+ GFC+ Process Contingency	30
	Royalty fees	% PFC	0.5
	Misc. capital cost	%TPI	40
	Inventory capital	%TPC	30
	Total maintenance cost	%TPC	5.0
	Labor fee	$/hr	34.65
	Solvent makeup cost	$/t	1000
	Electricity price	$/MWh	50

Table 1 summarizes the major technical and economic parameters and assumptions for the IL-based capture system. The capture system consists of two trains that are designed to be an isothermal process for 90% CO_2 capture. Both the absorption and stripping vessels are designed to operate at 30^oC. The CO_2 in the syngas is absorbed at 3000 kPa, whereas the CO_2-rich solvent is regenerated in the three flash drums with decreasing pressures from 1000 kPa to 80 kPa. Figure 2 also shows the mass flow rate and composition for each stream for the given process designs. The process simulation results show that the H_2-rich stream delivered as the fuel to turbines has 94.2% of H_2 and the combined CO_2 product stream has 99.4% of CO_2. The gas stream out of the HP flash drum has 18.5% of H_2 so that it is recycled back to the absorber. As shown in Figure 2, the losses of hydrogen and [hmim][Tf$_2$N] along with the combined CO_2 product stream are too small to be ignorable.

Table 2 Performance and Cost Results of an IL-based CO_2 Capture System

Category	Value
System power use (MW)	
Solvent pumping power	16.0
Process compression power	14.5
CO_2 product compression power	31.2
Hydraulic turbine recovery power	9.8
Total net system power use	52.0
Process Facilities Capital (2011 M$)	101.2
Absorbers	19.3
Flash Drums	7.9
Solvent Pumps	4.5
Heat Exchanger	2.5
Slump Tanks	3.9
Process Compressors	23.4
CO_2 Product Compressors	36.2
Power Recovery Turbine	3.6
Total Capital Requirement (2011 M$)	210.7
Annualized Capital Cost (2011 M$/yr)	23.8
Fixed O&M Cost (2011 M$/yr)	11.6
Variable O&M Cost (2011 M$/yr)	17.1
CO_2 Separation Cost of Capture System (2011 constant $/t CO_2)*	19.0
Overall cost of CO_2 avoided (2011constant $/t CO_2)	59.0

* This metric is estimated as the capture system's total annualized cost divided by the amount of CO_2 captured.

Table 2 summarizes the performance and cost results for the CO_2 capture system using [hmim][Tf$_2$N]. To measure the overall capture cost, the cost of CO_2 avoided is an more appropriate metric than the separation cost that employs an arbitrary electricity price assumption. Thus, the IECM is applied to estimate the emission rates and LCOE of Shell IGCC plants with and without CCS, which in turn, are used to estimate the

avoidance cost for the capture system. For a given total cost of $5/ton for transport and storage, the resulting cost of CO_2 avoided is $59.0/ton of CO_2 captured.

Results from a series of sensitivity analyses indicate that the overall system energy penalty and cost is sensitive to the process designs including the CO_2 capture efficiency and operating temperature and pressure. An improvement on the CO_2 solubility would remarkably improve the viability of this technology. *More details about the modeling, analyses, and results of the capture system are presented in a manuscript under preparation. This manuscript is available per the sponsor's request.*

Pre-combustion CO_2 Capture System Using Chemical Tunable Ionic Liquids
The chemically tunable IL selected for pre-combustion CO_2 capture is [P2228][2-CNPyr] synthesized by researchers at the University of Notre Dame. This IL achieves a 1:1 and reversible chemical reaction between [2-CNpyr]⁻ and CO_2, resulting in an efficient separation. The isothermal solubility of CO_2 in [P2228][2-CNPyr] was measured by the University of Notre Dame team under the pressure less than 1 bar. A Langmuir-type absorption model is fitted with the measured solubility to predict the equilibrium under different conditions. The typical absorption and stripping process with temperature swing is adopted for the IL-based carbon capture. The multi-stage equilibrium process model is used to simulate the absorption process. The team has been applying the newly developed models to conduct technical and economic assessments for the capture system using [P2228][2-CNPyr].

Results for Adsorption Processes
This section of the report focuses on the use of metal organic frameworks (MOFs) for post-combustion CO_2 capture. Preliminary performance and cost models are developed for the evaluation of a pressure/vacuum swing adsorption (PSA/VSA) –based CO_2 capture system using MOFs for post-combustion CO_2 capture. The models are described here in brief and a few case studies are presented so as to understand the effects of sorbent properties and operating conditions on the performance of the capture system as well as the power plant. The results are compared with a MEA-based CO_2 capture process.

Solid sorbents for CO_2 capture

Metal organic frameworks (MOFs) are solid sorbents which have metal-containing nodes linked by organic ligand bridges. Typical metals include transition metals such as Cu, Ni, Al, Sc, Co, Mn etc. Since these are manufactured sorbents, their properties are "tunable" to enhance CO_2 capture. There are over a hundred MOFs reported in literature. In general, MOFs have higher surface area and pore volume compared with other sorbents for CO_2 capture [10]. For this report, two materials were chosen to be analyzed – Mg₂-(dobdc) (called Mg-MOF-74) and Zeolitic Imidazolate Frameworks (called ZIF-78). ZIF-78 was suggested by our collaborators at Northwestern University [11] and Mg-MOF-74 is often cited in the literature as a suitable MOF for CO_2 capture [12].

Analysis of isotherms

Langmuir isotherm parameters for these two materials were obtained from literature [11, 12]. Isotherms for ZIF-78 and Mg-MOF-74 are plotted in Fig 3 and Fig 4, respectively.

The isotherms for both materials follow familiar patterns in that gas loading on the sorbent increases with increasing partial pressure of the gas and decreases with increasing temperature. CO_2 isotherms for ZIF-78 are less steep compared to those of Mg-MOF-74. Mg-MOF-74 has higher CO_2 and N_2-loading compared with that of ZIF-78 at all pressures and temperatures. N_2 loadings for ZIF do not change appreciably with temperature. Adsorption of N_2 along with CO_2 leads to a decrease in the purity of the CO_2 product stream. As shall be seen later, the absolute loading of N_2 on the sorbent is more important in determining the purity of the product stream.
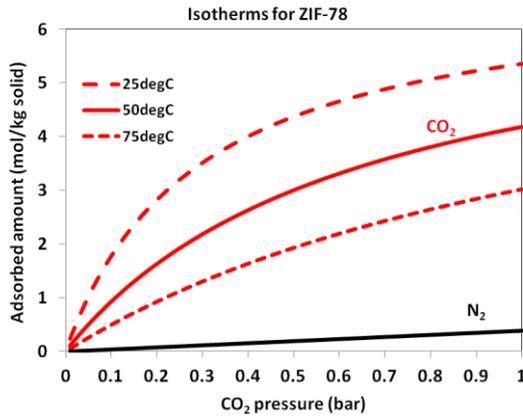
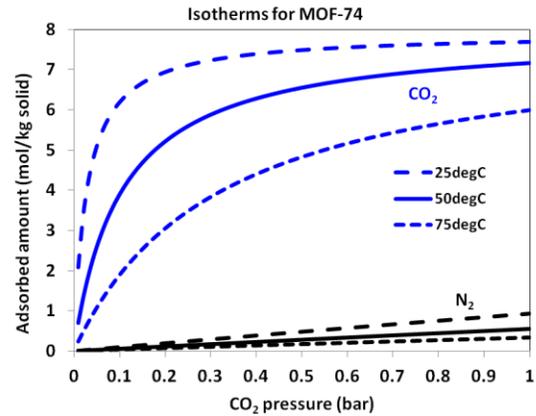

Figure 3. Isotherms for ZIF-78 [11]   Figure 4. Isotherms for Mg-MOF-74 [12]

Pressure Swing Adsorption (PSA) – Skarstorm cycle

In pressure swing adsorption (PSA) process, adsorption occurs at high pressure and desorption takes place at low pressure. In a modification of the PSA process, called vacuum swing adsorption (VSA), adsorption takes place at atmospheric pressure and desorption takes place under vacuum conditions. A typical simple PSA cycle is described by Skarstorm cycle, consisting of four individual steps – pressurization, feed, blowdown and purge (Fig 5) [13]. The variation of pressure in the column across these four steps is shown in Fig 6. Though the simple Skarstrom cycle consists of only four steps, additional steps have been used in different applications in order to increase the efficiency of the process. However, since the purpose of this work is a first order evaluation of materials for CO2 capture, the simple four-step cycle is used.
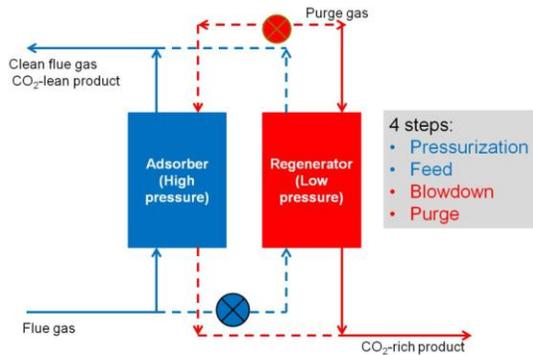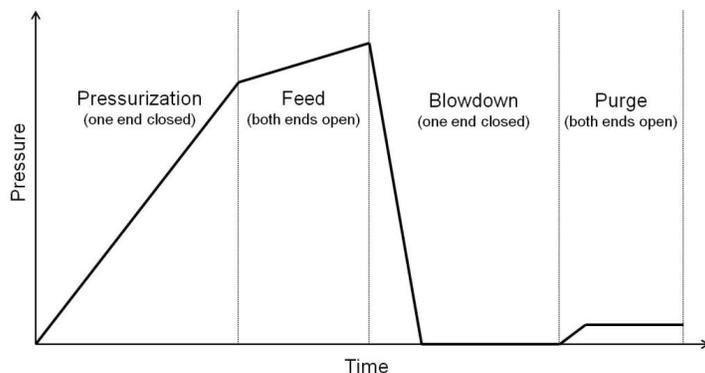

Figure 5. Schematic of a 2-column PSA process based on Skarstrom cycle

Figure 6. Pressure variation in the column of a PSA process

Simplified PSA/VSA model

Several models can be obtained in literature dealing with the evaluation of performance of a PSA process [14]. However, for the purpose of this analysis, a simplified PSA/VSA process model as described by Maring and Webley (2013) has been used for evaluating the performance of a PSA/VSA process [15]. In this simplified model, only three steps are considered – pressurization, feed and blowdown. In the pressurization and blowdown steps, pressure in the column ichanged between adsorption and desorption pressures in 100 equal increments, assuming that the bed reaches equilibrium at each step. At each step, mass and energy balance equations are solved. Details of the model are reported in Maring and Webley (2013). All equations are coded in MATLAB and the results were first validated with high accuracy with the results presented in Maring and Webley (2013). This model was used for the two sorbents selected for this work – ZIF-78 and Mg-MOF-74.

Application of simplified model to ZIF-78 and Mg-MOF-74.

The simplified performance model described in the previous section was applied to evaluate the performance of two solid sorbents – ZIF-78 and Mg-MOF-74 – in a PSA/VSA process. The model was run to solve the mass and energy balance equations over a range of operating conditions. The results of the model were used to develop reduced order regression models which would be useful for conducting design studies and sensitivity analyses. Specifically, reduced order models were developed for five performance variables – molar flow rates of CO_2 and N_2 products, molar flow rate of flue gas in the feed and pressurization steps and also the vacuum work needed during the blowdown step. The estimator variables are operating conditions such as the mole fraction of CO_2 in the feed, temperature of feed gas, adsorption and desorption pressures. These were used to calculate key performance metrics which are important for evaluation of a CO_2 capture process:

- CO_2 product purity – the volume fraction of CO_2 in the product stream. CO_2 purity should be high for pipeline transport.
- CO_2 product recovery – amount of CO_2 removed from the flue gas stream by the CO_2 capture process. A typical CO_2 capture process is expected to capture 90% of CO_2 from the flue gas.

- Specific work requirement – the amount of work required for blower, vacuum pump and CO_2 compressor per unit mass of CO_2 captured. It is desirable to minimize the amount of work required by the CO_2 capture process.

The reduced order models described in the previous section are exercised for the two solid sorbent materials. The impacts of varying operating conditions on the performance metrics for the two sorbents are presented in this section.

It was observed that ZIF-78 had better performance metrics (purity, recovery and specific work) than Mg-MOF-74. Hence, only the results for ZIF-78 are presented here. Comparison with results for Mg-MOF-74 will be presented later on in a detailed report. Generally, sorbents with higher adsorption capacity and higher selectivity are believed to give higher CO_2 product purity and recovery. However, this analysis showed that CO_2 product purity and recovery are higher when ZIF-78 is used despite the fact that Mg-MOF-74 has higher CO_2 adsorption capacity (Fig 4) and higher CO_2/N_2 selectivity. The main difference between the sorbents appears to be the N_2 adsorption capacity, which is much lower for ZIF-78 compared to that for Mg-MOF-74. Thus it can be concluded that for a PSA/VSA process, it is the absolute adsorption capacity of N_2 on a sorbent, rather than CO_2 adsorption capacity and CO_2/N_2 selectivity, which determines CO_2 purity and recovery. Hence, research should be focused on developing sorbents which have a high CO_2 adsorption capacity and very low N_2 adsorption capacity.

ZIF-78 Analysis

Figure 7 shows the CO_2 product purity for the ZIF-78 case, at different desorption pressure, inlet CO_2 concentration, inlet flue gas temperature and adsorption pressure. From the figure it is clear that CO_2 product purity is in general low ($< 75\%$) under all operating conditions. The desorption pressure has to be lower in order to increase higher purity. Lower temperature leads to higher purity. Lower adsorption pressure results in higher purity. On the other hand, higher inlet concentration of CO_2 gives higher product purity. Hence it can be concluded that in order to increase CO_2 product purity, the desorption pressure has to be very low, inlet temperature of the flue gas and adsorption pressure need to be low and the inlet concentration of CO_2 should be high.
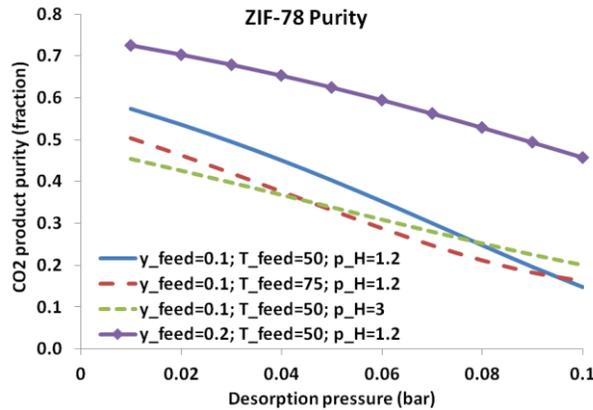
Figure 7. CO$_2$ product purity for ZIF-78

Figure 8 shows the recovery (capture rate) of CO$_2$ from the flue gas when ZIF-78 is used as a sorbent in the PSA/VSA process. Similar to purity, it can be observed that CO$_2$ recovery from the PSA process is also in general low. Higher recovery rates can be achieved only at low desorption pressures. Lower temperature gives higher recovery, which is similar to the trend seen for purity. The effect of temperature on recovery, however, is not significant. Unlike for purity, higher adsorption pressure gives higher recovery. Similar to its effect on purity, higher inlet CO$_2$ concentration leads to higher recovery. Hence it can be concluded that low desorption pressure, low feed temperature, high inlet CO$_2$ concentration and high adsorption pressure are needed to improve CO2 product recovery.
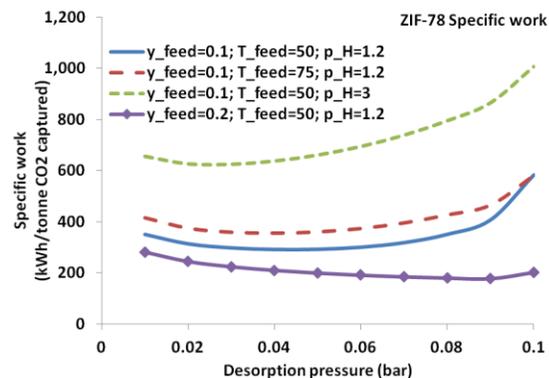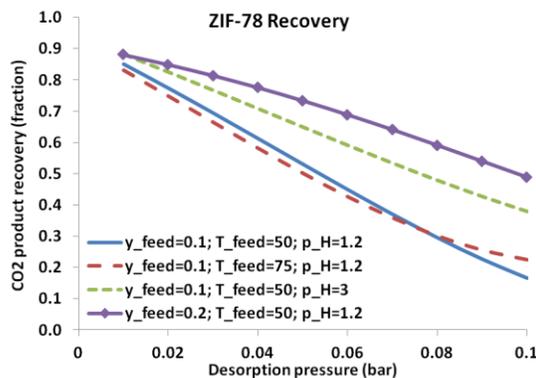
Figure 8. CO$_2$ product recovery for ZIF-78   Figure 9. Specific work requirement for ZIF-78.

Figure 9 shows the specific work required by the capture process per unit mass of CO$_2$ captured, when ZIF-78 is used as a sorbent in the PSA/VSA process. Lower desorption pressure leads to higher specific work requirement, though the change is not significant. Lower temperature results in lower specific work, similar to the trend seen for purity and recovery. Higher adsorption pressure significantly increases the specific work requirement. Higher inlet CO$_2$ concentration leads to lower specific work requirement. Hence it can be concluded that low feed temperature, high inlet CO$_2$ concentration and low adsorption pressure are needed to lower specific work requirement.

In practical applications to a power plant, inlet CO_2 concentration is fixed by the type of coal used in the power plant and pollution control equipment used upstream of the CO_2 capture process. Flue gas temperature can be lowered in pre-treatment units but the amount of cooling of flue gas is limited by size and cost of cooling equipment. Hence, for the design of a CO_2 capture process, adsorption and desorption pressures are the variables which can be easily varied to achieve purity requirements.

Constant CO_2 capture efficiency

CO_2 capture systems are typically designed to achieve a given capture efficiency (recovery). Figures 10 shows the combination of adsorption and desorption pressures required to achieve specific CO_2 capture efficiencies (recovery) for ZIF-78. To achieve a high CO_2 capture efficiency, the desorption pressure needs to be very low, for all adsorption pressures. Figure 11 shows the specific work requirement to achieve a given capture efficiency as a function of adsorption pressure for ZIF-78. Higher capture efficiency requires higher specific work and higher adsorption pressure increases the specific work significantly. It can be concluded that lower adsorption pressure will lead to low specific work requirement.
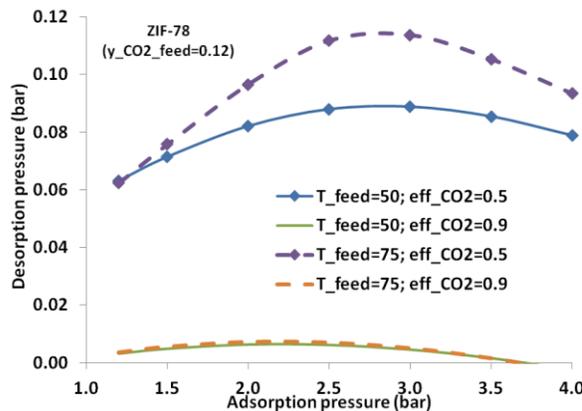
Figure 10. Combination of adsorption and desorption pressures for fixed CO_2 capture efficiency for ZIF-78
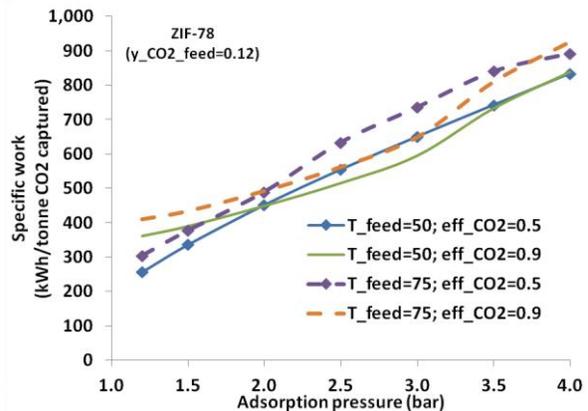
**Figure 11. Specific work requirement for fixed CO_2 capture efficiency for ZIF-78**

Case study – application to a power plant

The performance models developed above are applied to a power plant case study. The input conditions are given in the following table:

Table 3 Assumptions for Case Study

Gross electrical output	650 MW
Coal type	Appalachian medium sulfur
Total thermal input	1,546 MW
CO_2 flow rate in flue gas	11,310 kmol/hr
CO_2 concentration in flue gas (assuming dry flue gas)	14%
Inlet flue gas temperature	50^oC
Inlet flue gas pressure	1.2 bar
Sorbent used	ZIF-78

CO_2 capture efficiency was varied between 50% and 95%. Figure 12 shows the desorption pressure required to achieve a desired CO_2 capture efficiency and the resulting net plant efficiency. As can be seen from the figure, increasing capture efficiency leads to significant loss of plant efficiency. For example, 90% CO_2 capture rate would reduce the net plant efficiency to 15%, which is much lower than the net plant efficiency obtained when an MEA-based CO_2 capture system is used (close to 30%). Figure 13 shows the CO_2 product purity and the amount of sorbent required as function of CO_2 capture efficiency. CO_2 product increases with increasing capture efficiency because the required desorption pressure is also very low. The amount of sorbent required decreases with the capture efficiency.
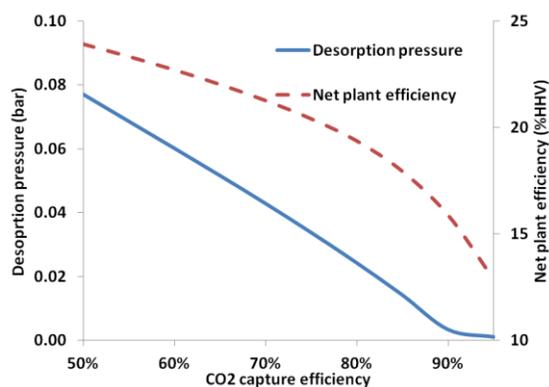
Figure 12. Variation in the required desorption pressure and net plant efficiency as a function of CO2 capture efficiency
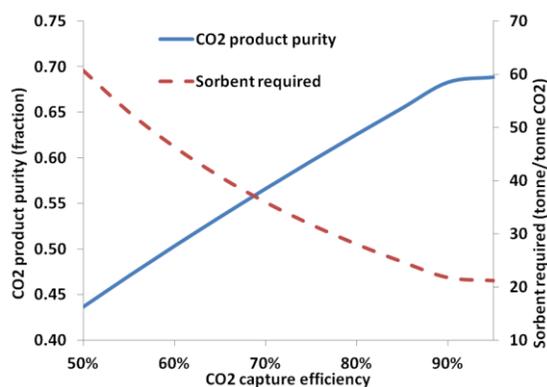
Figure 13. Variation in CO2 product purity and sorbent required as a function of CO2 capture efficiency

Summary

Performance models for a PSA process using Mg-MOF-74 and ZIF-78 are developed. Based on the results, it was demonstrated that ZIF-78 is a better sorbent than Mg-MOF-74, mainly because of the lower adsorption capacity of N_2 for ZIF-78. It was also shown that low desorption pressure, low temperature, high inlet CO_2 concentration lead to better performance of the PSA process. Higher adsorption pressure leads to a significant

increase in work requirement. Hence the system should be operated at a low adsorption pressure close to atmospheric pressure.

Application of the performance model to a power plant case study showed that using MOFs for post-combustion CO_2 capture leads to a very high energy penalty. Energy penalty increases with increasing CO_2 capture efficiency. Material and process improvements should be achieved in order to make MOFs-based systems competitive with conventional MEA-based CO_2 capture systems.

Development of a New Life Cycle Module for IECM
The task draws on the literature and life cycle inventory databases to estimate supply chain water inventories and their uncertainties. The inventories of all power plant mass flows were calculated by the IECM, including resource requirements and waste or byproduct streams. The task started with estimating the water use inventory. Water use factors for coal production and transport supply chains were estimated based on the existing data from peer-reviewed literature. The team applied the CMU's Economic Input-Output Life Cycle Assessment tool to estimate water use factors for coal-fired power plant infrastructures and the EcoInvent database to estimate water use factors for production of chemicals used for CO_2 capture and conventional emission control systems at coal-fired power plants.

Future Plans
Here we outline the set of planned tasks for fulfilling the goals of this project:
- Continue developing/improving technical and economic models and systems analysis for the three CO_2 capture technologies under study.
- Develop reduced-order performance models as needed and incorporate them into the IECM, assess plant-level attributes and targets, and characterize variability and uncertainty of key process parameters;
- Establish a life cycle analysis module for the IECM;
- Conduct comparative techno-economic assessments for the three CO_2 capture technologies under study.

Publications
Manuscripts are under preparation for journal publication.

References
[1]   Intergovernmental Panel on Climate Change (IPCC). (2005). IPCC Special Report on Carbon Dioxide Capture and Storage. Prepared by Working Group III of the Intergovernmental Panel on Climate Change; Cambridge University Press: New York.
[2]   Rubin, E. S., Chen, C., & Rao, A. B. (2007). Cost and performance of fossil fuel power plants with CO_2 capture and storage. *Energy policy*, *35*(9), 4444-4454.
[3]   Rubin, E.S., H. Zhai and K. Kietze, Integrated Environmental Control Model, Version 8.0.2, Public Release, available at: www.iecm-online.com (2012).
[4]   Shiflett, M. B., & Yokozeki, A. (2007). Solubility of CO_2 in room temperature ionic liquid [hmim][Tf2N]. *The Journal of Physical Chemistry B*, *111*(8), 2070-2074.

[5]   Yokozeki, A., & Shiflett, M. B. (2009). Separation of carbon dioxide and sulfur dioxide gases using room-temperature ionic liquid [hmim][Tf2N]. *Energy & Fuels*, *23*(9), 4701-4708.

[6]   Gurkan, B., Goodrich, B. F., Mindrup, E. M., Ficke, L. E., Massel, M., Seo, S., ... & Schneider, W. F. (2010). Molecular design of high capacity, low viscosity, chemically tunable ionic liquids for CO_2 capture. *The Journal of Physical Chemistry Letters*, *1*(24), 3494-3499.

[7]   Electric Power Research Institute (EPRI). TAGTM − Technical Assessment Guide Vol.1: Electricity Supply, Rev.7; Report TR-102276-VIR7; Electric Power Research Institute: Palo Alto, CA, June 1993.

[8]   Chen, C. (2005). A Technical and Economic Assessment of CO2 Capture Technology for IGCC Power Plants. PhD Thesis, Department of Engineering and Public Policy, Carnegie Mellon University, Pittsburgh, PA.

[9]   Basha, O. M., Keller, M. J., Luebke, D. R., Resnik, K. P., & Morsi, B. I. (2013). Development of a Conceptual Process for Selective CO_2 Capture from Fuel Gas Streams Using [hmim][Tf_2N] Ionic Liquid as a Physical Solvent. *Energy & Fuels*, *27*(7), 3905-3917.

[10]   Li, J-R., Ma, Y., McCarthy, M.C., Sculley, J., Yu, J., Jeong. H-K., Balbeuna, P.B., Zhou, H-C. (2011). Carbon dioxide capture-related gas adsorption and separation in metal-organic frameworks. *Coordination Chemistry Reviews*, 255, 1791-1823.

[11]   Leperi, K., Gao, H., Snurr, R.Q., You, F. (2014). Modeling and optimization of a two-stage MOF-based pressure/vacuum swing adsorption process coupled with material selection. *Chemical Engineering Transactions*, 39, 277-282.

[12]   Mason, J.A., Sumida, K., Herm, Z.R., Krishna, R., and Long, J.R. (2011). Evaluating metal-organic frameworks for post-combustion carbon dioxide capture via temperature swing adsorption. *Energy and Environmental Science*. 4, 3030-3040.

[13]   Grande, C.A. (2012). Advances in pressure swing adsorption for gas separation. ISRN Chemical Engineering. 1-13.

[14]   Knaebel, K.S., and Hill, F.B. (1985). Pressure swing adsorption: Development of an equilibrium theory for gas separation. *Chemical Engineering Science*. 40 (12), 2351-2360.

[15]   Maring, B.J. and Webley, P.A. (2013). A new simplified pressure/vacuum swing adsorption model for rapid adsorbent screening for CO2 capture applications. *International Journal of Greenhouse Gas Control*. 15, 16-31.

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Appendix

Nomenclature in Results for Absorption Processes
a: parameter in Redlich-Kwong equation of state
b: parameter in Redlich-Kwong equation of state
C_3:   measure of reaction site density
D: diffusion coefficient
g: gravity
h: enthalpy of liquid flow
H: enthalpy of gas flow
Hn: Henry's law constant
ΔH: reaction heat
k_1:   reaction equilibrium constant
K: phase equilibrium ratio
L: solvent flow rate
n: number of moles
Q: cooling duty
P: pressure
R: gas constant
T: temperature
V: gas flow rate or molar volume
x: mole fraction in liquid phase
X: mole ratio in liquid phase
y: mole fraction in gas phase
μ: viscosity
ρ: density
$\emptyset$:   fugacity coefficient

Subscripts:
i: component
j: stage number
G: gas phase
L: liquid phase
V: vapor phase