

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 CO₂. 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 (CO₂) emissions from fossil fuel power plants [1]. Adding today's amine-based CCS to pulverized coal (PC) power plants for 90% CO₂ 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 CO₂ 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 biomimetic sorbents (Stanford University) for post-combustion capture. In this project we propose to substantially expand the IECM to explicitly include models of these advanced CO₂ capture processes, plus the capability to include a life cycle analysis of substances used for CO₂ capture.

Results to Date

The team started with researching such new materials as ILs and MOFs used for CO₂ capture. As elaborated below, the team has assessed the status of available data on material properties and process in consultation with other GCEP researchers and developed preliminary technical and economic models for capture processes. All the models are currently coded in the MATLAB environment.

Results for Absorption Processes

This section report our research results to date on ILs, which employ physical or chemical absorption processes to capture CO₂ from a mixed gas stream.

Development of a Multistage Equilibrium Model for Gas Absorption

Absorption of CO₂ 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. As discussed below, the multi-stage process model takes into account the mass balance (M), equilibrium (E), summation (S), and enthalpy balance (H). The Newton-Raphson simultaneous correction algorithm is applied to solve the MESH equations and then provide the profiles of vapor and liquid compositions and temperatures across all equilibrium stages.

Mass balance for each component at each stage (j):

$$L_{j-1}x_{i,j-1} - L_jx_{i,j} + V_{j+1}y_{i,j+1} - V_jy_{i,j} = 0$$

Equilibrium 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:

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

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]:

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

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 CO₂ uptake on the basis of mole ratio is predicted in terms of CO₂ pressure, Henry's law constant, and reaction equilibrium constant as [6]:

$$X_{\text{CO}_2,j} = \frac{n_{\text{CO}_2}}{n_{\text{IL}_0}} = \frac{P_{\text{CO}_2,j} / H_{n_j}}{1 + \frac{k_{1,j} P_{\text{CO}_2,j} C_3}{H_{n_j}}}$$

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.

Estimation of Absorber Size

To size the absorber, the height is estimated in terms of the overall mass transfer coefficient, which is estimated as:

$$\frac{1}{K_G} = \frac{1}{k_G} + \frac{m}{k_L}$$

The physical mass transfer coefficients of gas and liquid phases are estimated using empirical mass transfer correlations developed by Onda et al [7] for randomly packed columns. The following equations describe the correlations of interfacial area, gas-phase mass transfer coefficient, and liquid-phase mass transfer coefficient as a function of physical properties and flow velocity designs.

$$\frac{\dot{a}}{a_p} = 1 - \exp \left\{ -1.45 \left(\frac{\sigma_c}{\sigma_L} \right)^{0.75} \left(\frac{v_L}{\dot{a}_p \mu_L} \right)^{0.1} \left(\frac{v_L^2 \dot{a}_p}{\rho_L^2 g} \right)^{-0.05} \left(\frac{v_L^2}{\rho_L \sigma_L \dot{a}_p} \right)^{0.2} \right\}$$

$$\frac{k_G RT}{\dot{a}_p D_G} = \epsilon \left(\frac{v_G}{\dot{a}_p \mu_G} \right)^{0.7} \left(\frac{\mu_G}{\rho_G D_G} \right)^{1/3} (\dot{a}_p d_p)^{-2}$$

Where ϵ is 2 if $d_p < 0.012$ and 5.23 otherwise.

$$k_L \left(\frac{\rho_L}{\mu_L g} \right)^{1/3} = 0.0051 \left(\frac{v_L}{\dot{a}_p \mu_L} \right)^{2/3} \left(\frac{\mu_L}{\rho_L D_L} \right)^{-0.5} (\dot{a}_p d_p)^{0.4}$$

To account for the effect of chemical reaction on the mass transfer, the physical mass transfer coefficient of the liquid phase is adjusted by an enhancement factor that reflects the reaction kinetics as:

$$\frac{1}{K_G} = \frac{1}{k_G} + \frac{H_{n_{\text{CO}_2}}}{k_L E}$$

Development of Engineering-Economic Models

The performance models 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 the IL-based CCS system. This study employs the costing method and nomenclature of the Electric Power Research Institute’s Technical Assessment Guide. The total capital requirement of an IL-based capture system takes into account the direct costs plus a number of indirect costs such as the general facilities cost, engineering and home office fees, contingency costs, and owner’s costs. As given in Table 1 for a post-combustion capture system, the major direct cost components include the direct contact cooler, flue gas blower, circulation pump, lean-solvent cooler, absorber and stripper, lean/rich solvent heat exchanger, steam extractor and reboiler, solvent processing unit, solvent reclaimer, as well as CO₂ product compression. Table 2 summarizes major fixed and variable operating and maintenance (O&M) cost components. Fixed O&M costs include operating labor, maintenance costs, and administrative and support labor costs. Variable O&M costs include IL makeup, chemicals, solid waste treatment, power use, and CO₂ transport & storage.

Table 1 Capital cost components

CO₂ Capture Process Area Costs	CO₂ Capture Plant Costs
Direct contact cooler	Process facilities capital
Flue gas blower	General facilities capital
Absorber	Engineering. & home office fees
Heat Exchangers/coolers	Project contingency cost
Solvent pumps	Process contingency cost
Sorbent regenerator	Interest charges
Reboiler	Royalty fees
Steam extractor	Preproduction (startup) cost
Sorbent reclaimer	Inventory capital
Sorbent processing	
CO ₂ product compression	
Process Facilities Capital (sum above)	Total Capital Requirement (sum above)

Table 2 Operating and maintenance cost components

Variable Cost Component	Fixed Cost Component
Solvent makeup	Operating labor
Chemicals	Maintenance labor
Reclaimer waste disposal	Maintenance material
Electricity	Admin. & support labor
CO ₂ transport and storage	
Total Variable Cost (sum above)	Total O&M Cost (sum above)

Application of Ionic Liquids to Post-combustion CO₂ Capture

The pre-combustion capture process using ILs is still under development by the University of Notre Dame (UND). Thus, in consultation with the UND research group, our initial effort has focused on a post-combustion process model which can later be extended to the pre-combustion case. The chemically tunable IL, trihexyl-(tetradecyl)phosphonium 2-cyanopyrrolide ([P66614][2-CNpyr]) synthesized by the UND research group [6,8], is selected for this systems analysis. This IL achieves a 1:1 and reversible chemical reaction between [2-CNpyr]⁻ and CO₂, resulting in an efficient separation. The typical absorption and stripping process is adopted for the IL-based carbon capture. The multi-stage equilibrium process model is used to simulate the adiabatic absorption process. The CO₂ of flue gas is assumed to be the only component transferred from the gas phase to liquid phase. A generalized Sherwood/Leva/Eckert correlation is adopted to estimate the gas-phase pressure drop across the absorber. Given that no water is used to dilute the solvent and the solvent vapor loss is nearly zero in the capture process, a single-stage flash drum in equilibrium is employed for the stripping process. The size of flash drum is determined in terms of empirical gas velocity and liquid surge time designs.

The technical and cost models are applied to evaluate the IL-based system for capturing CO₂ from the flue gas out of a 650 MW (gross) supercritical pulverized coal power plant. The team greatly appreciates the collaboration of the University of Notre Dame who shared the property data of [P66614][2-CNpyr]. Table 3 summarizes the preliminary performance and costs of the IL-based system for 90% CO₂ capture. Figure 1 further presents the “cost of CO₂ captured” for a range of CO₂ removal efficiencies, excluding CO₂ transport and storage costs. This metric is currently being used by the U.S. Department of Energy for purpose of capture technology assessment with a benchmark cost of \$40/ton CO₂ captured. For 90% CO₂ capture the cost of an IL-based capture system would be higher than the DOE benchmark or that of a comparable amine-based CCS system, mainly due to a higher capital cost. However, current process designs for the IL-based capture system are not yet optimized. Other more robust metrics for comparing the cost of plants employing different CCS systems, such as added LCOE for CCS and CO₂ avoidance cost, will be used for future comparative cost assessments.

Table 3 Preliminary performance and costs of an IL-based capture system

Variable	Unit	Value
Flue gas flow rate	kmole/hr	94980
CO ₂ concentration	mol. fraction	0.12
CO ₂ removal efficiency	%	90
Number of trains	#	4
Temperature of flue gas into absorber	°C	40
Temperature of lean solvent into absorber	°C	35
Absorber operating pressure	bar	1.00
CO ₂ concentration in lean solvent stream	mol. fraction	0.050
CO ₂ concentration in rich solvent stream	mol. fraction	0.224
Lean solvent flow rate	kmole/hr	11433
Number of equilibrium stages in absorber	#	5
Cold-side temperature approach for rich/lean heat exchanger	°C	5
Pressure drop across absorber	kPa	12.5
Absorber height	m	44.7
Absorber diameter	m	10.5
Stripping temperature	°C	160
Stripping pressure	bar	1.03
Stripper height	m	25.8
Stripper diameter	m	7.4
Steam use for solvent regeneration	kJ/kg CO ₂	3864
Blower power use	MW	10.6
Pump power use	MW	8.3
CO ₂ product compression	MW	47.6
Total equipment power use	MW	66.5
Total capital requirement	2011M\$	772.5
Fixed O&M cost	2011M\$/yr	20.4
Variable O&M cost	2011M\$/yr	28.8
Total O&M cost ^a	2011M\$/yr	49.2
Cost of CO ₂ captured ^{a,b}	2011\$/t	46.1

^a This item does not include the CO₂ transport and storage costs.

^b The cost of CO₂ captured in constant dollars is estimated as the total annual levelized cost divided by the total amount of CO₂ captured, in which the value of fixed charge factor is 0.113 and the capacity factor is 75%.

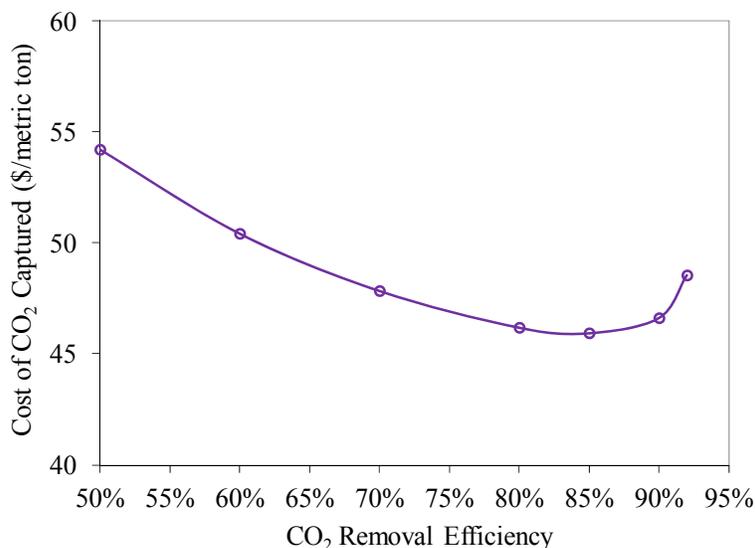


Figure 1. Cost of CO₂ captured as a function of removal efficiency

Application of Ionic Liquids to Pre-combustion CO₂ Capture

The systems analysis for a pre-combustion process has started with physical absorption for CO₂ capture. The ionic liquid, 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([hmim][Tf₂N]), is selected for capturing CO₂ from the shifted fuel gas mixture mainly because of its stability, low viscosity, and low water solubility [9]. As Shiflett and Yokozeki did [4], the generic RK EOS is employed to predict the solubility behavior of CO₂ and H₂ in [hmim][Tf₂N] under different pressures and temperatures. Figure 2(a) and (b) shows the solubility of CO₂ and H₂ in a binary system, respectively. The VLE model based on the RK EOS is further adjusted by incorporating additional binary interaction parameters of CO₂ and H₂ and then applied to predict the simultaneous solubility of CO₂ and H₂ in a tertiary system. The predicted pressure of the tertiary system is validated with an experimental study conducted by Kumelan et al [10], which results in a high R² value (0.996).

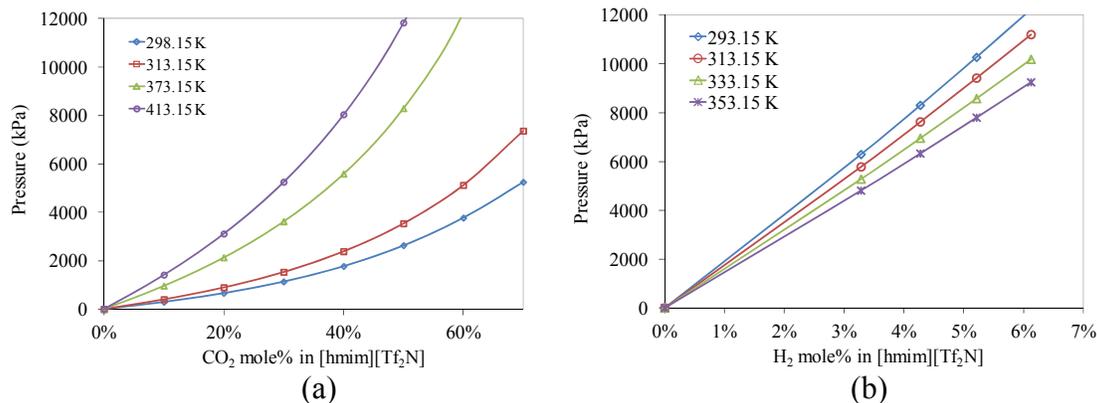


Figure 2. PT-x phase diagram of CO₂ and H₂ in [hmim][Tf₂N]

The phase equilibrium correlations of CO₂ and H₂ in [hmim][Tf₂N] will be integrated in the newly developed multi-stage process model for the gas absorption that uses [hmim][Tf₂N] as the solvent for pre-combustion CO₂ capture. Figure 3 presents a

conceptual capture process proposed by Basha et al [9], in which CO₂ is absorbed by the physical solvent, and then the solvent is regenerated in a series of pressure-swing flash drums. The research team plans to apply the performance and cost models to systematically evaluate this capture process design.

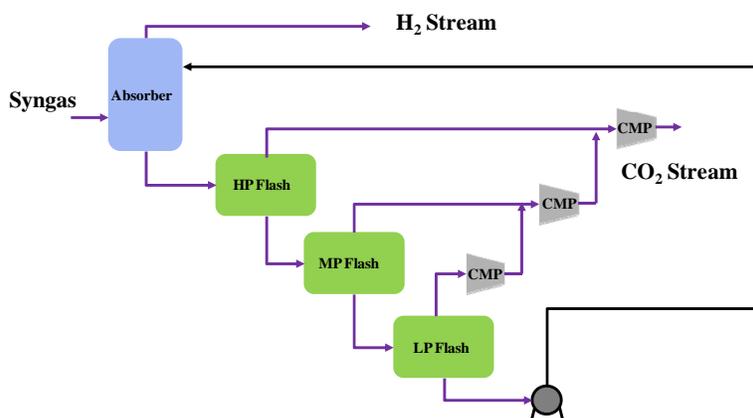


Figure 3. Conceptual capture process for CO₂ and H₂ separation

Results for Adsorption Processes

This section reports our research results to date on metal organic frameworks (MOFs) developed in consultation with GCEP researchers at Northwestern University. MOFs are porous solid sorbents consisting of organic-inorganic hybrid networks. The nodes are made of metals (single ions or clusters), which are connected by organic linking groups to form 1-D or 2-D or 3-D coordination networks (Figure 4). Owing to their extraordinary surface areas and tunable pore surface properties, MOFs have gained a lot of attention recently for separation of CO₂ from gas streams, both in pre-combustion and post-combustion applications [11-12].

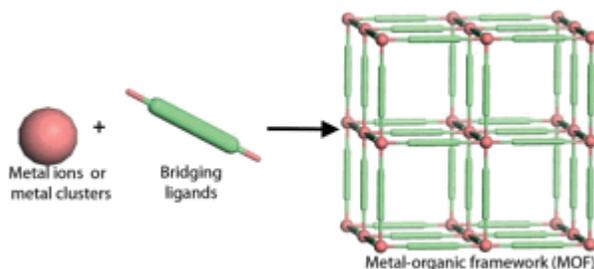


Figure 4. Schematic of metal organic framework [13]

The main advantage of MOFs is that their pore surface properties are tunable. They also possess extraordinary surface areas compared to other solid sorbents. Their potential scalability for industrial use makes them an attractive choice as a solid sorbent. Because of their lower heat capacity compared with aqueous amines, the energy penalty for regeneration is likely to be lower. MOFs have high adsorption capacities both at low and high pressures, making them suitable for both pre-combustion and post-combustion CO₂ capture applications. However, the adsorption capacity is much smaller at low pressures than at high pressures.

In this report, a preliminary model of a pressure swing adsorption (PSA) process for post-combustion CO₂ capture using MOFs is described.

Langmuir Models for Adsorption

In this study, Langmuir adsorption models are used to calculate the loadings of CO₂ on MOFs at different pressures and temperatures. According to this model, the amount of gas adsorbed on a sorbent at a given temperature and pressure (called an isotherm) is given by:

$$n_{\text{CO}_2, \text{ads}} \left(\frac{\text{mol}}{\text{kg}} \right) = \frac{m_{\text{CO}_2} b_{\text{CO}_2} P_{\text{CO}_2}}{1 + b_{\text{CO}_2} P_{\text{CO}_2}}$$

$$b_{\text{CO}_2} = b_0 e^{\frac{Q_{\text{CO}_2}}{RT}}$$

where, m_{CO_2} (mol/kg) is the saturation loading, b_0 (1/bar) is the Langmuir parameter and Q_{CO_2} (kJ/kmol) is the heat of adsorption.

Pressure Swing Adsorption

Regeneration of CO₂ from MOFs can be achieved either by temperature swing adsorption (TSA) or pressure swing adsorption (PSA). However, particularly for MOFs, PSA seems to be the preferred regeneration method [14-15]. Hence, a PSA system is modeled here. A schematic of a PSA system is shown in Fig 5.

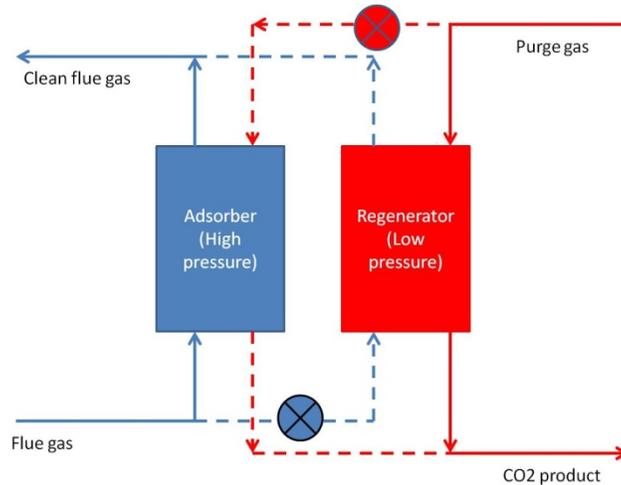


Figure 5. A schematic of pressure swing adsorption process.

PSA is a cyclic process, consisting of two vessels packed with MOF (or other solid sorbent) pellets, each acting as an adsorber or regenerator in turn. When CO₂ adsorption is saturated at high pressure, gas flow to the adsorber is stopped and the pressure is released from the adsorber, releasing the CO₂, which is then purged by a purge gas stream. In this step, the adsorber acts as a regenerator. A parallel reactor acts as an adsorber when the first vessel is in regeneration stage and as a regenerator when the first

vessel is in adsorption stage. Thus, a continuous operation is achieved. Gas flows are controlled by valves. Figure 6 shows these stages and the pressure variation in each step.

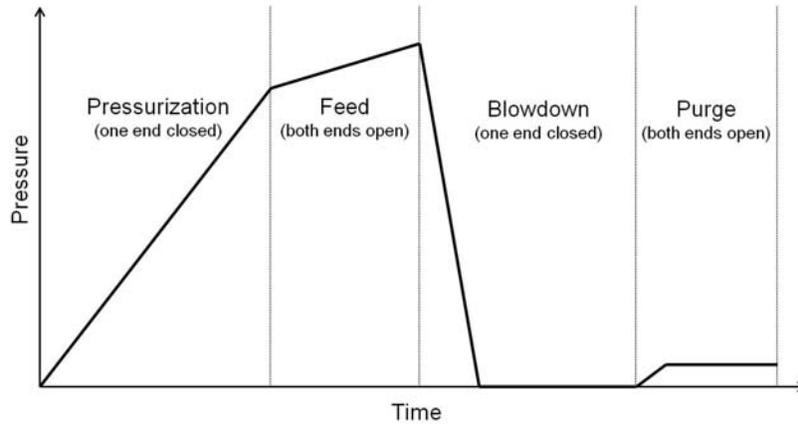


Figure 6. Stages in a PSA process [16]

In the first step, the bed is pressurized by feeding the flue gas with one end closed. Once the pressure reaches a certain value, the other end is opened and the feed step takes place at a fairly constant pressure. Adsorption of CO_2 onto MOF occurs in these two steps. Once breakthrough happens, the outlet end is closed and gas is removed from the other end, thereby reducing pressure in the reactor. Consequently, the CO_2 adsorbed on the MOF is released. In an optional purge step, the CO_2 in the reactor is purged using a gaseous stream [16].

Since PSA involves compressing flue gas to a high pressure, a vacuum swing adsorption (VSA) process is recommended for post-combustion capture applications [17]. The steps in VSA process are essentially the same as in a PSA process except that adsorption happens at close to atmospheric pressure and desorption happens at lower pressures achieved using a vacuum pump.

Simplified Process Model for PSA/VSA

A process model is needed to estimate the mass of sorbent and energy required to capture CO_2 . CO_2 purity and recovery are also important parameters that need to be calculated. In this study, a simplified PSA/VSA process model is used, as described by Maring and Webley [18]. The simplified model consists of three steps – blowdown, repressurization, and feed.

The initial condition is assumed to be a bed saturated with feed (flue gas) after breakthrough at adsorption pressure and temperature. In the blowdown step, the pressure is reduced from high pressure (P_H) to a lower pressure (P_L) by removing gas from the reactor using a vacuum pump when necessary. For modeling purposes, it is assumed that blowdown happens in 100 equal increments. After blowdown, in the repressurization step, flue gas is added incrementally to the bed till the bed pressure reaches P_H again. Then in the feed step, the other end of the bed is open and there is a flow of gas through the bed. The final pressure, temperature and composition are equated with the initial values to close the mass balance. Adsorption is assumed to take place at equilibrium, i.e.

the adsorbed phase is always at equilibrium with the gas phase. When there is data, co-adsorption of N₂ is also considered.

The total number of moles of CO₂ at any given point of time is given by the following equations:

$$n_{CO_2, total} = n_{CO_2, ads} + n_{CO_2, gas}$$

$$n_{CO_2, ads} = \frac{m_{CO_2} b_{CO_2} p_{CO_2}}{1 + b_{CO_2} p_{CO_2}}$$

$$b_{CO_2} = b_0 e^{\frac{Q_{CO_2}}{RT}}$$

$$n_{CO_2, gas} = \frac{y_{CO_2} PV}{RT}$$

Similar equations can be written for N₂.

For preliminary modeling, isothermal conditions are assumed. Since pressure is reduced incrementally, the pressure at each step is known. So, only the bed composition needs to be solved for.

Solving mass balance equations gives the following expression for mole fraction of CO₂ in the gas in the bed, for each pressure step:

$$y_{CO_2} = y_{CO_2, i} + \left(\frac{RT}{P}\right) \left((n_{CO_2, ads, i} + y_{CO_2, i} n_{total, ads, i}) - (n_{CO_2, ads} + y_{CO_2, i} n_{total, ads}) \right)$$

where, the subscript 'i' denotes the condition from the previous step.

This equation can be solved for each incremental pressure drop in the blowdown step to calculate the purity of product CO₂, recovery of CO₂ and vacuum work required.

$$n_{CO_2, product} = \sum_1^{blowdown} y_{CO_2, i} (n_{total, i} - n_{total})$$

$$W_{vacuum} = \sum_1^{blowdown} (n_{total, i} - n_{total}) \times \frac{1}{\eta} \left(\frac{k}{k-1}\right) T_{feed} \left(\left(\frac{P_i}{P}\right)^{\frac{k-1}{k}} - 1 \right)$$

$$Purity = \frac{n_{CO_2, product}}{n_{CO_2, product} + n_{N_2, product}}$$

$$Specific\ work = \frac{(W_{vacuum} + W_{blower})}{n_{CO_2, product}}$$

A blower is needed to increase the pressure beyond atmospheric pressure.

Case Study

A case study was performed to study the application of this model for a sample MOF. Mg-MOF-74, also known as Mg₂(dobdc), is chosen for the sample calculation because it has been extensively studied in the literature [19-20]. Langmuir data for this MOF are

easily obtained. Since the primary adsorption mechanism in MOFs is physical, polyethylenimine (PEI, a chemical sorbent) was also chosen to compare with the MOF [21]. Langmuir data for these two sorbents are presented in Table 4. The composition of flue gas is assumed to be 12% CO₂ and the rest N₂.

Table 4 Langmuir parameters of sorbents used in this case study

	MOF-74		PEI	
	CO ₂	N ₂	CO ₂	N ₂
b ₀ (1/bar)	1.557e-6	4.96e-5	1.07e-6	0
Q (kJ/mol)	42	18	50	0
m (mol/kg)	7.9	14	2.89	0

The isotherms for these two sorbents at three different temperatures are given in Fig 7.

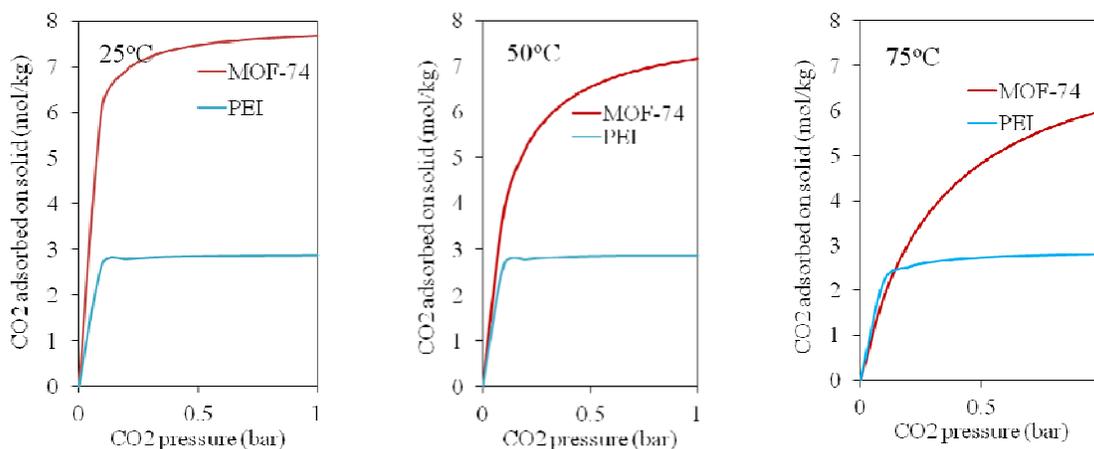


Figure 7. Isotherms for Mg-MOF-74 and PEI at different temperatures

Using the simplified PSA/VSA model described previously, purity and specific work requirements for these two sorbents at 75°C are calculated. Results are shown in Fig 8 and 9. Red lines are for PEI and blue lines are for MOF-74.

From preliminary assessment, MOFs lead to lower purity of CO₂ product than PEI and consume slightly higher energy for product removal than PEI. Since PEI is a chemisorbent, purity can be expected to be higher, which is also the reason for its lower specific work.

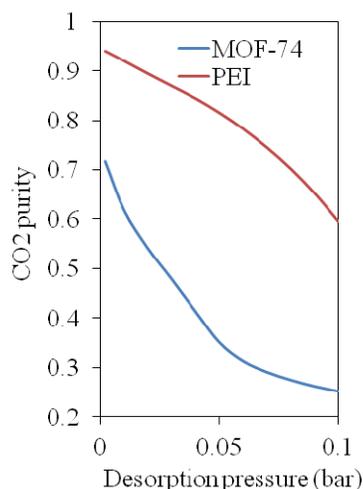


Figure 8. Purity of CO₂ product for MOF-74 (blue) and PEI (red)

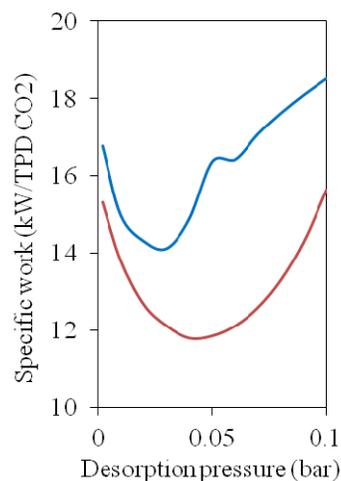


Figure 9. Specific work requirement for MOF-74 (blue) and PEI (red)

Progress

For processes using ionic liquids, preliminary performance and cost models have been developed based on physical and chemical properties of a chemically tunable IL used for post-combustion CO₂ capture. The team has developed the phase equilibrium model for [hmim][Tf₂N] used as a physical solvent for pre-combustion carbon capture and will integrate it into the process modeling framework for the systems analysis. The team will improve the performance and cost models to evaluate chemically-complexing ILs for pre-combustion carbon capture once the property data are provided by the collaborators.

A preliminary performance model also has been developed for a PSA/VSA process using MOF as sorbent for post-combustion CO₂ capture. So far the focus has been to develop a working model for a PSA process which can later be integrated into a larger framework of a power plant. Since the results are preliminary, no conclusions about MOFs can be drawn yet. The model will be further developed to make it robust. Multiple MOFs will be compared in order to study the relative importance of various parameters for performance. The model will be integrated with a power plant. More literature review will be conducted to incorporate the effects of impurities such as SO_x and water vapor. Depending on the data available, reaction kinetics will be incorporated to develop a reactor design in consultation with the Northwestern University research group. This will later be used as input to a cost model.

The Stanford team has sent us a preliminary set of isotherm data for a nitrogen-enriched carbon-based sorbent that is likely to be the foundation for their biomimetic sorbent. Their data includes nitrogen and CO₂ adsorption isotherms at a few temperatures. The team will perform regression analysis to fit a two-site Langmuir model to this data. The regressed parameters will allow us to compare the performance of this sorbent to MOFs and chemisorbents in the simplified PSA model.

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 CO₂ capture technologies under study.
- Develop reduced-order performance models as needed and incorporate them into the IECM.
- Establish a life cycle analysis framework for CO₂ capture materials.
- Assess plant-level attributes and targets.
- Characterize variability and uncertainty of key process parameters.
- Conduct comparative techno-economic assessments for the three CO₂ capture technologies under study.

Publications

None to report at this time.

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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_p :	nominal packing diameter
D :	diffusion coefficient
E:	enhancement factor
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
k_G :	gas-phase mass transfer coefficient
K_G :	overall gas-phase mass transfer coefficient
k_L :	liquid-phase mass transfer coefficient
L:	solvent flow rate
n:	number of moles
m:	slope
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
\hat{a} :	wetted packing area
\hat{a}_p :	total packing area
σ_c :	critical surface tension of packing material
σ :	surface tension
μ :	viscosity
ρ :	density
\emptyset :	fugacity coefficient

Subscripts:

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