Post Combustion Based CO_2 Capture using Solid Sorbents

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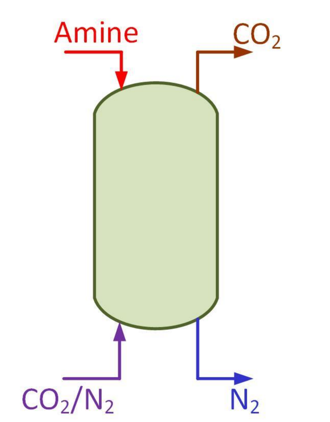
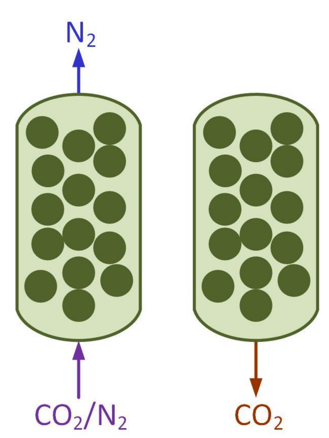
BACKGROUND



Absorption

- Employs liquid solvents, e.g. amines
- Commercialized technology
- High energy penalty for solvent regeneration
- Corrosion and degradation of solvent



Adsorption

- Employs solid-sorbents
- Pilot-scale demonstrations for CO_2-capture
- Explosive growth in ability to synthesize novel solid sorbents, e.g. MOF
- Proven ability to reduce parasitic energy consumption
- Process design and optimization challenging

SHORT-TERM OBJECTIVES

FULL PSA CYCLE

- Stiff PDEs
- Cyclic Process
- Convergence Complexities

Gas phase component and total mass balances:

$$\frac{\partial y_i}{\partial t}+\frac{y_i}{P}\frac{\partial P}{\partial t}-\frac{y_i}{T}\frac{\partial T}{\partial t}=\frac{T}{P}D_L\frac{\partial}{\partial z}\left(\frac{P}{T}\frac{\partial y_i}{\partial z}\right)-\frac{T}{P}\frac{\partial}{\partial z}\left(\frac{y_iP}{T}v\right)-\frac{RT}{P}\frac{1-\varepsilon}{\varepsilon}\frac{\partial q_i}{\partial t}$$

$$\frac{1}{P}\frac{\partial P}{\partial t}-\frac{1}{T}\frac{\partial T}{\partial t}=-\frac{T}{P}\frac{\partial}{\partial z}\left(\frac{P}{T}v\right)-\frac{RT}{P}\frac{1-\varepsilon}{\varepsilon}\sum_{i=1}^{ncomp}\frac{\partial q_i}{\partial t}$$

Energy balance:

$$\left[\frac{1-\varepsilon}{\varepsilon}\left(\rho_s C_{p,s}+C_{p,a}\sum_{i=1}^{ncomp}q_i\right)\right]\frac{\partial T}{\partial t}=\frac{K_z}{\varepsilon}\frac{\partial^2 T}{\partial z^2}-\frac{C_{p,g}}{R}\frac{\partial(vP)}{\partial z}-\frac{C_{p,g}}{R}\frac{\partial P}{\partial t}-\frac{1-\varepsilon}{\varepsilon}C_{p,a}T\sum_{i=1}^{ncomp}\frac{\partial q_i}{\partial t}$$
$$+\frac{1-\varepsilon}{\varepsilon}\sum_{i=1}^{ncomp}(-\Delta H_i)\frac{\partial q_i}{\partial t}-\frac{2h_{in}(T-T_w)}{\varepsilon r_{in}}$$

Darcy's Law for pressure drop:

$$v=\frac{4}{150\mu}\left(\frac{\varepsilon}{1-\varepsilon}\right)^2 r_p^2\left(-\frac{\partial P}{\partial z}\right)$$

Linear driving force (LDF)

$$\frac{\partial q_i}{\partial t}=\alpha_i(q_i^*-q_i)$$

≥120 hours of computation

Optimizer

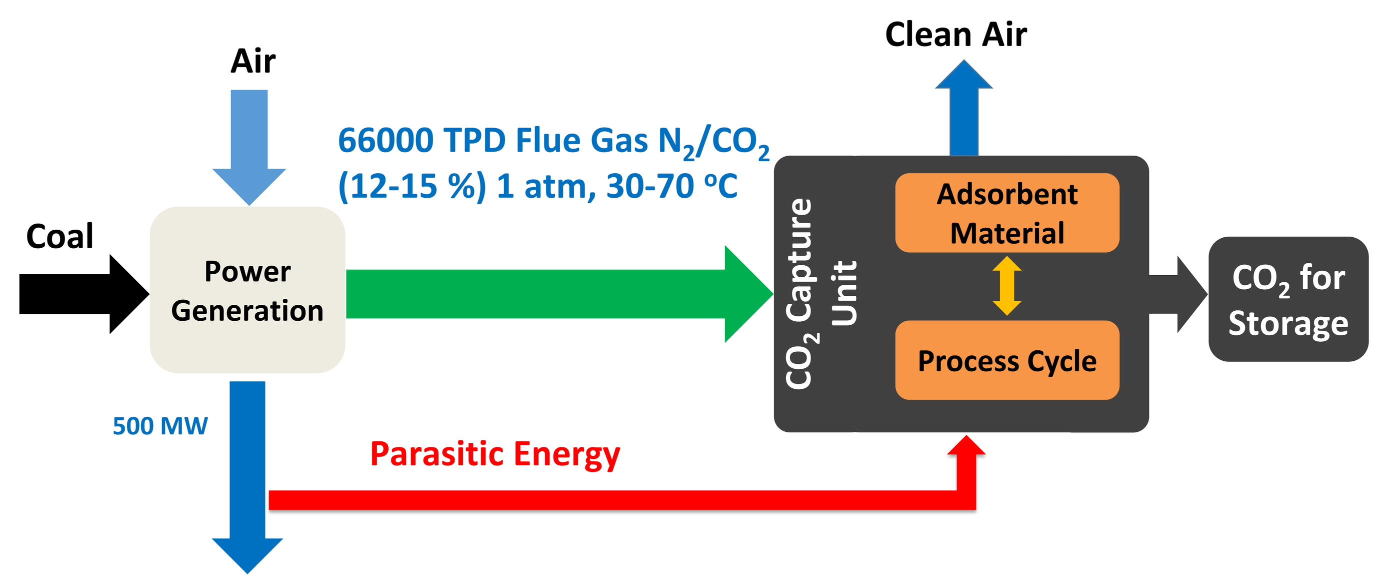
- Genetic Algorithm
- Multi Objective Optimization
- Stochastic Output

Simplified Model

- Model Reduction
- Proxy Modeling

PROJECT OVERVIEW

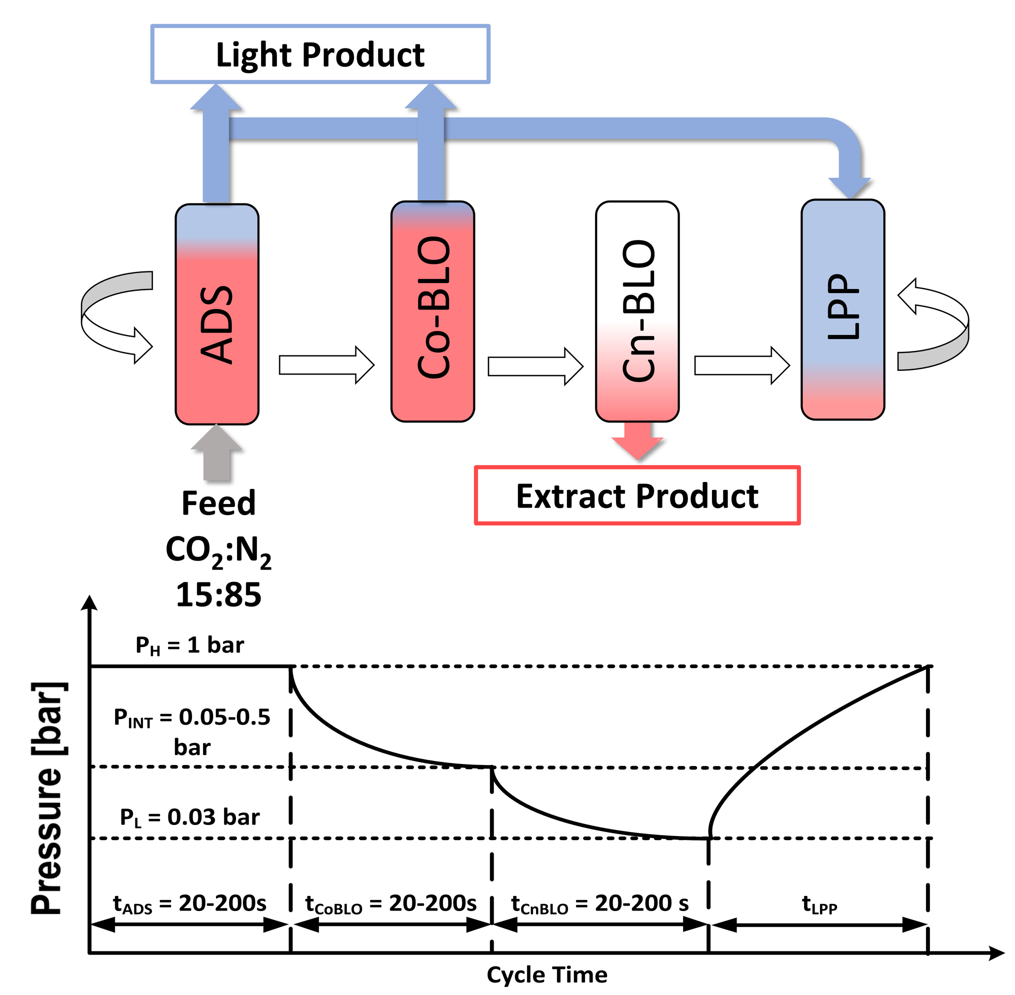
SCHEMATIC OF POST-COMBUSTION CO_2 CAPTURE



CHALLENGES IN POST-COMBUSTION CO_2 CAPTURE

- Low CO_2 concentration in flue gas
- Large volumes – unprecedented, even for industrial operations
- Achieving high purity along with recovery
- Reducing parasitic energy
- Reducing plant footprint

SCHEMATIC OF A SIMPLE PRESSURE SWING ADSORPTION UNIT FOR CO_2 CAPTURE



CHALLENGES IN ADSORPTION PROCESS DESIGN:

- Unsteady state operation- No explicit design methods
- Movement of heat and mass fronts in space and time – Computationally intensive to solve
- Multiple operating configurations with many operating variables subject to operational constraints – Optimization is a challenge

THEME OVERVIEW

Power plant → CO_2 capture → CO_2 compression & transportation → CO_2 sequestration / CO_2 utilization

EXPECTED OUTCOMES

Material Input

- Material Kinetics
- Binary Isotherm Measurements

Material

- Material characterization
- Filtering Materials

Lab Scale Demonstration

- Breakthrough Experiments
- Cycle Experiments

Reduced order Model Simulator

- Design of Process cycles
- Optimization of Process Conditions

Reduce Parasitic Energy

- Higher level optimizations
- Plant level energy optimization

Systems Level Process optimization & Integration

- Reduction in parasitic energy
- Integration of the CO_2 Capture process

Scale up and Industrial level simulations and Implementation

EXTERNAL PARTNERS

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