CCSI^2
Carbon Capture Simulation for Industry Impact

Multi-Objective Optimization of Solid Sorbent-based CO2 Capture Systems

Miguel Zamarripa, John Eslick, David Miller
National Energy Technology Laboratory (NETL)

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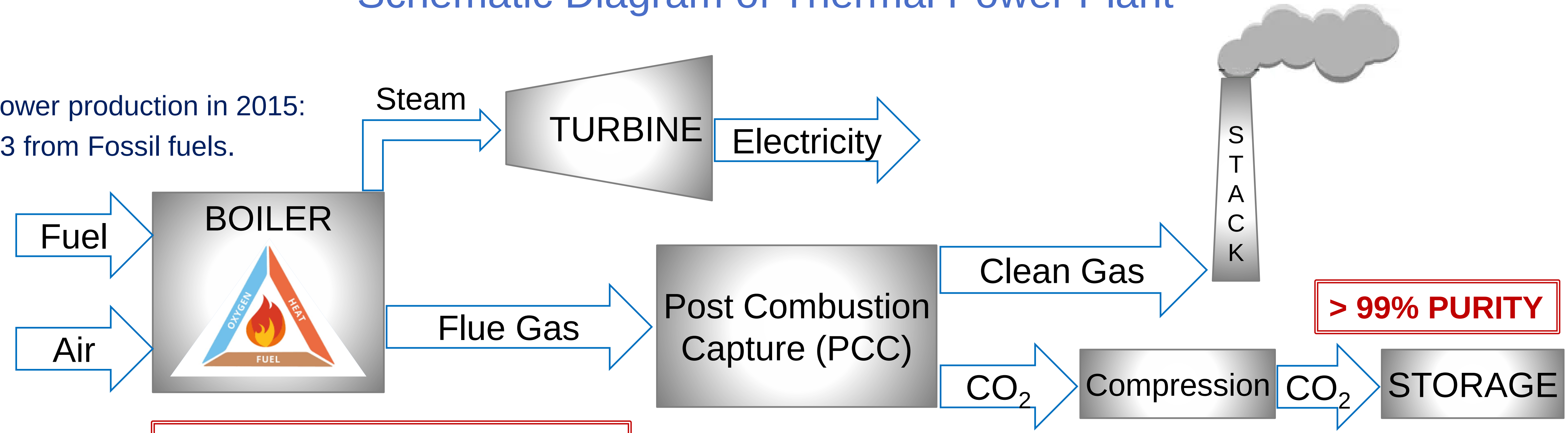
Importance of Post-combustion Carbon Capture

- Schematic Diagram of Thermal Power Plant -

US power production in 2015:

- 2/3 from Fossil fuels.



Fuel

Air

BOILER

OXYGEN

HEAT

FUEL

Steam

TURBINE

Electricity

Flue Gas

Post Combustion Capture (PCC)

Clean Gas

STACK

CO_2

Compression

CO_2

STORAGE

> 99% PURITY

Flue Gas:

- Coal Power plant, 650 MW (**~27 kmol/s**)

PCC:

- Low CO_2 concentration **(~12 % vol)**
- Multiple components (**H_2O**, N_2, CO, O_2)
- **Capture target 90%**

Post-Combustion Carbon Capture Technologies

Liquid Solvents – absorption

Membranes – gas permeation

Solid Sorbents – adsorption

Current studies often do not **rigorously optimize** complete systems considering

- multiple technology options
- process configurations
- operating conditions

Goals:

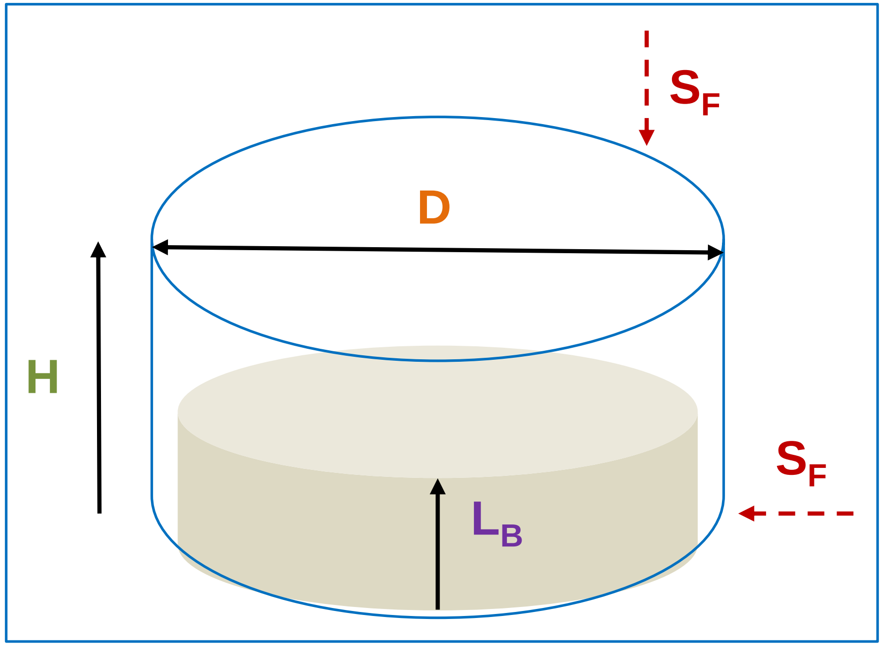
- Simultaneously optimize the **process configuration**, **process design** and **operating conditions** based on rigorous models.
- Explore changes in the **optimal results** (plant design, configuration, and operation) as a function of different **capture rates** (i.e., 40%, 60%, or 90%)

Solid Sorbent Technologies

[1] Lee, A., & Miller, D. C. (2012). *Industrial & Engineering Chemistry Research*,*52*(1), 469-484.

Gas – Solid contactors (adsorption and regeneration):

- Bubbling fluidized bed reactors:
  - 1D model (3 regions: Emulsion, Cloud-Wake, Bubble)[1].
  - PDE's + algebraic equations (~14,000 equations).
  - Sorbent properties (Arrhenius constant & activation energy, heat of adsorption).



Reactor design:

- Solids Feed (**S_F**, top or bottoms)
- Overflow and underflow operation
- Diameter (**D**), height (**H**), solid bed depth (**L_B**)
- Heat exchanger: # tubes and tube spacing

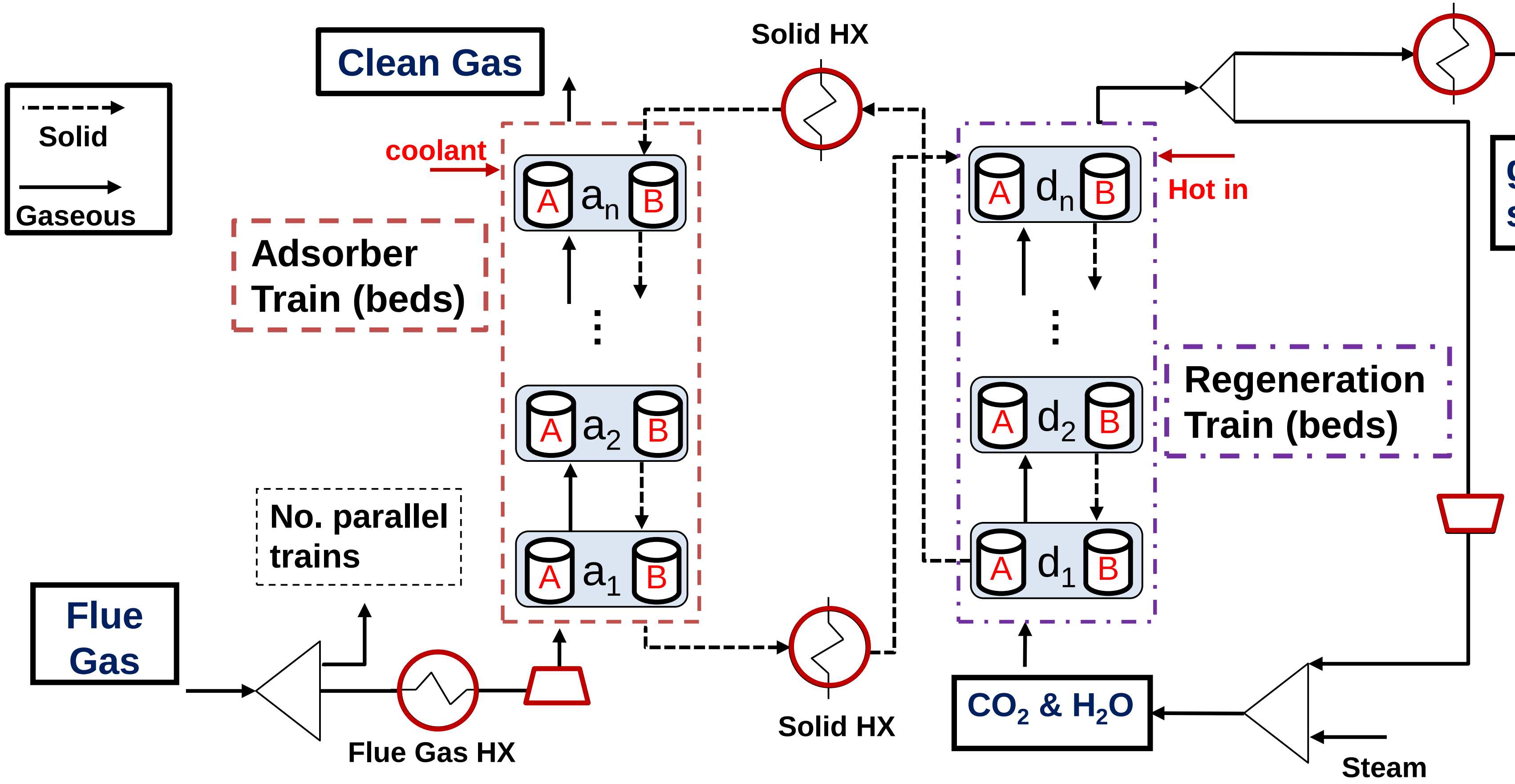
Unit level:

↑ H, D, LB
Gas – Solid contact

System level:

↑ Pressure Drop
Costs: Operation + Investment

Superstructure Optimization Framework



MINLP

Problem **Complexity** Increases with:

- \# of technologies
- \# of stages
- Non-linearities of the problem

- Discrete Decisions: **No. of Parallel trains?** **How many beds (Ads and Rgn)?** **What technology used for each reactor (A or B)?**
- Continuous decisions: **Unit Dimensions (D, h, HX area)** **Operating conditions (T, P, F, z)**

Fixed & Operating Cost

Cost of Electricity

$$\min COE = \frac{(Investment\ + Operating_{fix} + Operating_{var})}{(Net\ Power)}$$

$$\begin{aligned} \mathbf{s.t.}\quad & Material\ Balances \\ & Energy\ Balances \\ & Equipment\ Design \\ & Process\ Configuration \\ & Capture\ Target \end{aligned}$$

Costing Methodology:

- **Investment cost**
  - Sorbent, Power Plant, Capture (ads, rgn, HX, cmp).
- **Operating cost:**
  - Fixed: labor, maintenance, others.
  - Variable: utilities “coolant & steam”, waste water, others.
- **Net power**:
  - Power PP – (kW for compression, blowers, pumps, etc).

Quality Guidelines for Energy System Studies: Performing a Techno-economic Analysis for Power Generation Plants (DOE/NETL-2015/1726)

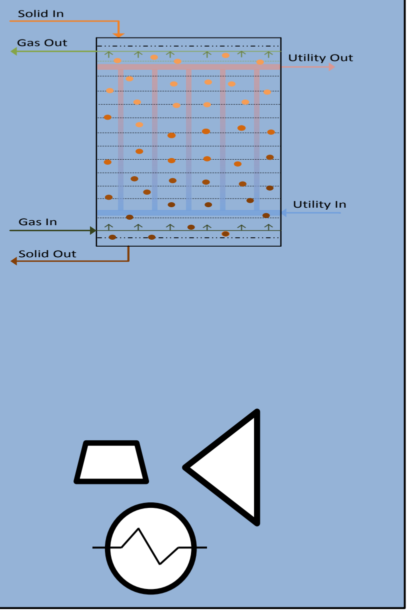
- ➢ Capital cost levels and their elements

Product and Process Design Principles Synthesis (Seider et al., 2009)

- ➢ Purchase cost calculations

Multi-objective Analysis

Process Models

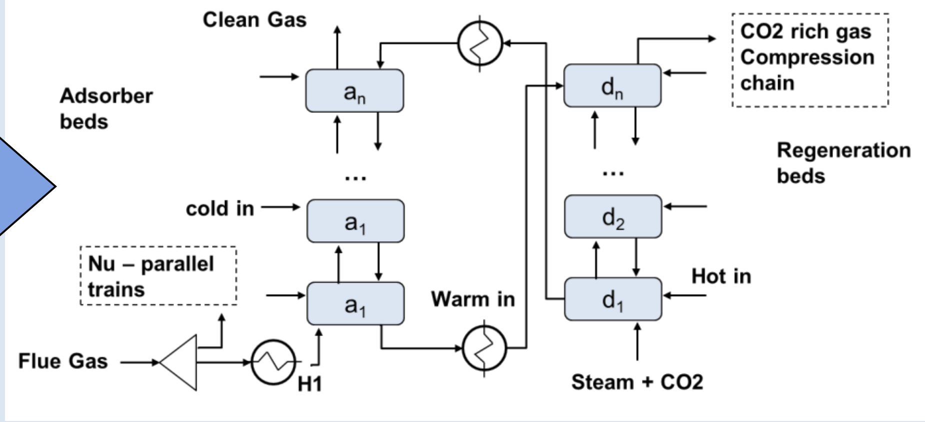


Surrogate Models
(nonlinear models
suitable for optimization)

+

First Principle Models

Superstructure Opt. Model

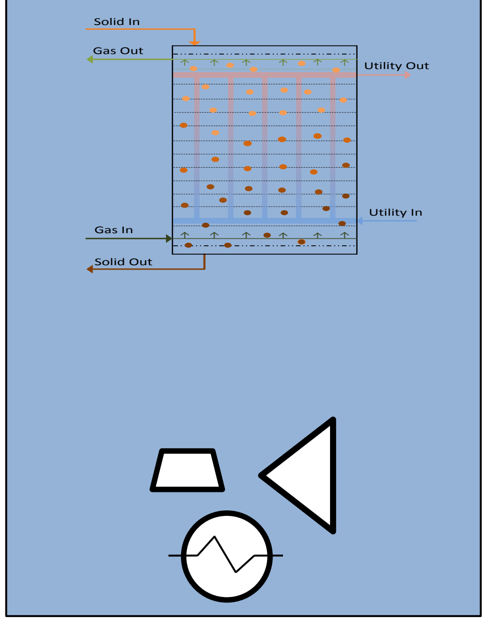


Surrogate Model
Generation and
Validation

FOQUS + ALAMO
a black-box modeling tool

Multi-objective Analysis

Process Models



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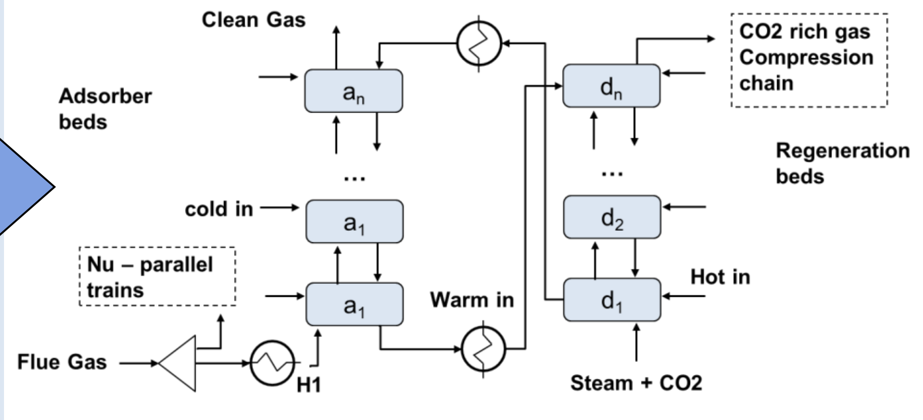
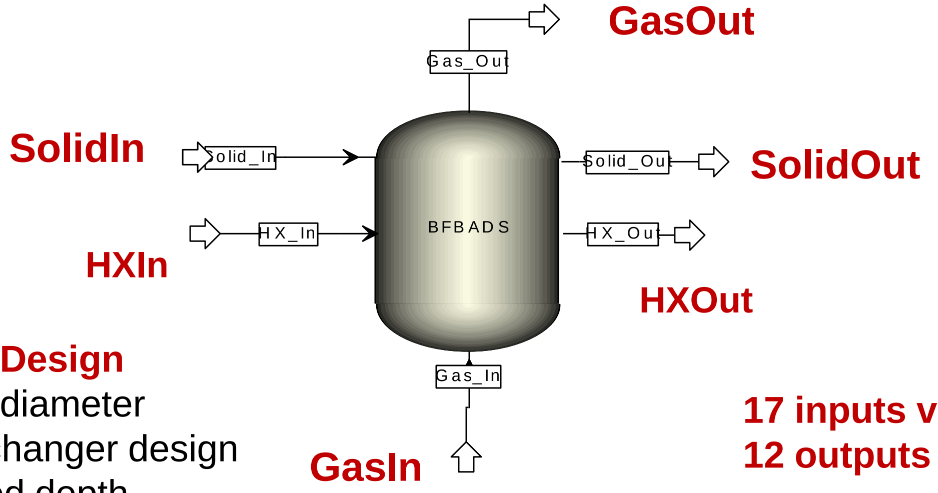


FOQUS

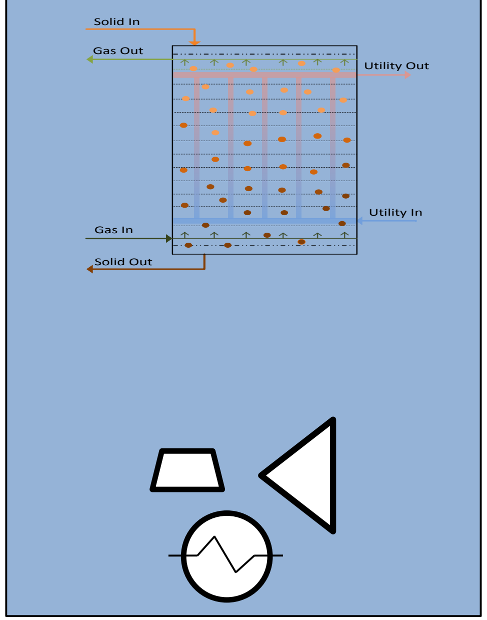
- BFB for Adsorption & Regeneration
  - Detailed ACM simulation.



~~~14,000 equations~~

12 EQUATIONS

Reactor Design
Dt – unit diameter
Heat Exchanger design
Solids bed depth

17 inputs vars
12 outputs vars
~~~

Multi-objective Analysis

Process Models



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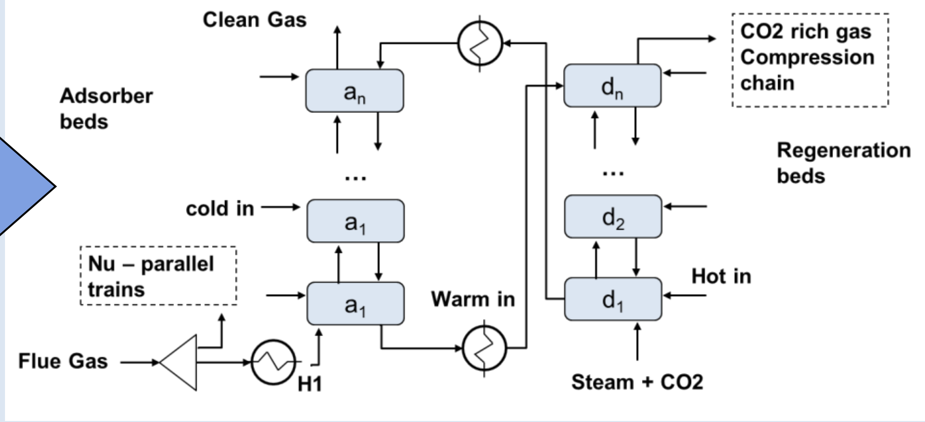
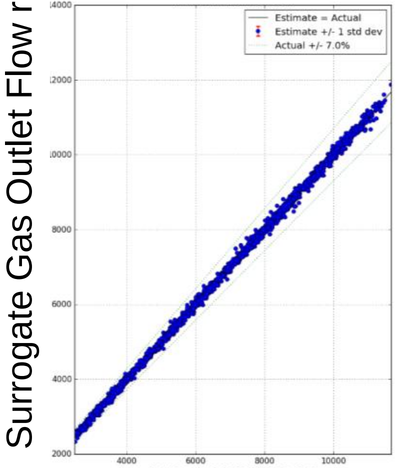


FOQUS

- BFB for Adsorption & Regeneration
    - Detailed ACM simulation.
- **Data Management**
- **Run ALAMO**
- Validation

- **Data Set:**
    - 2000 samples
    - Latin Hypercube Sampling method

Fit data



Rigorous Gas Outlet Flow rate

R^2= 0.99

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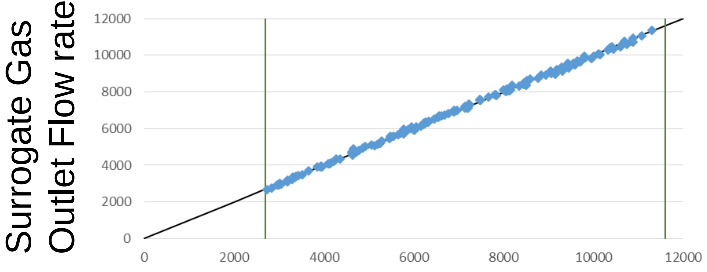


Rigorous Gas Outlet Flow rate

- Cross-Validation
    - 200 samples
    - LHS method

Solid Sorbent System – Case Study

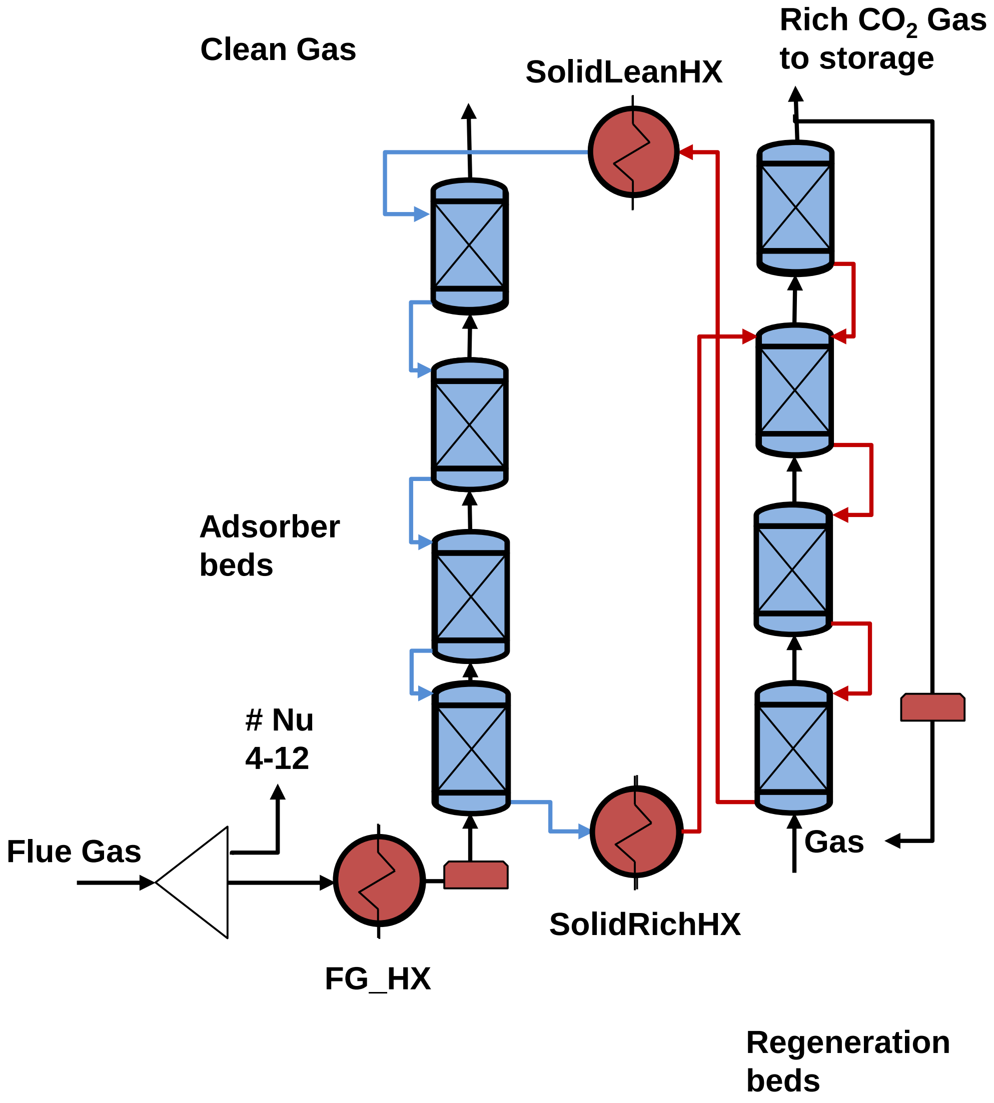
Adsorption system

Plant consists of:

- Flue gas (**650 MW power plant**)
- 90 % capture needed
- CO_2 ~12% (molar fraction)
- 4 adsorber & regeneration beds
  - 2 technologies (reactor configuration)
- 4 – 12 parallel units.

Mathematical Model

- **First principle**
- **Surrogate models**.



Optimal Solutions

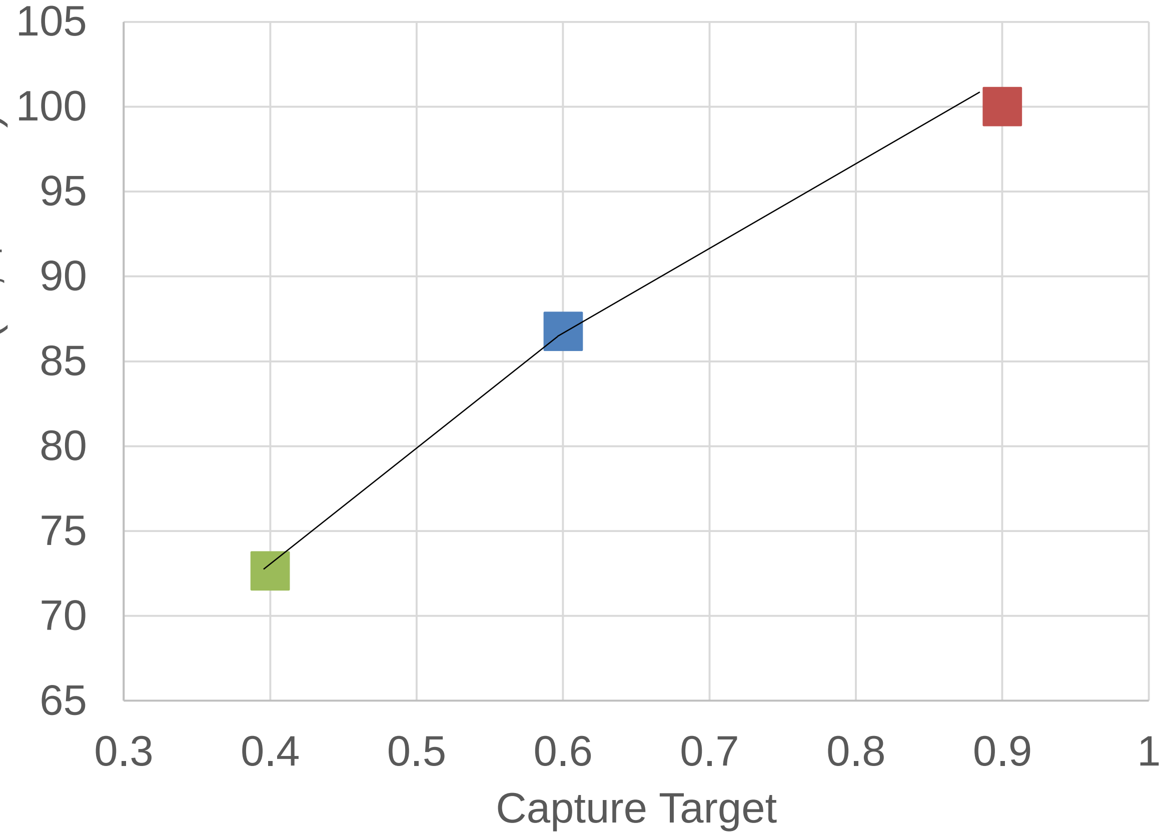
Summary:

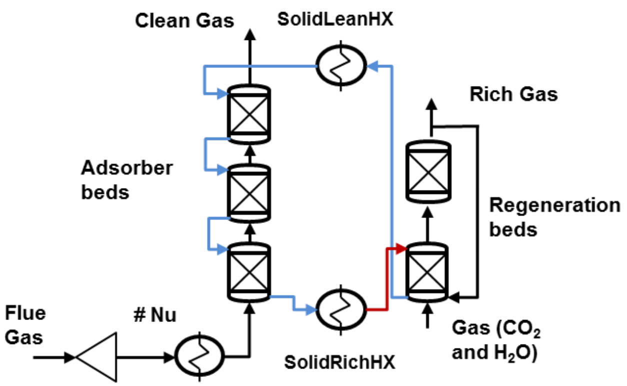
- Superstructure optimization allow us to explore all the possible plant **layouts**.
- Optimization problem (GAMS/Dicopt):
  - 383 equations
  - 588 variables (24 Discrete)
- 90% CO_2 Capture.

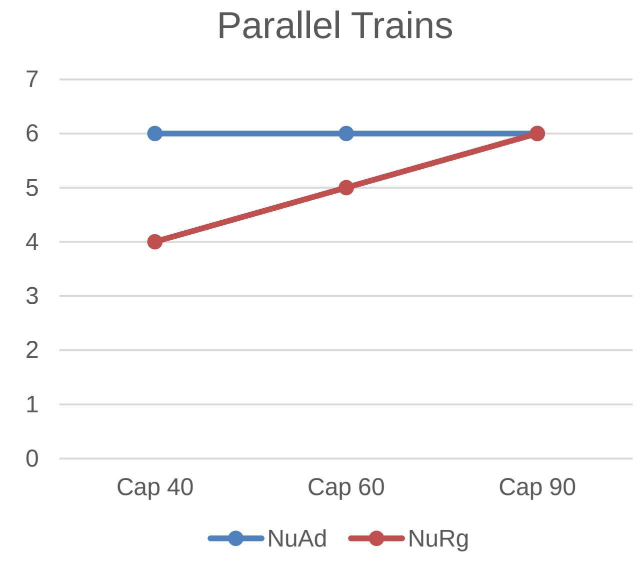
	Different initialization			Fixed layout			
	Optimal	**Case 1**	**Case 2**	**Case 4**	**Case 5**	**Case 6**	**Case 7**
% COE increase	-	0.347	0.766	3.689	3.68	4.536	6.23
Adsorber beds		3	3	3	2	3	3
Regeneration beds		3	2	1	3	2	2
Ads parallel units		6	6	6	6	6	7
Rgn parallel units		6	6	6	5	4	7

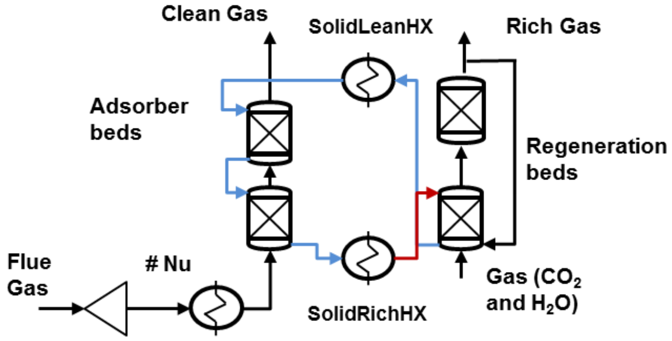
COE vs Capture Target

- Cost of electricity due to capture
- Capture target (90% - Base Case)









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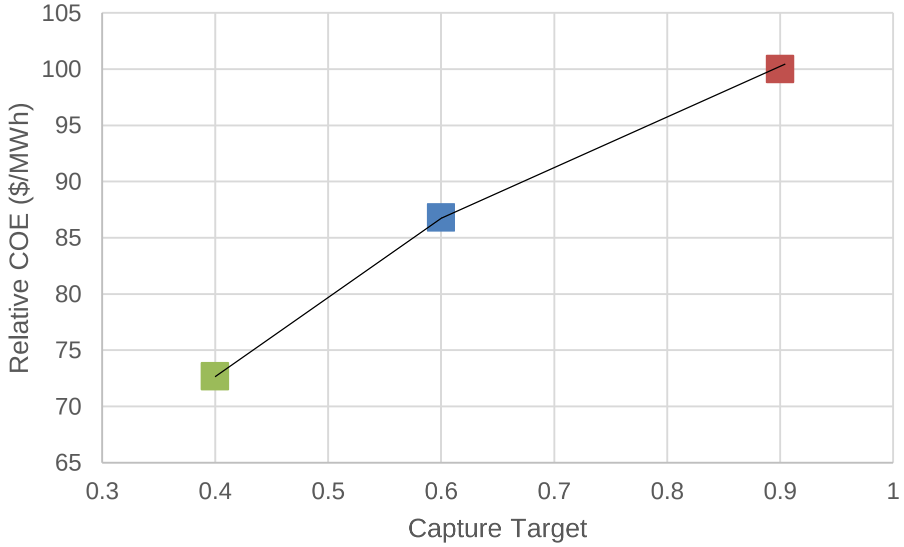
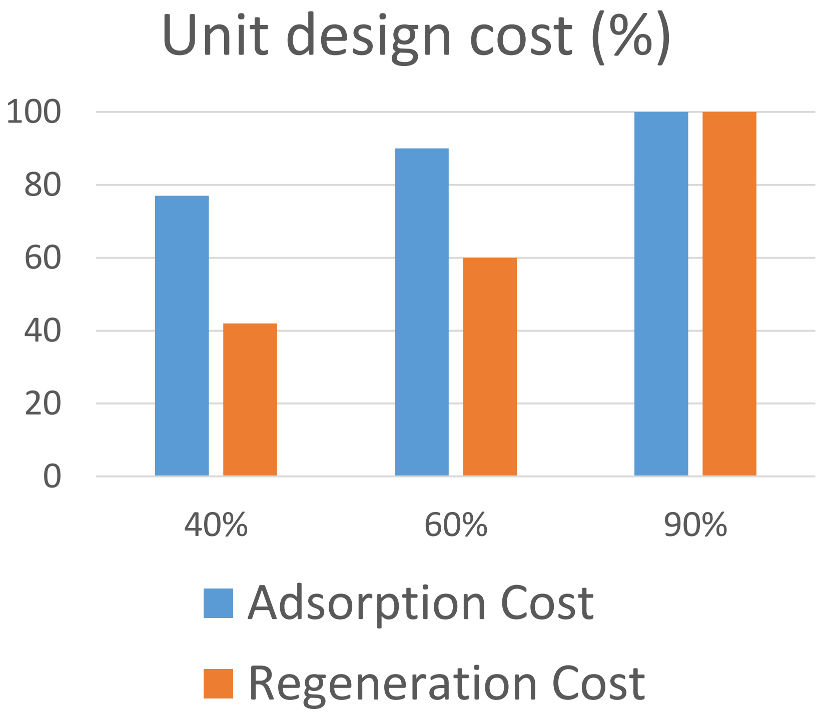
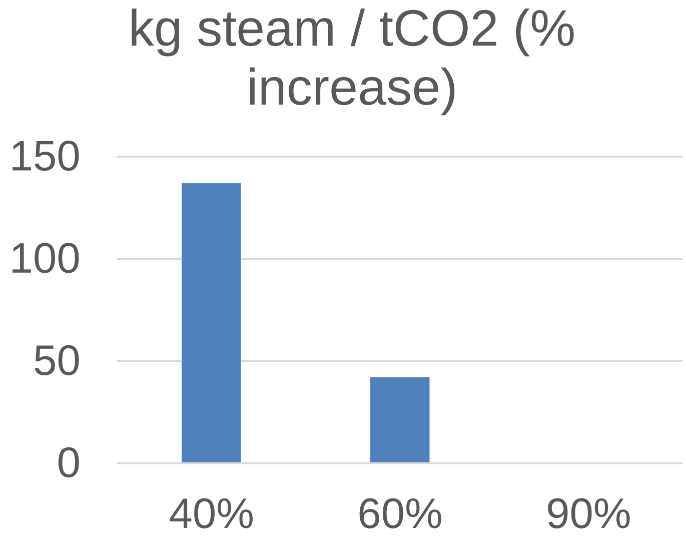
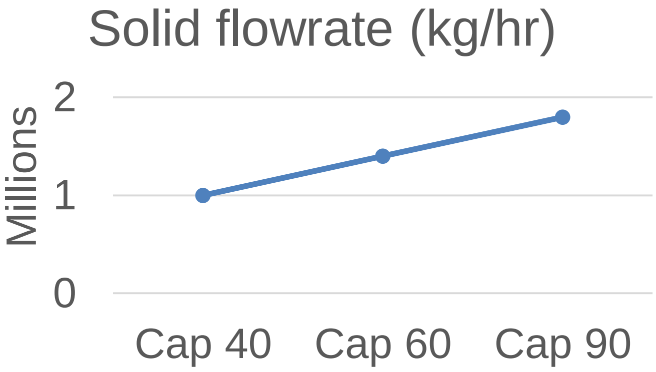



Unit design cost (%)


kg steam / tCO2 (% increase)


Solid flowrate (kg/hr)

Remarks

- Superstructure optimization is challenging
  - PDE models replaced by surrogates

- Integrated conceptual design and process synthesis tools
  - **Facilitate** rapid development
- Robust mathematical optimization framework
  - Optimal process configuration changes with capture target
  - Demonstrates importance of conceptual design
    - Complements typical flowsheet optimization
- Potential extension for multiple technologies

Acknowledgments

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Thank you for your attention

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Carbon Capture Simulation for Industry Impact

For more information
https://www.acceleratecarboncapture.org/

David C. Miller, Ph.D., Technical Director
David.Miller@netl.doe.gov

Michael S. Matuszewski, Associate Technical Director
Michael.Matuszewski@netl.doe.gov