CCSI

Carbon Capture Simulation Initiative

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Optimal Design and Operation of Hybrid CO_2 Capture Systems

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Post Combustion Technologies

Post Combustion CO2 Capture

- **Solid Sorbents – adsorption**

  Issues
  - Energy Intensive
  - Plant complexity
- **Solvents - absorption**

  Issues
  - Energy Intensive
  - Plant complexity
- **Membrane-based – gas permeation**

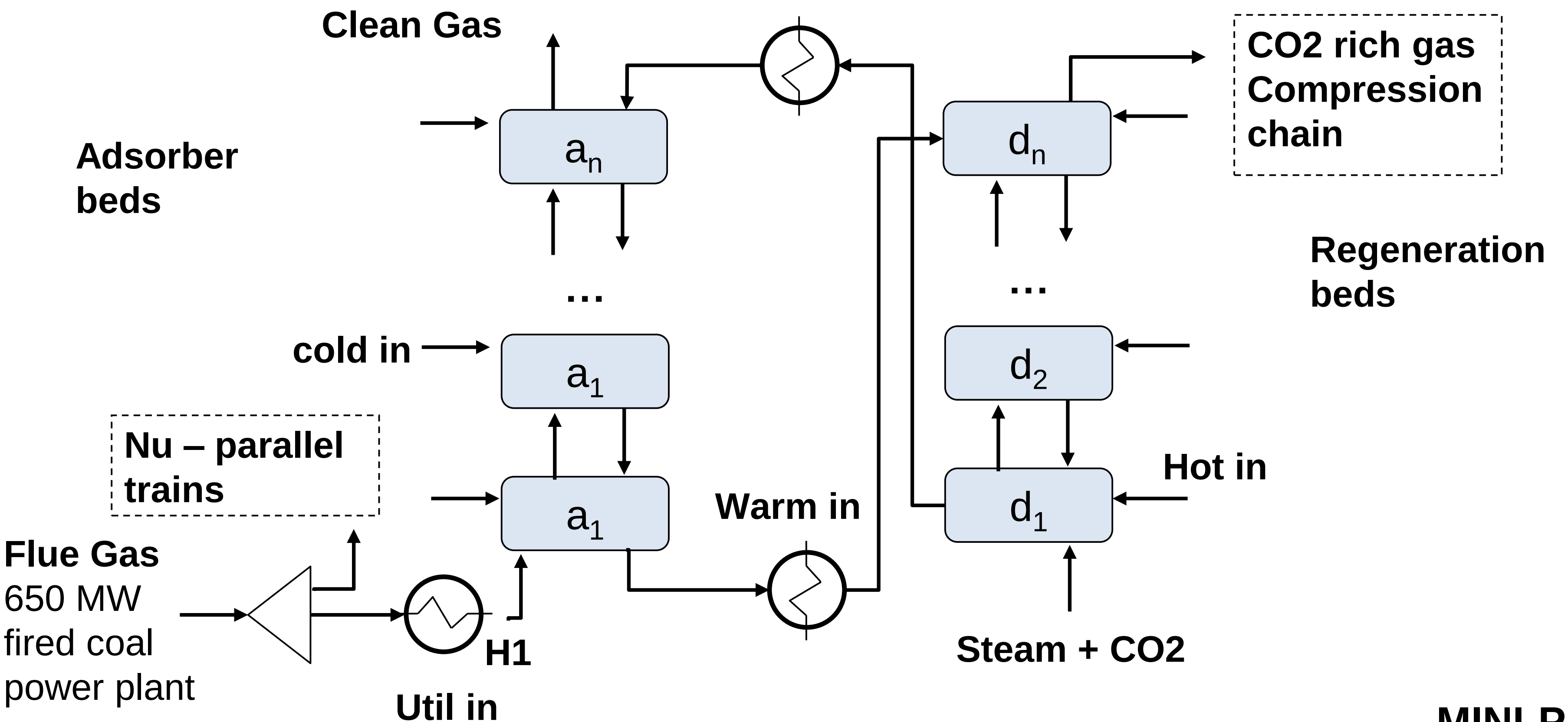
  Issues
  - Flue gas with low CO_2 concentration

Studied independently

➢ Hypothesis
- **Hybrid CO_2 capture plants** could reduce the capture costs.

➢ Intermediate GOALS
- Establish a consistent framework to optimize the structure and design of capture technologies
  - Superstructure optimization framework
- **Robust Mathematical** models

Superstructure Optimization Framework



MINLP

- Discrete Decisions: **How many units? Parallel trains? What technology used for each reactor?**
- Continuous decisions: **Unit geometries, Operating conditions (temp, pressure, flow rates, compositions)**

Problem Statement

Cost of Electricity (COE)

$$\min COE$$

$s.t.$ Material Balances
Energy balances
Equipment design

Adsorption model

- Design:
  - # of parallel units,
  - # of adsorbers and # of regenerators,
  - Size of equipment (Heat exchangers, reactors, blowers)
- Operation:
  - Flows (molar and mass flow rates)
  - Temperatures (Coolant, steam, gas, solids)
  - Pressure (gas and solids)
  - Concentrations (gas and solids)

$$\min COE$$

$s.t.$ Material Balances
Energy balances
Equipment design

- Operating Cost
- Variable Cost
- Fixed annual investment cost
- Net power cost

Membrane separation model

- Design:
  - # of membranes to be installed,
  - Size of equipment (Heat exchangers, pumps, expanders, membranes)
- Operation:
  - Flows (permeate, retentate)
  - Temperature (gas, coolant)
  - Pressure (retentate and permeate sides)
  - Concentrations (gas)

Solid Sorbent System

Adsorption system

Plant consists on:

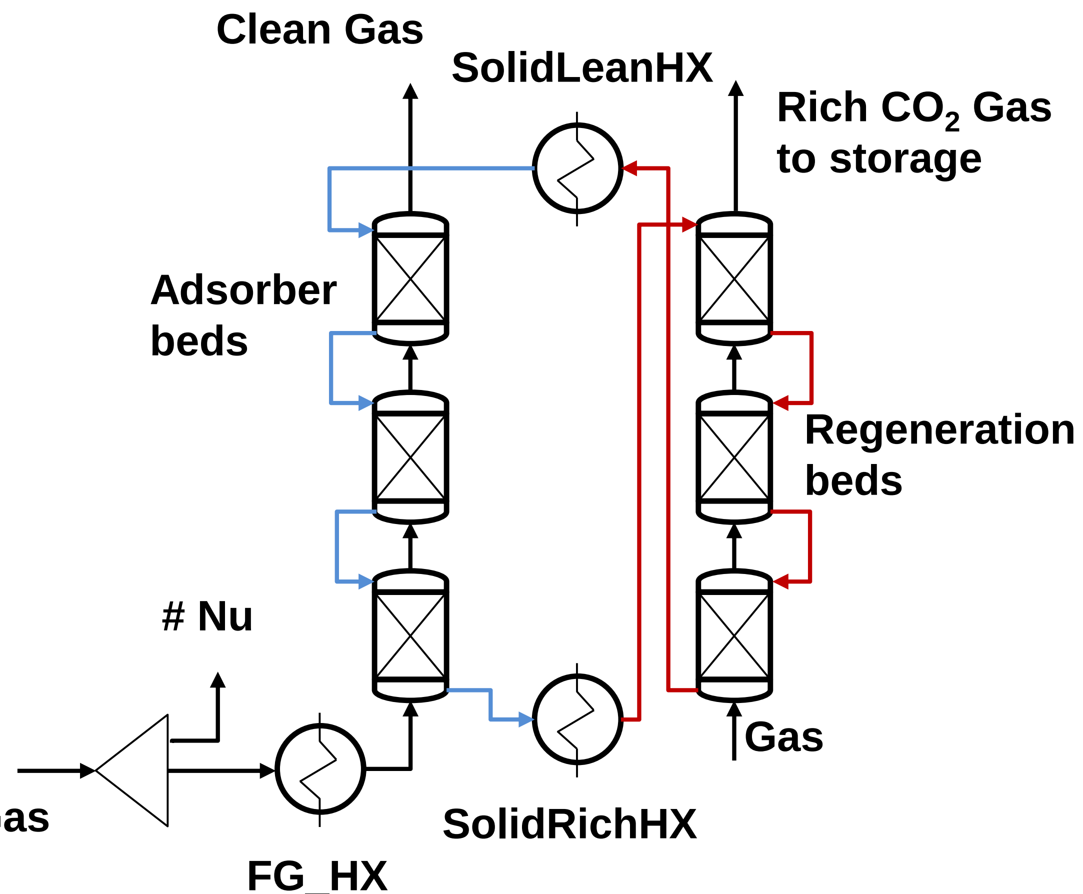
- Flue gas (**650 MW power plant**)
- 90 % capture

Design Decisions:

- # number of parallel units,
- Flue gas heat exchanger,
- Adsorber and Regeneration trains,
- SolidLean and SolidRich Heat exchangers

Operation

- Flows, temperatures, concentrations



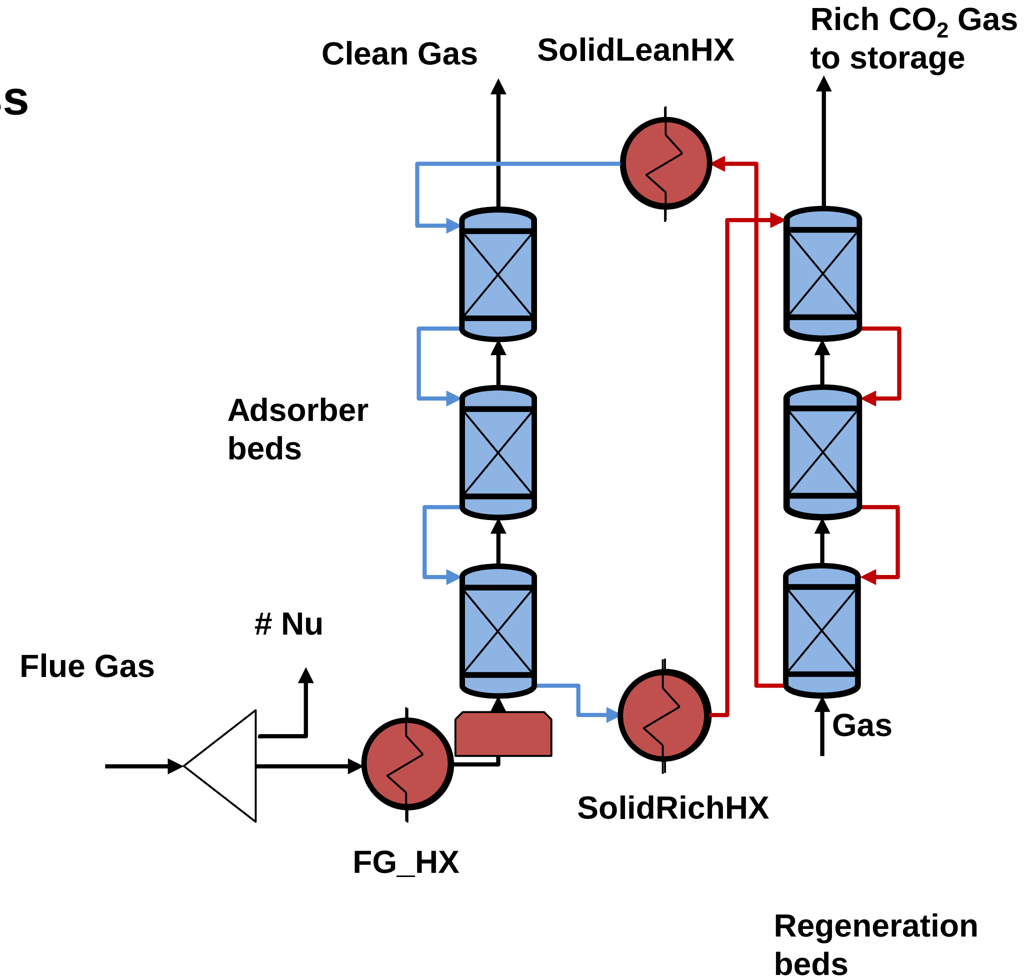
Solid Sorbent System

Adsorption & Regeneration process

- ➢ Bubbling fluidized bed reactor
  - Lee and Miller 2013[1]
  - One dimensional model
  - Mass & energy balances
  - Integrated heat exchanger
  - PDEs 10,000 Equations

Mathematical Model

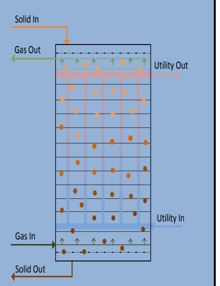
- Mix of **first principle**
- and **Surrogate models** to describe the process.



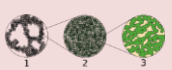
[1]Lee A, Miller, D.C. I&ECR 2013.

Solid Sorbent System

Process Models



Basic Data Submodels



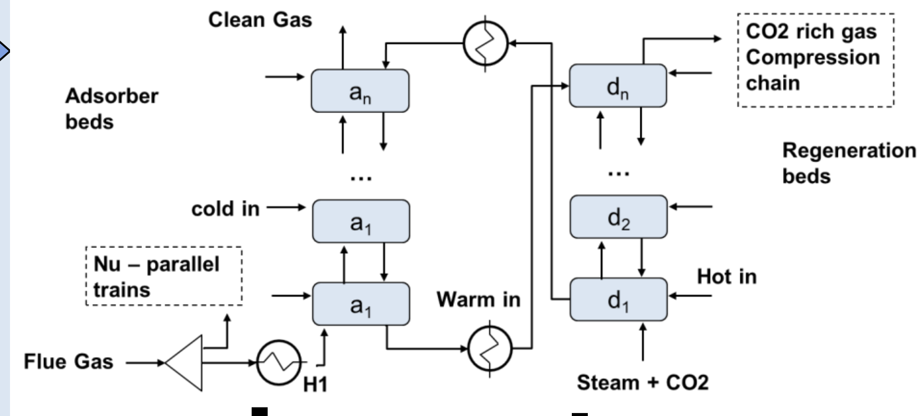
Algebraic Surrogate Models

ALAMO
a black-box modeling tool

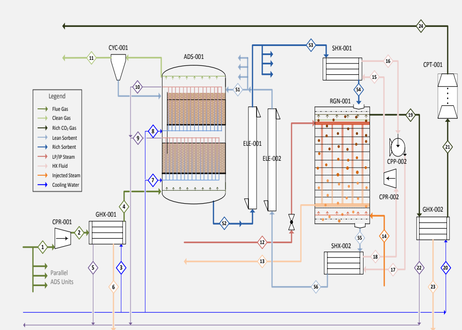
First Principle Models

- Heat exchangers, blowers, pumps, etc.
- Nonlinear algebraic equations

Superstructure Optimization



Carbon Capture Process



Optimized Process

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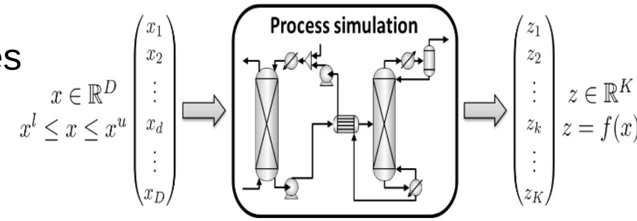
Solid Sorbent System

ALAMO “Surrogate models correlate the input and output variables of the process“

Adsorption system

- First principle:
  - Heat exchangers, blowers, pumps, etc.

Input variables



Output variables

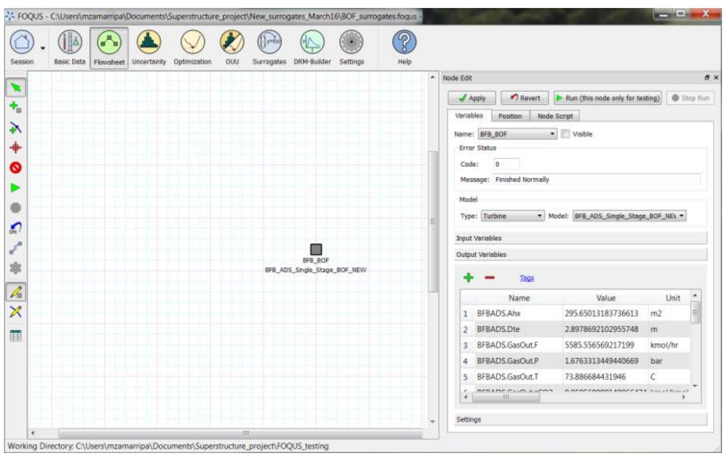
Data set (simulations)

Final surrogate Model:

$$z_i = f(x_1, \ldots, x_D) \;\; \forall\, i \in K$$

- Surrogate models:

Framework for Optimization and Uncertainty Quantification and Surrogates - FOQUS



FOQUS

Process Simulation	Surrogate model	Optimization
• Data sampling • Data analysis • Data refining	• Generation • Validation	• **GAMS** • Validation (FOQUS)

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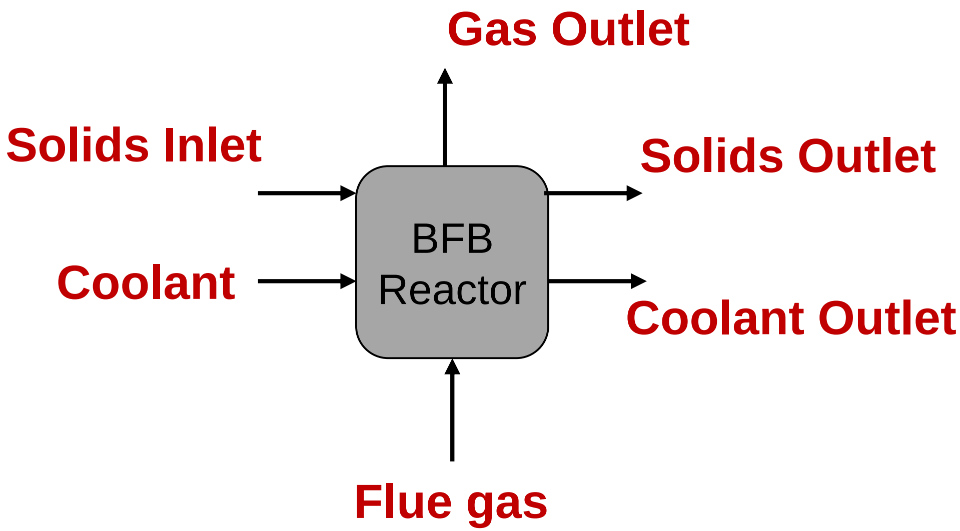
Solid Sorbent System

Reactor Design
- Dt – unit diameter (m)
- Heat Exchanger design
- Solids Fluidization bed

Adsorption system

- First principle:
  - Heat exchangers, blowers, pumps, etc.

- Surrogate models:
  - Simulation
    - Model 10,000 PDE's
    - Aspen Custom Modeler
  - Data set
    - 2000 samples
    - Latin Hypercube Sampling method



- **Flow rate**
- **Pressure**
- **Temperature**
- **Concentration**

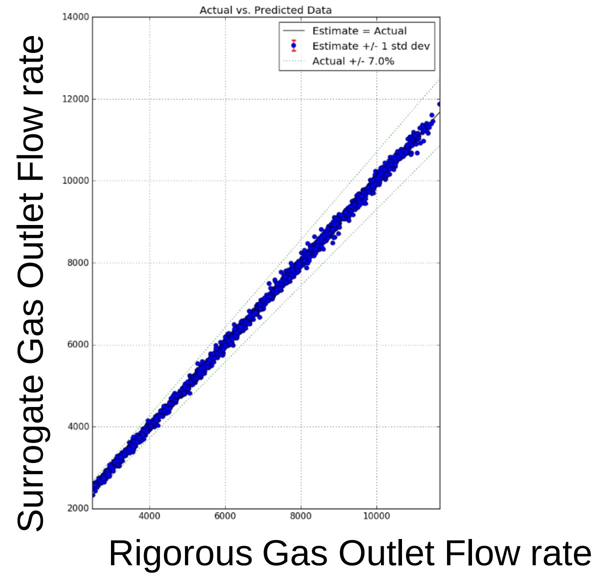
Solid Sorbent System

Adsorption system

- First principle:
  - Heat exchangers, blowers, pumps, etc.

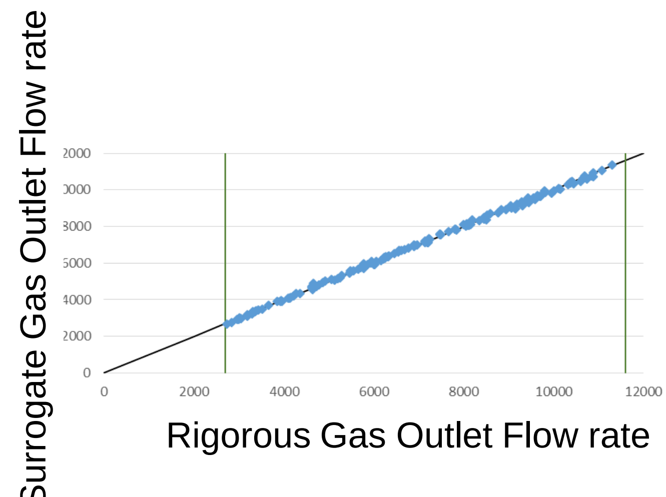
- Surrogate models:
  - Simulation
    - Model 10,000 PDE's
    - Aspen Custom Modeler
  - Data set
    - 2000 samples
    - Latin Hypercube Sampling method
  - **Surrogate model generation**
    - **Validation and cross-validation**

Fit data



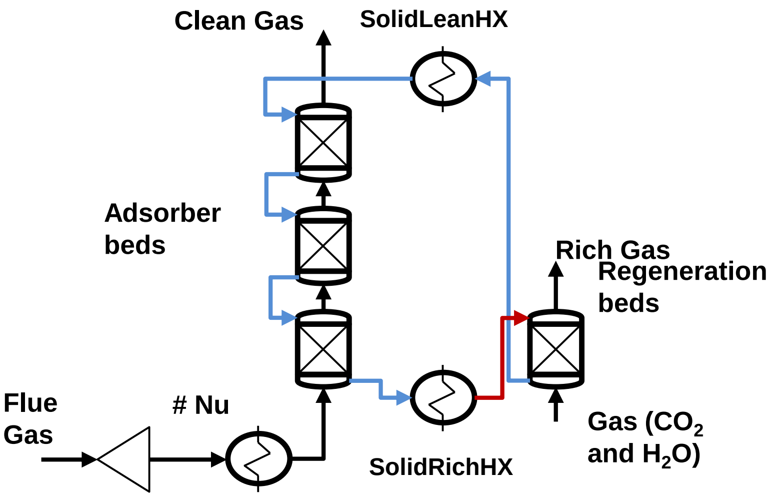
R^2= 0.99

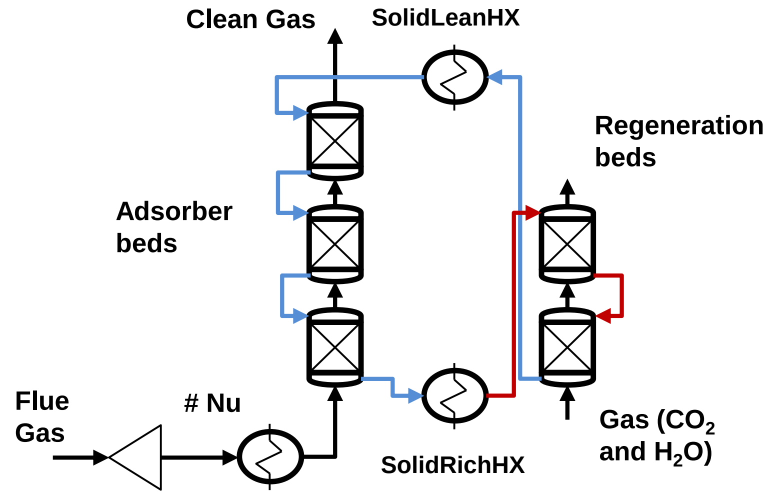
Cross-validation



R^2= 0.99

Optimal Solutions





Optimization:

- Superstructure optimization allow us to explore all the possible plant layouts.
- 90% CO_2 Capture.

Fixed layout

	Best Case	Case 1	Case 2
COE increase relative to best case	-	5.12 %	3.63 %
Adsorber beds	3	3	3
Regeneration beds	1	2	1
Ads parallel units	6	6	8
Rgn parallel units	4	4	6

Membrane based systems

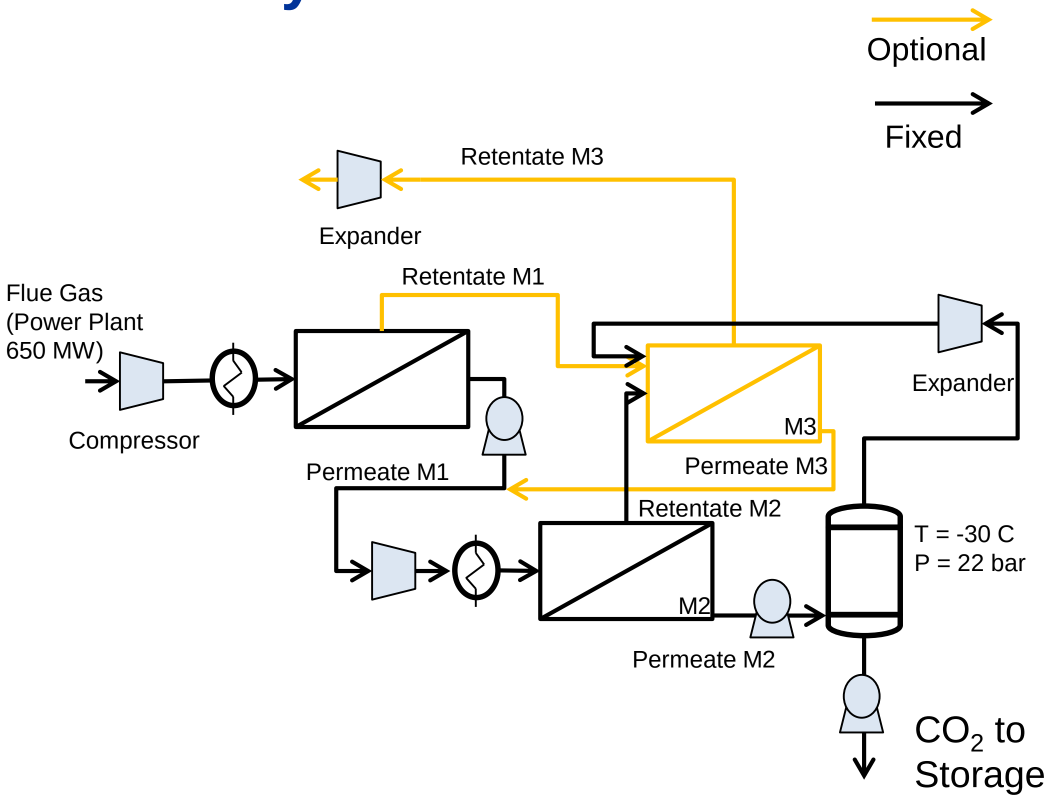
Membrane separation

Design:

- # of membranes to be installed
- Membrane area
- Size/cost of Heat exchanger, pumps, compressors, expanders

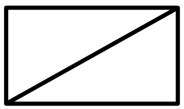
Operation:

- Flows (feed, permeate, retentate)
- Temperature (gas, coolant)
- Pressure
- Concentrations (gas)



90% Capture

97 % CO_2 pure to Storage



T_{mem} = 25 C

Permeance = fixed (kgmol/m2 s bar)

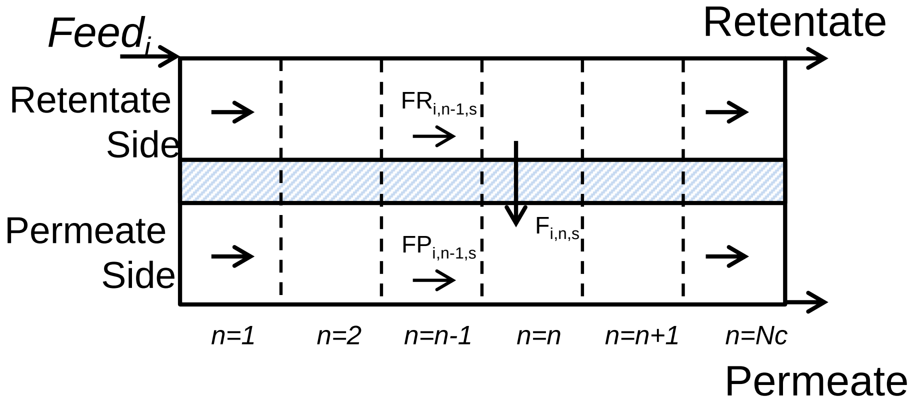
Operation = co-current flow

Pressure ratio = Pin (bar) /Pout (bar)

Membrane based systems

- Separation stage

Co-current flow[2]



$FR_{i,n,s}$ – molar flow rate **retentate side**

$FP_{i,n,s}$ – molar flow rate **permeate side**

$F_{i,n,s}$ – molar flow rate **moving** from the **retentate to** the **permeate** side

Material Balances:

$$FR_{i,n,s} = \text{Inlet} - F_{i,n,s}$$

$$FP_{i,n,s} = \text{Inlet} + F_{i,n,s}$$

$$F_{i,n,s} = \frac{A_s}{|Nc|} \frac{P}{\delta} \left(P1_s xr_{i,n,s} - P2_s xp_{i,n,s} \right)$$

Membrane Area

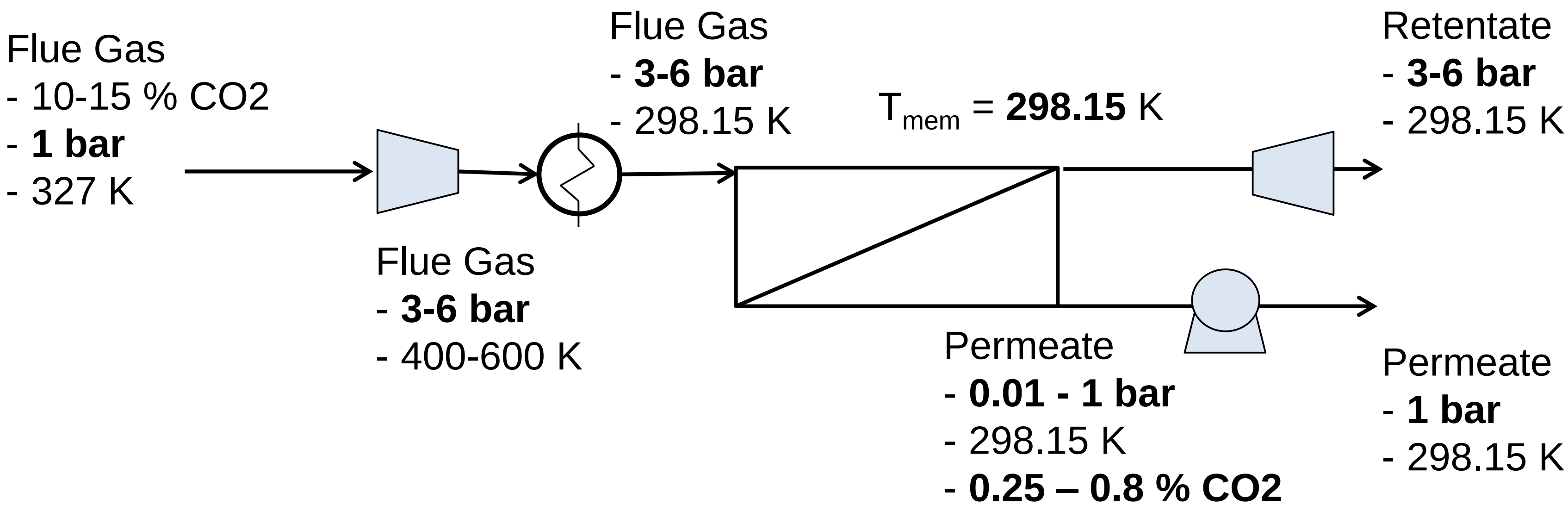
Membrane material design
Permeance (kgmol/m² s bar)

Driving force
(Partial pressure difference)

[2]Hasan, Baliban, Elia and Floudas, I&ECR, 2012.

Membrane based systems

- Separation stage

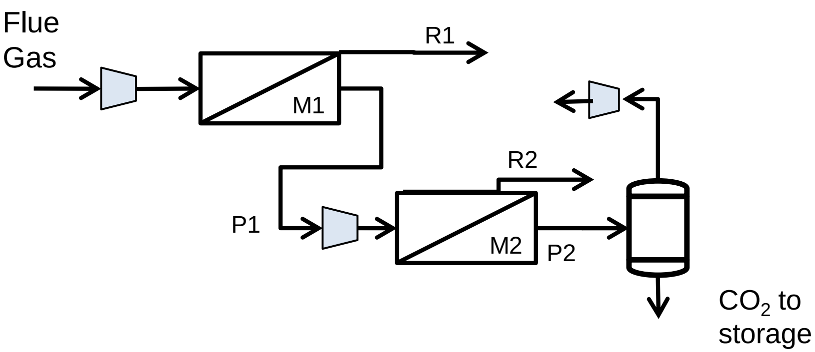


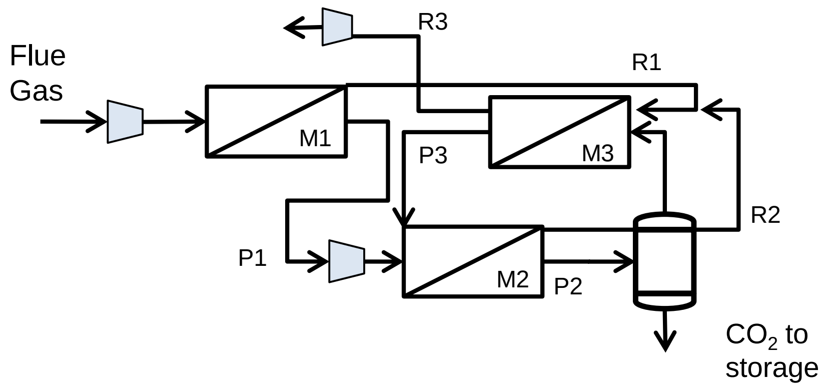
Stage:
- Compression system
- Heat exchanger
- Membrane
- Vacuum pump
- Expander

$$\min_{x} f(x)$$
$$\begin{aligned} s.t.& \\ & g_i(x) \leq 0, \quad i = 1, \dots, n \\ & h_j(x) = 0, \quad j = 1, \dots, m \\ & x \in X \end{aligned}$$

Optimal Solutions

P – Permeate
R – Retentate
M – Membrane





Optimization:
- Configuration: 2 membrane stages, flash unit, recirculation R1 and R2 to M3
- 15% COE increase relative to best case
- **70% CO_2 Capture**

Optimization:
- Configuration: 3 membrane stages, flash unit, recirculation R1 and R2 to M3
- 90% CO_2 Capture

Remarks

- A robust mathematical optimization framework has been developed to optimize the structure and design of CO_2 capture technologies.
- Establishing a consistent basis for analyzing the cost of electricity due to capture is a critical issue to compare different Post Combustion Capture Technologies.
- Further work has been simplified and a hybrid model is under study.

Solid Sorbents

- Rigorous models have been replaced by surrogate models.
  - Surrogate model generation, validation and cross-validation have been simplified with the Framework for Optimization and Uncertainty Quantification and Surrogates.

Membrane-based systems

- Optimization of multiple membrane configurations is a critical issue to enhance the separation performance.

Acknowledgments

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Thank you for your attention