CCSI

Carbon Capture Simulation Initiative

16AIChE

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Optimal Design and Operation of Hybrid CO_2 Capture Systems

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Post Combustion Technologies

General issues:
- **Costing Methodologies**
- **Optimization frameworks**

Post Combustion CO_2 Capture

Studied independently

- Solid Sorbents – adsorption
- Solvents - absorption
- Membrane-based – gas permeation

Solid Sorbents – adsorption

Issues
- Energy Intensive
- Plant complexity

Solvents - absorption

Issues
- Energy Intensive
- Plant complexity

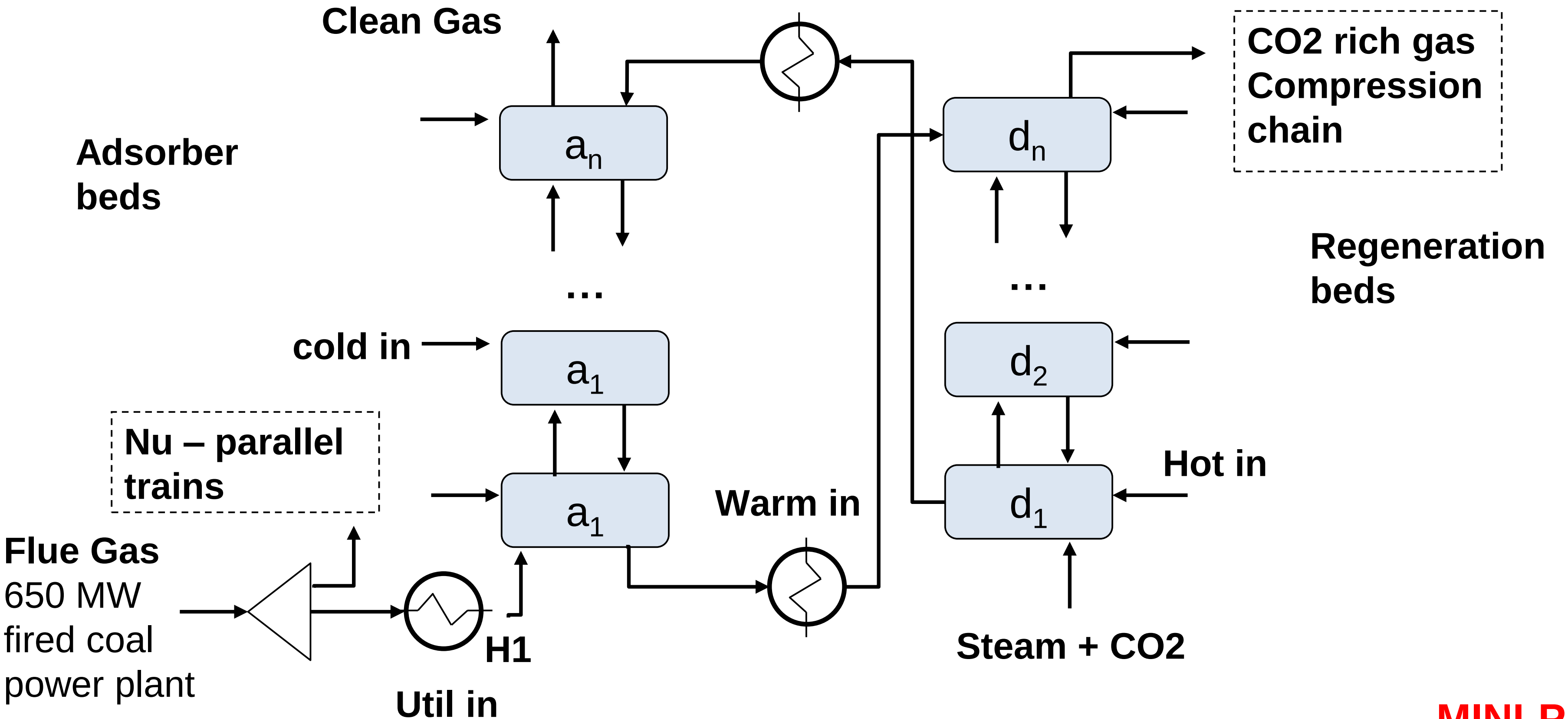
Membrane-based – gas permeation

Issues
- Flue gas with low CO_2 concentration

- 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

$$\min COE$$

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

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

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)

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:

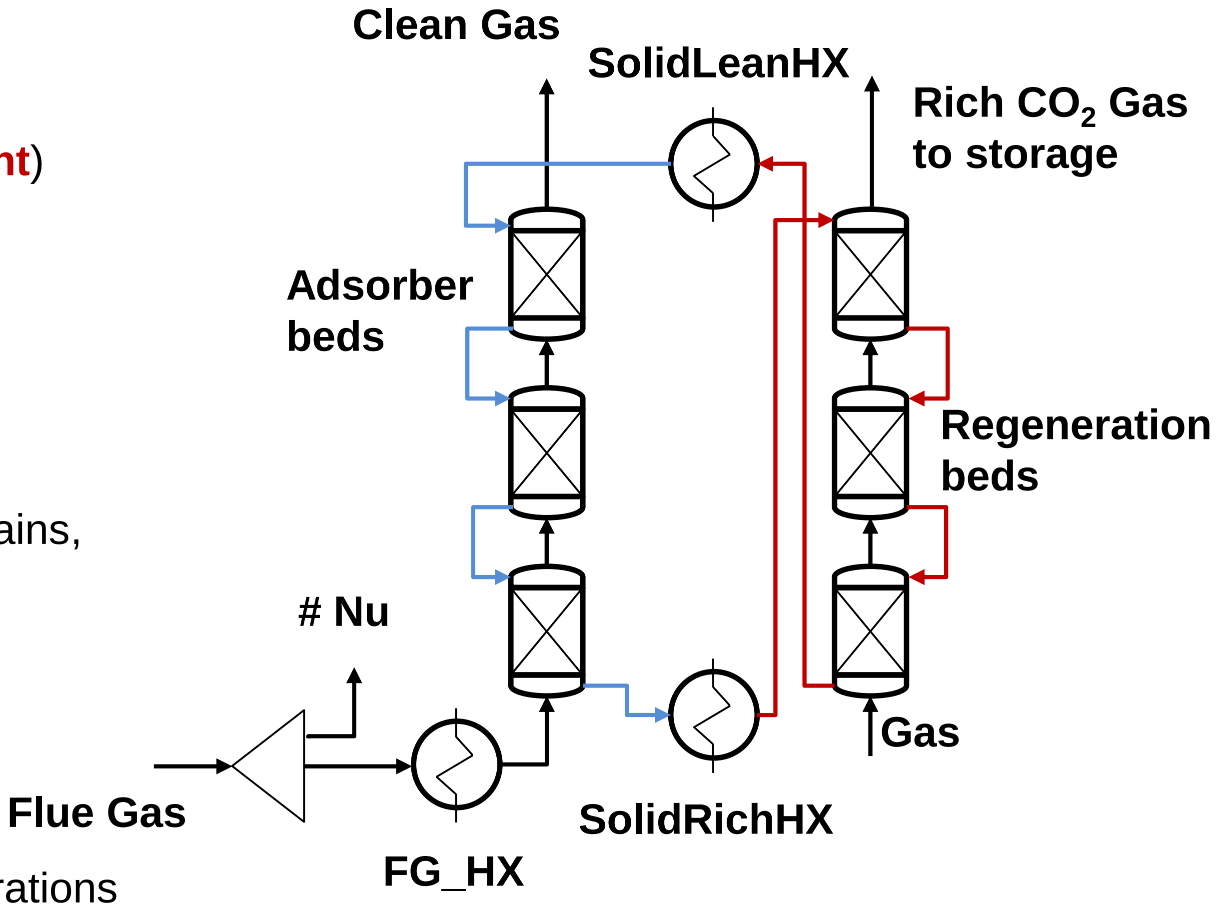
- Flue gas (**650 MW power plant**)
- 90 % capture

Design Decisions:

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

Operation

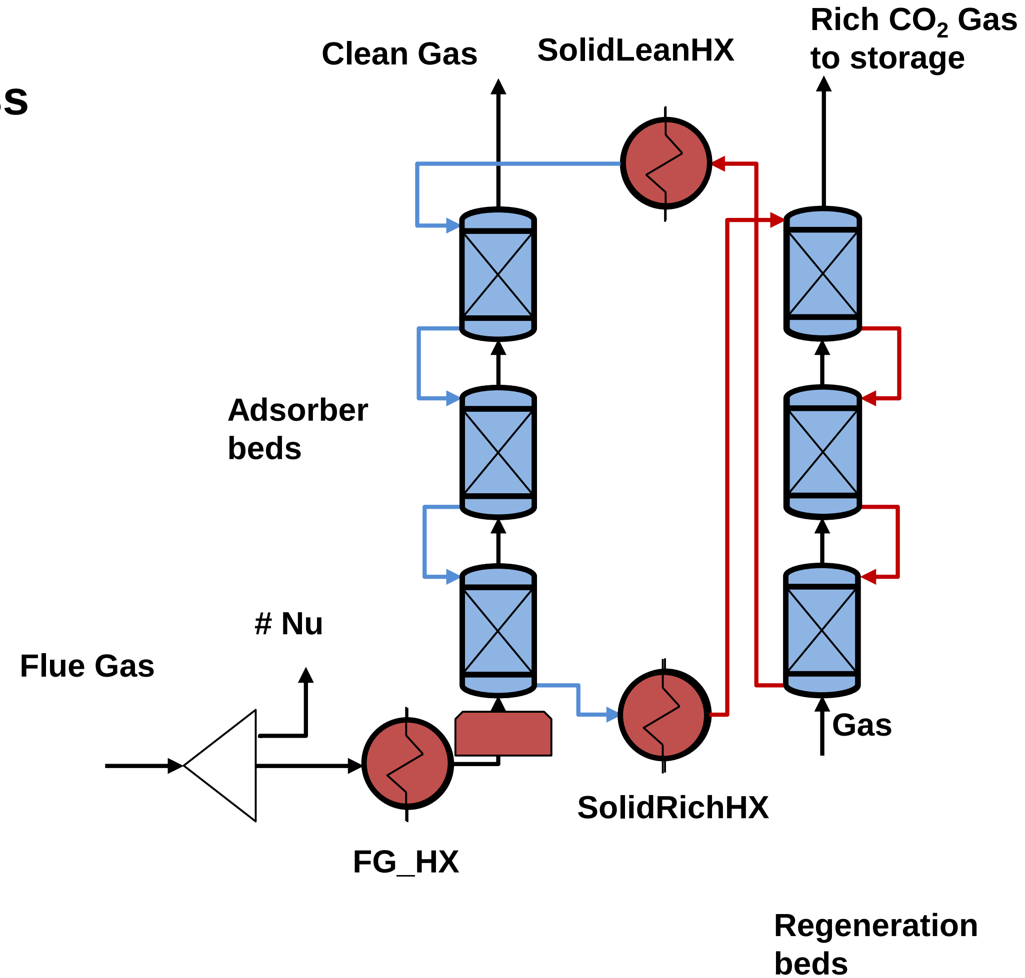
- Flows, temperatures, concentrations



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



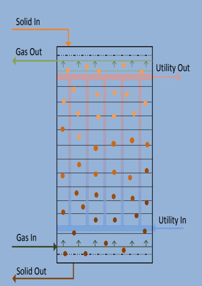
Mathematical Model

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

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

Solid Sorbent System

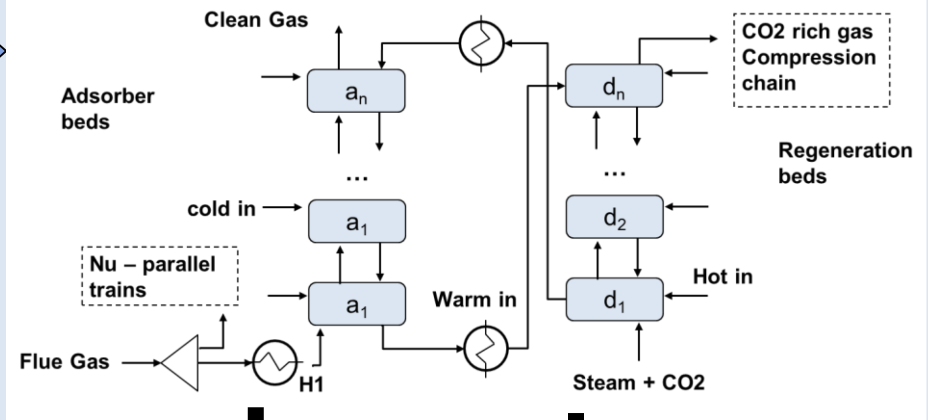
Process Models



Algebraic Surrogate Models

ALAMO
a black-box modeling tool

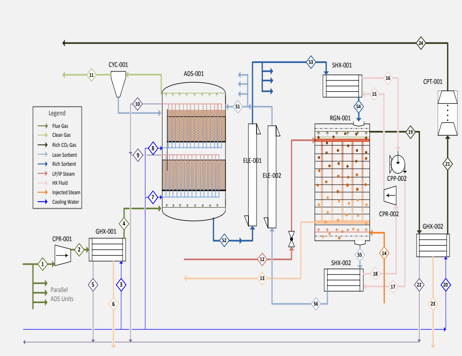
Superstructure Optimization



First Principle Models

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

Carbon Capture Process



Optimized Process

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Framework for Optimization and Uncertainty Quantification and Surrogates - FOQUS

- Carbon Capture Simulation Initiative tool set
  - Simulation, Statistics, Uncertainty Quantification, Optimization, Surrogate Modeling, Dynamic Models.

Process Simulation
- Data sampling
- Data analysis
- Data refining

Surrogate model
- Generation
- Validation

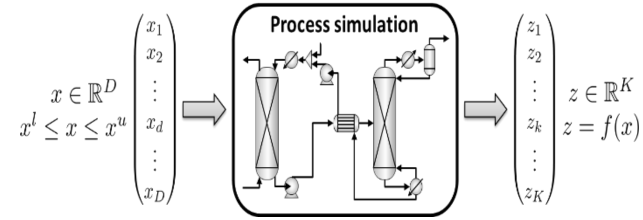
Optimization
- **GAMS**
- Validation (FOQUS)

ALAMO – Automated Learning of Algebraic Models

"**Surrogate** models correlate the input and output variables of the process"

Input variables

Output variables



Data set (simulations)

Final surrogate Model:

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

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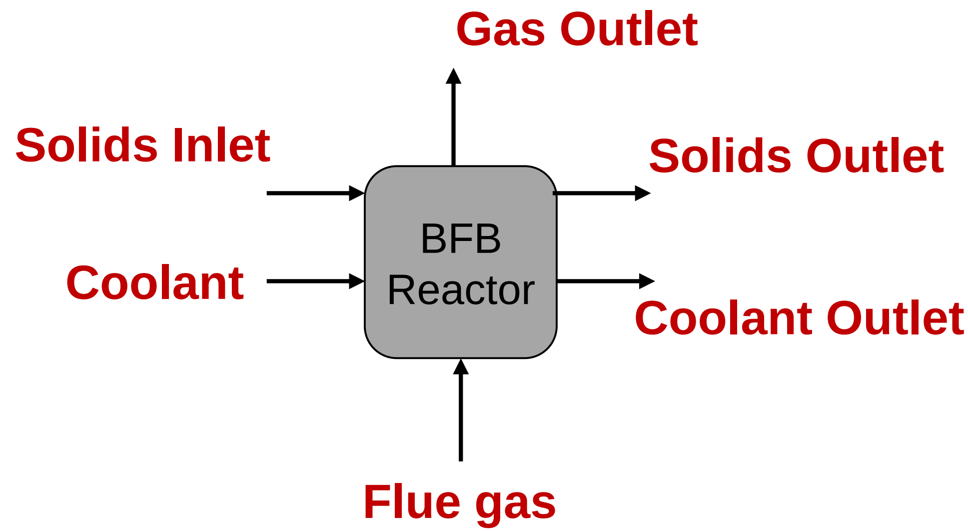
Surrogate Model Generation

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

Reactor Design

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



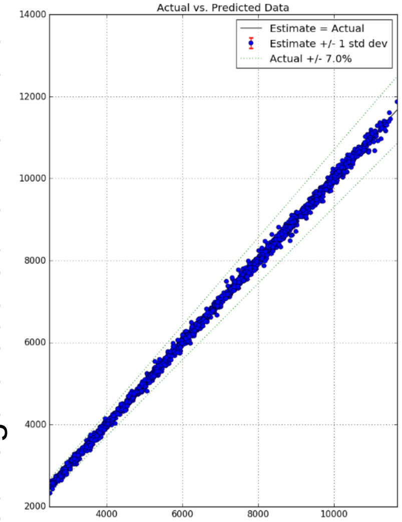
- **Flow rate**
- **Pressure**
- **Temperature**
- **Concentration**

Solid Sorbent System

- 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

Surrogate Gas Outlet Flow rate

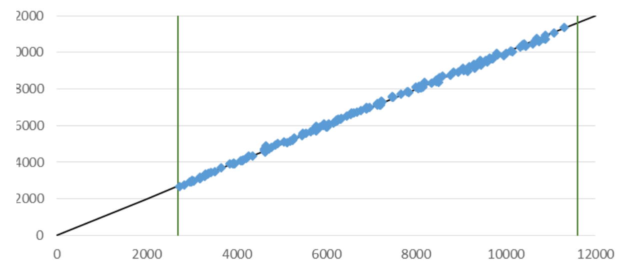


Rigorous Gas Outlet Flow rate

R^2= 0.99

Cross-validation

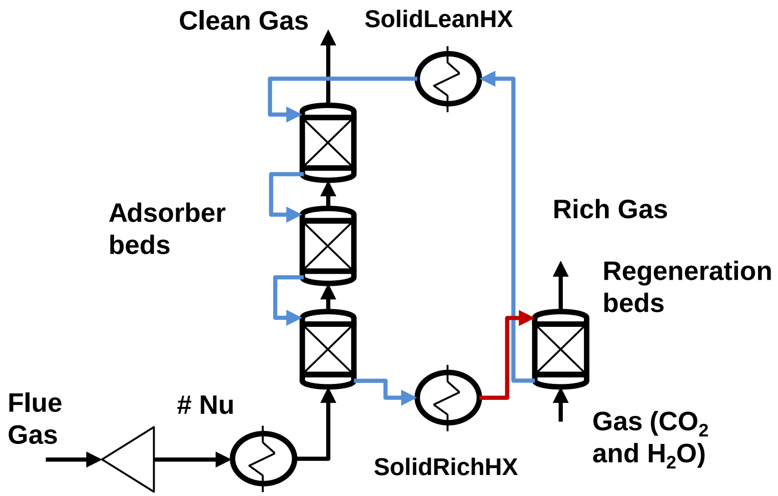
Surrogate Gas Outlet Flow rate

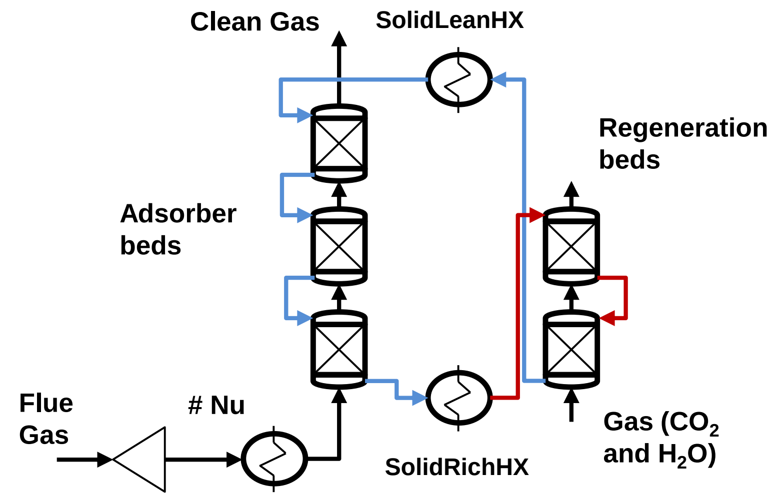


Rigorous Gas Outlet Flow rate

R^2= 0.99

Optimal Solutions





Optimization:

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

Fixed layout (Case 1 – Case 3)

	Best Case	Case 1	Case 2	Case 3
% COE increase	-	3%	4 %	5 %
Adsorber beds		2	3	3
Regeneration beds		2	1	2
Ads parallel units		6	8	6
Rgn parallel units		4	6	4

Membrane based systems

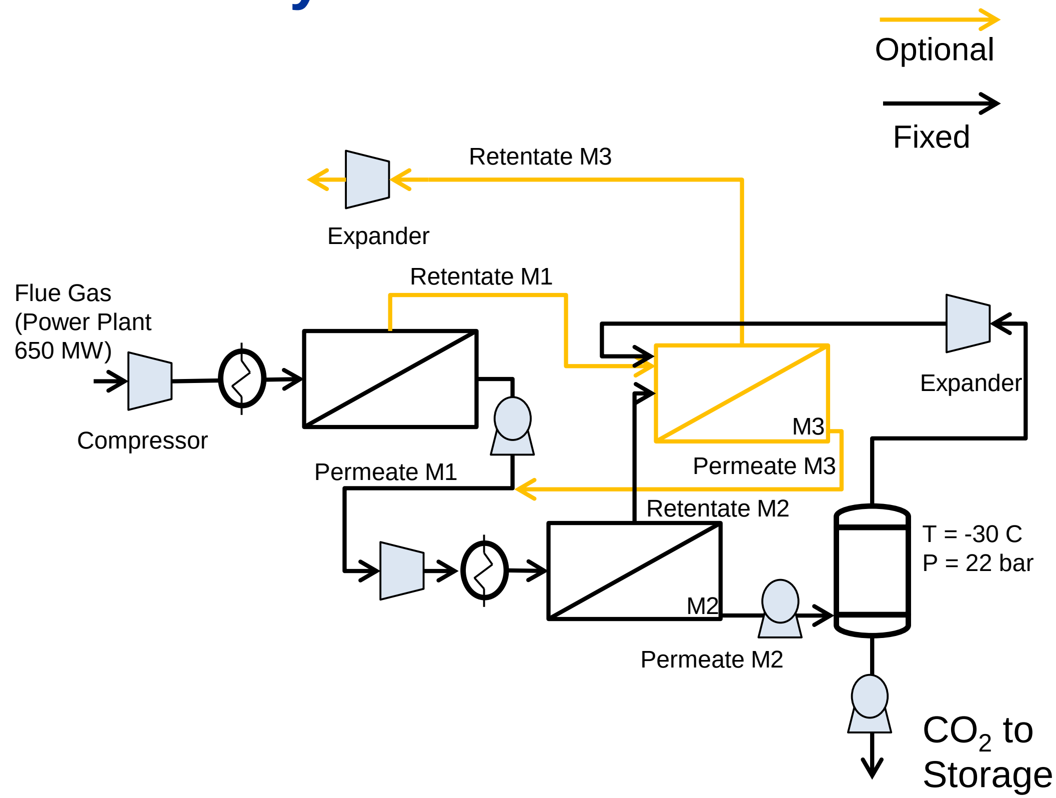
Membrane separation

Design:

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

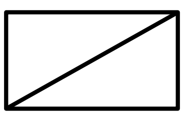
Operation:

- 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)

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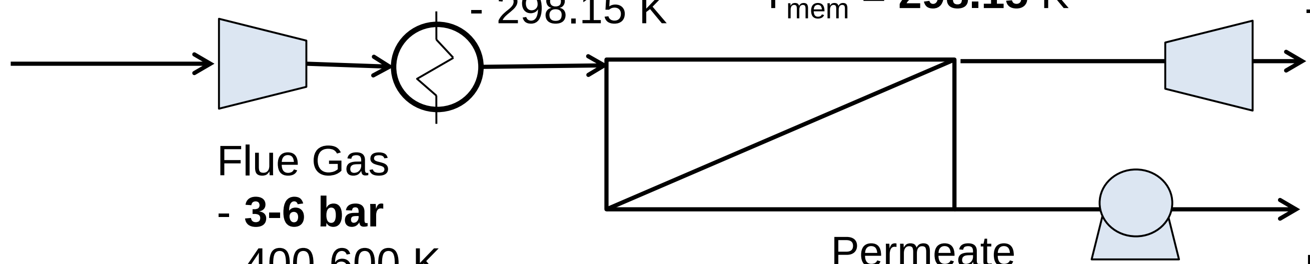
Membrane based systems

- Separation stage

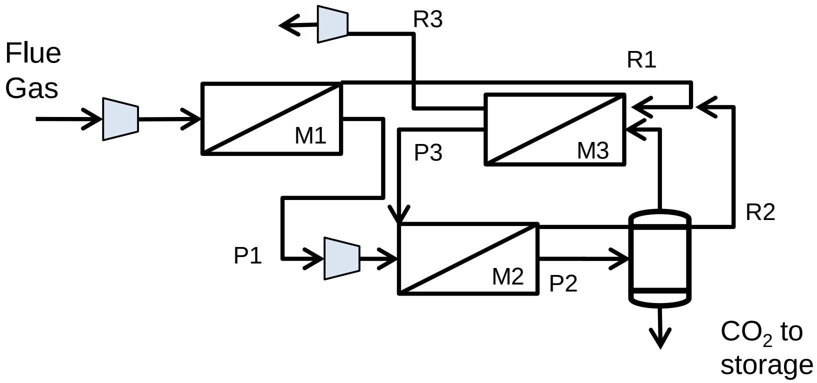


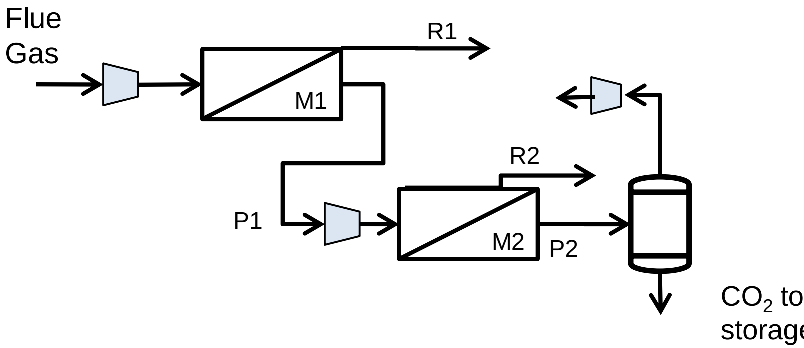
Stage:
- Compression system
- Heat exchanger
- Membrane
- Vacuum pump
- Expander

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

Optimal Solutions

P – Permeate
R – Retentate
M – Membrane



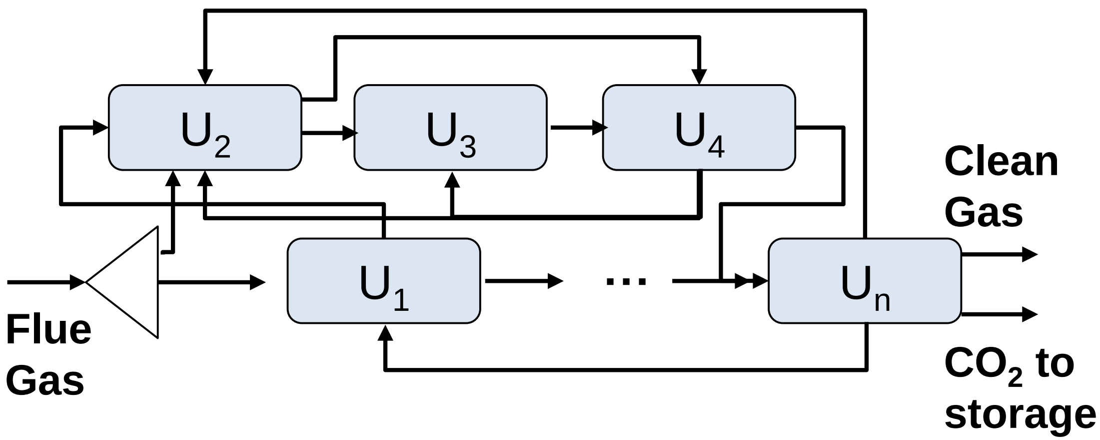


Optimization:
- Configuration: 3 membrane stages, flash unit, recirculation R1 and R2 to M3
- 90% CO_2 Capture

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

Conclusions and Future Work

- Configuration of CO_2 systems is extremely **important** for individual technologies.
- Establish a **consistent framework** for evaluating multiple technologies is a critical task
- Combined technologies could lead to improvements in the separation performance while reducing the energy penalty.



Given is:

- Set of **separation stages** (U)
  - Adsorber, regenerator, membrane, **others**.
  - Heat exchanger, pump, compressor, expander.
- Minimize **Cost of Electricity**

Similar to Superstructure Optimization of Water Networks (Yang & Grossman 2011)

MINLP: Mix of First Principle and Surrogate Models

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Thank you for your attention