CCSI^2
Carbon Capture Simulation for Industry Impact

Superstructure-based Optimization of Membrane-based Carbon Capture Systems

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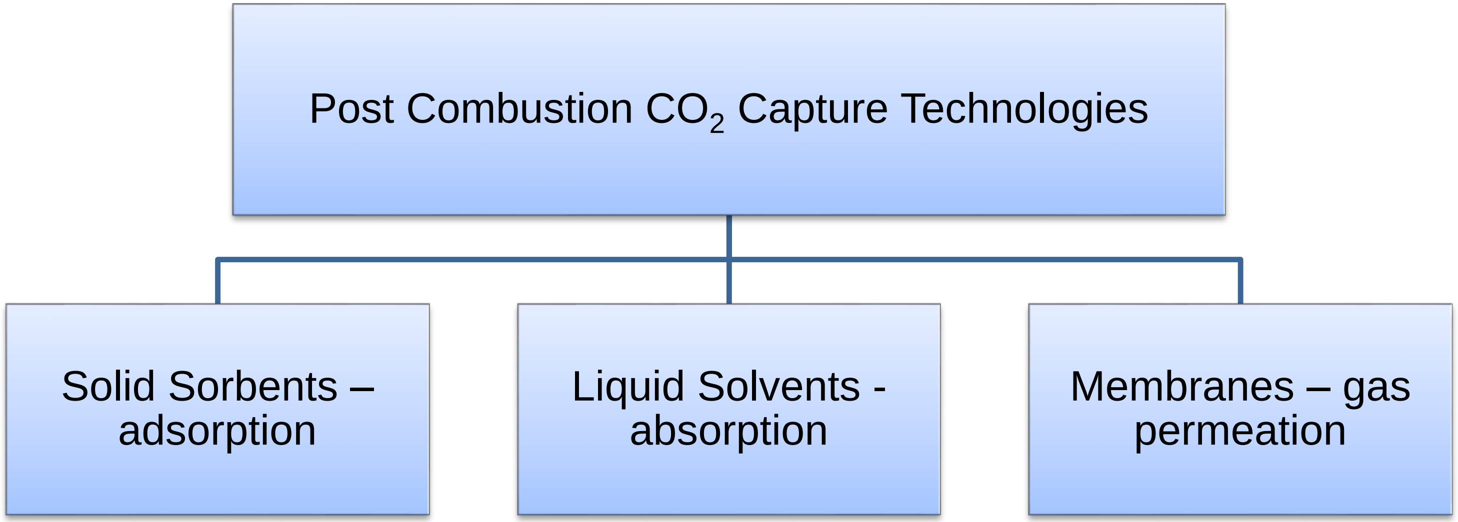
Introduction



Post Combustion CO_2 Capture Technologies

Solid Sorbents – adsorption

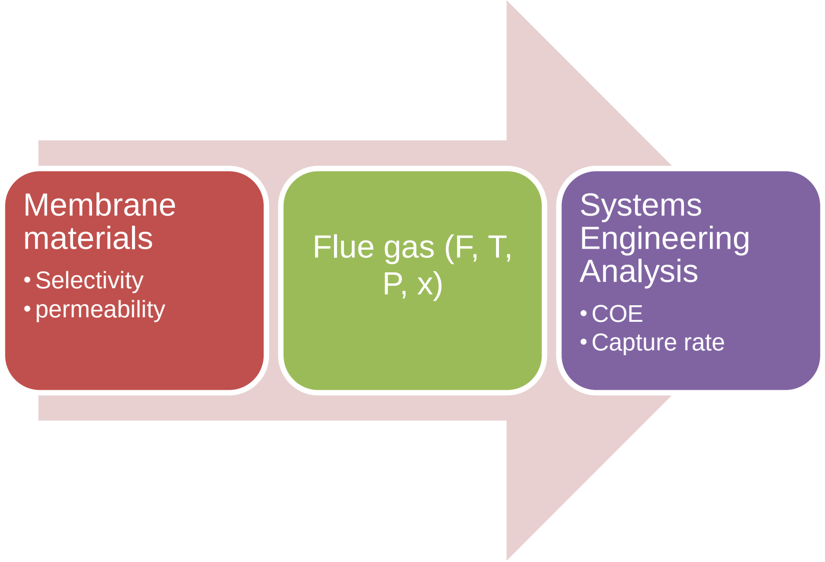
Liquid Solvents - absorption

Membranes – gas permeation

Motivation: Current applications are insufficient to simultaneously **optimize** multiple technologies, process configurations, and operating conditions while minimizing the cost of electricity (COE).

Goal:

- Develop a **superstructure-based** mathematical optimization framework.
  - Simultaneously optimize the **process configuration**, **process design** and **operating conditions** based on rigorous models.

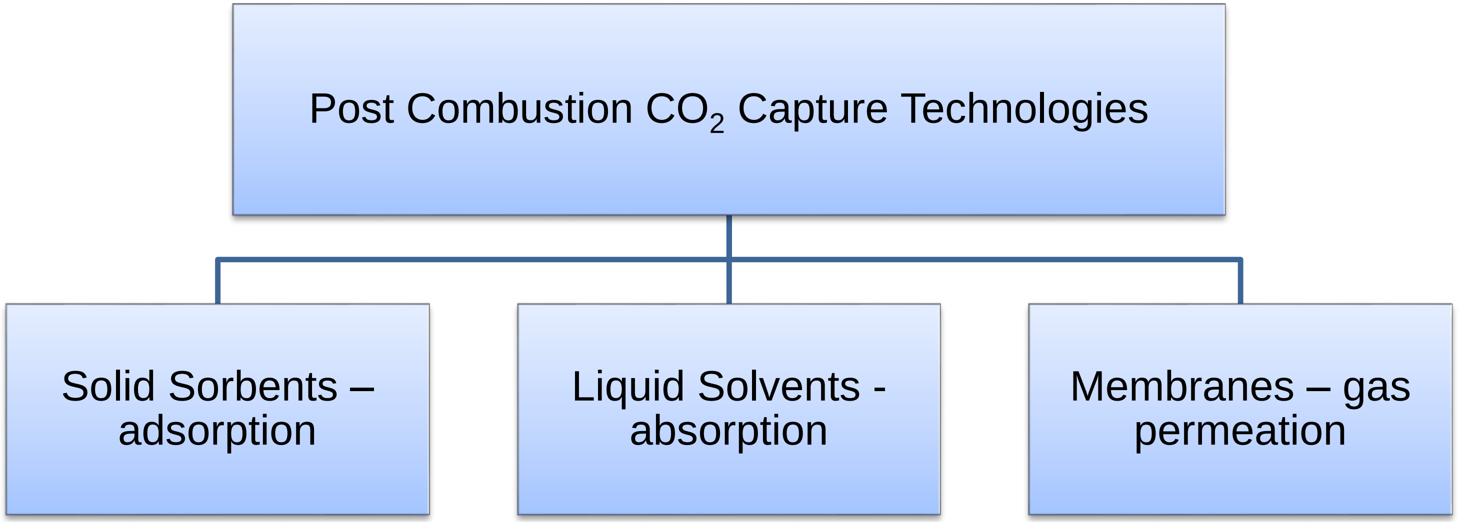


Membrane materials
- Selectivity
- permeability

Flue gas (F, T, P, x)

Systems Engineering Analysis
- COE
- Capture rate

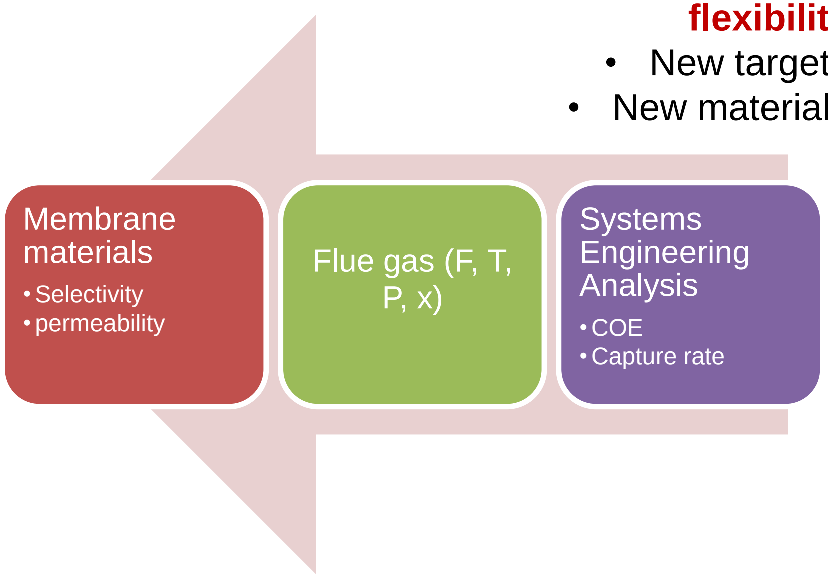
Introduction



Motivation: Current applications are insufficient to simultaneously **optimize** multiple technologies, process configurations, and operating conditions while minimizing the cost of electricity (COE).

Exploit the model flexibility

- New targets
- New materials



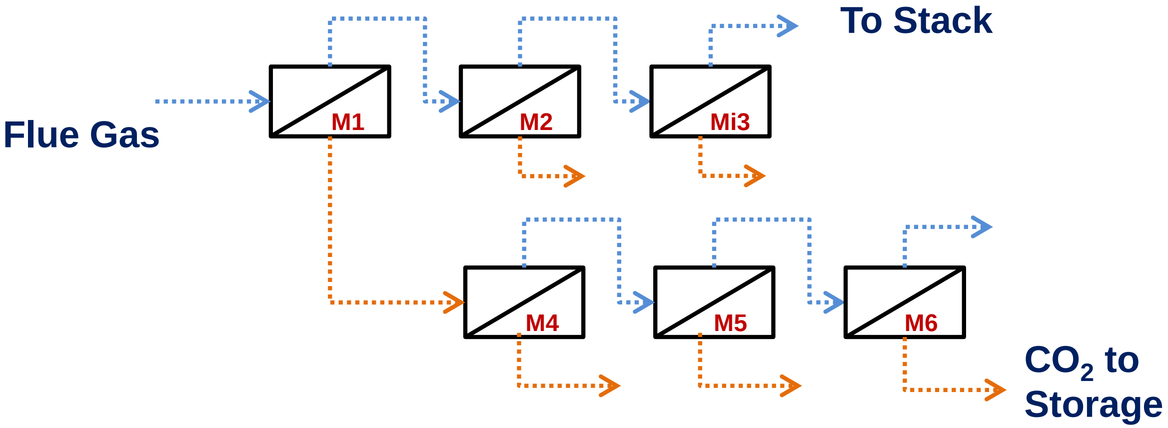
Goal:

- Develop a **superstructure-based** mathematical optimization framework.
  - Simultaneously optimize the **process configuration**, **process design** and **operating conditions** based on rigorous models.

Membrane systems optimization

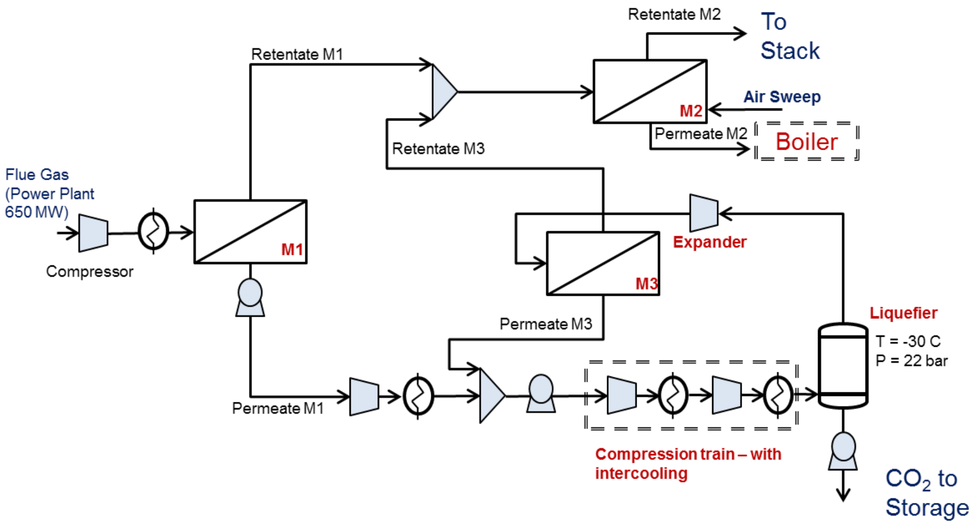
Superstructure based optimization

- First principles + simplified models.
- Studies focus on **multi-stage configurations**.
- The number of **process configurations** analyzed by the optimizer is limited. (Hasan et al., 2012 and Arias et al., 2016)

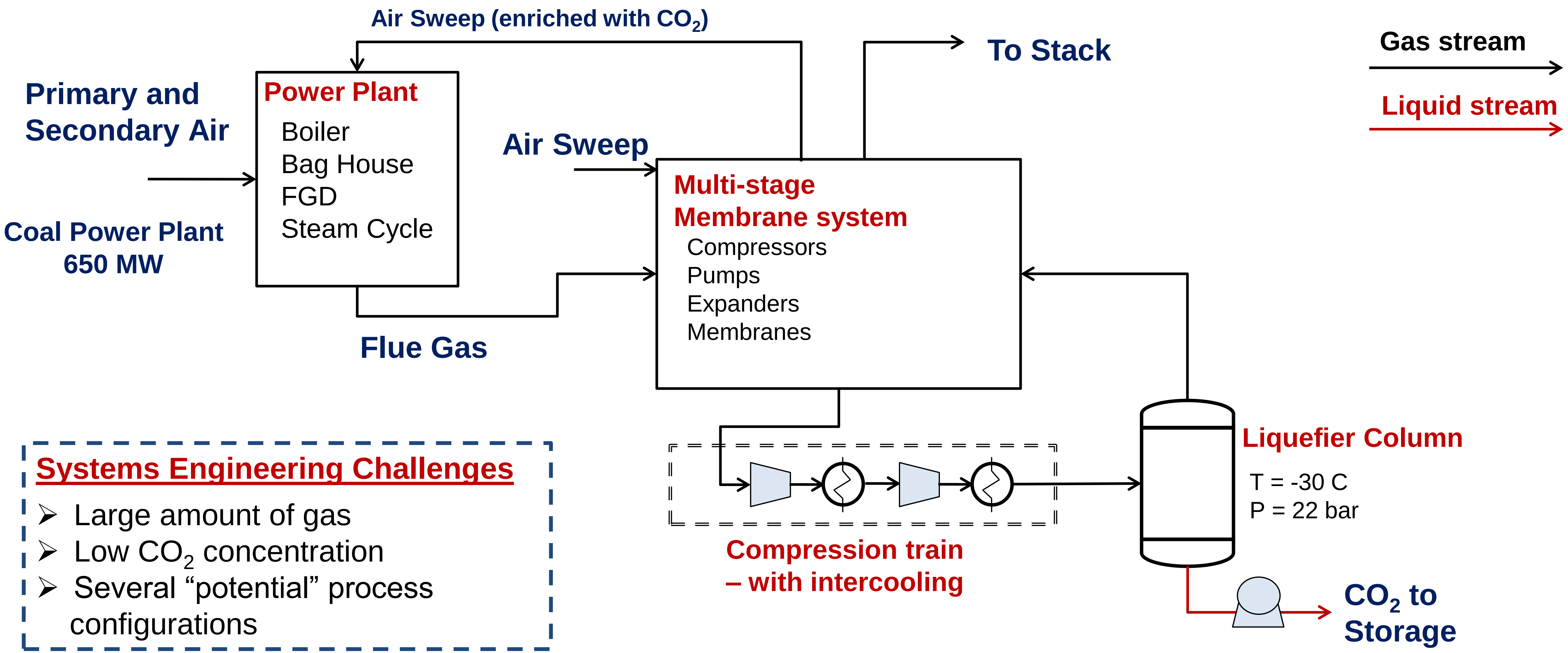


Advanced process configurations

- Rigorous models.
- **Fixed process configurations** (simulation-optimization frameworks).
  - ➢ (Merkel et al., 2010; Morinelly & Miller 2011 & 2012).



Advanced Process Configurations



Air Sweep (enriched with CO_2)

To Stack

Gas stream

Liquid stream

Primary and Secondary Air

Coal Power Plant
650 MW

Power Plant
Boiler
Bag House
FGD
Steam Cycle

Air Sweep

Flue Gas

Multi-stage Membrane system
Compressors
Pumps
Expanders
Membranes

Liquefier Column
T = -30 C
P = 22 bar

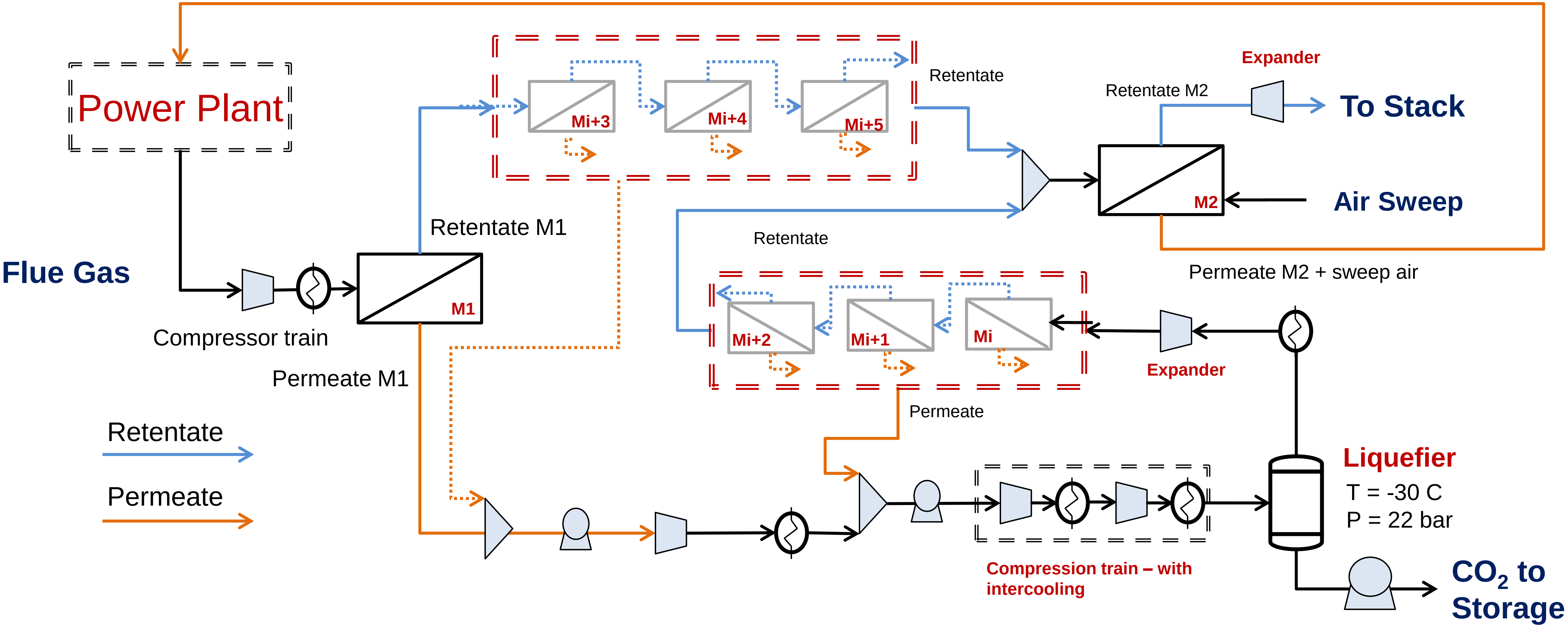
Compression train – with intercooling

CO_2 to Storage

Systems Engineering Challenges

- Large amount of gas
- Low CO_2 concentration
- Several “potential” process configurations

Superstructure Optimization Framework



- Discrete Decisions: **How many units?** **NLP – bypassing the units not installed**
- Continuous decisions: **Unit design, Operating conditions (temp, pressure, flow rates, compositions)**

Cost of Electricity

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

$$\boldsymbol{s.t.}\quad \begin{array}{l} Material\ Balances \\ Energy\ Balances \\ Equipment\ Design \\ Process\ Configuration \\ Capture\ Target \end{array}$$

Costing Methodology:

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

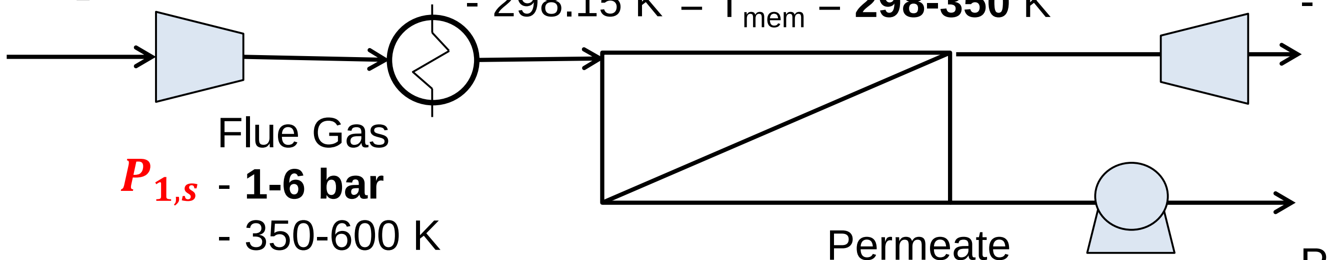
Quality Guidelines for Energy System Studies: Performing a Techno-economic Analysis for Power Generation Plants (DOE/NETL-2015/1726)

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

➢ Purchase cost calculations

Single Stage

- Separation stage



$FF_{i,s}$ Flue Gas
- 10-15 % CO_2
P_f - **1 bar**
T_f - 327 K

$W_{j,s}$

Flue Gas
$P_{1,s}$ - **1-6 bar**
- 350-600 K

Flue Gas
- **1-6 bar**
- 298.15 K = T_{mem} = **298-350** K

Retentate
- **3-6 bar**
- 298.15 K

Permeate
- **0.2 - 1 bar**
- 298.15 K
- **0.25 – 0.8 % CO_2**

Permeate
- **1 bar**
- 298.15 K

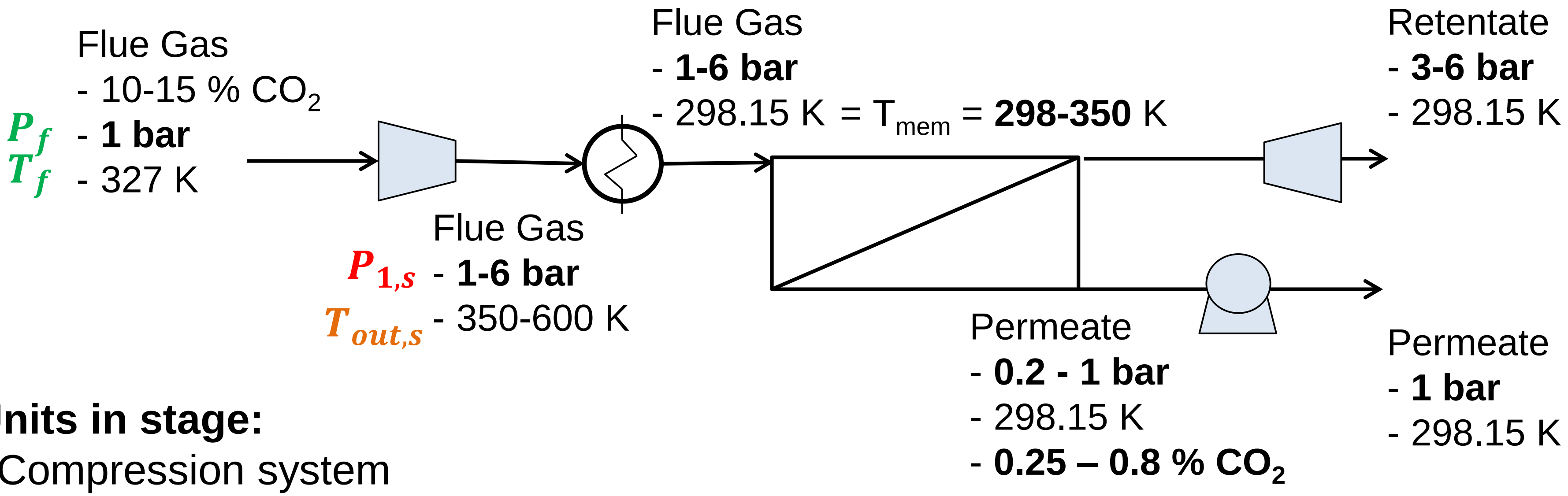
Units in stage:
- Compression system
- Heat exchanger
- Membrane
- Vacuum pump
- Expander

Compressor duty (Hp):

$$W_{j=1,s} = \frac{1}{\eta}\sum_i FF_{i,s}\left(\frac{8314}{745.3}\right)T_f\frac{\gamma}{\gamma-1}\left[\left(\frac{P_{1,s}}{P_f}\right)^{(\gamma-1)/\gamma}-1\right]$$

Single Stage

- Separation stage



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Flue Gas
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$T_{out,s}$ - 350-600 K

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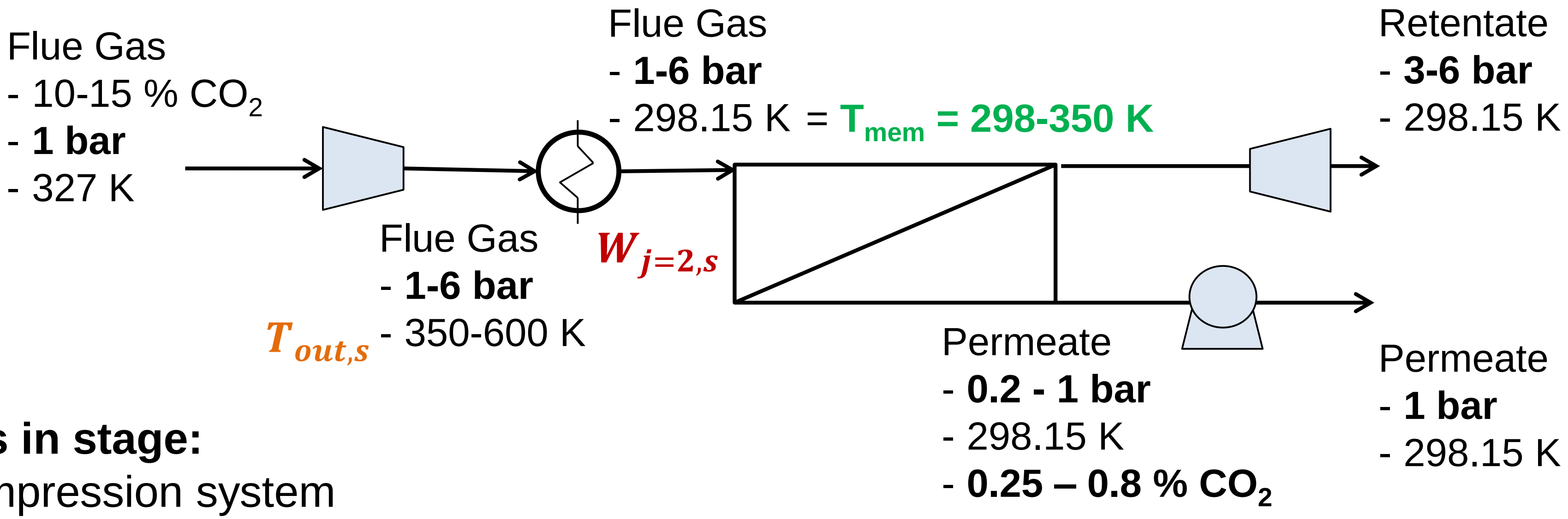
Outlet Temperature (after compression) (K):

$$T_{out,s} = T_f \left(\frac{P_{1,s}}{P_f}\right)^{(\gamma-1)/\gamma}$$

Single Stage

- Separation stage



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Flue Gas
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$W_{j=2,s}$

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- **3-6 bar**
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Permeate
- **1 bar**
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Units in stage:
- Compression system
- Heat exchanger
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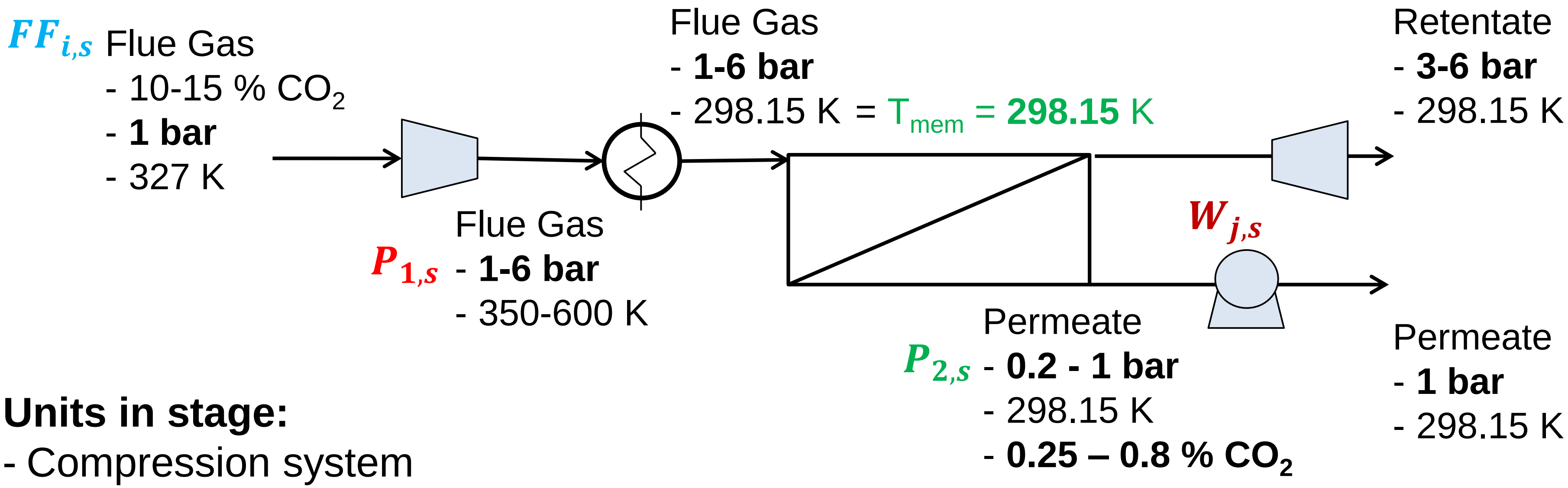
- Expander

Heat exchanger duty (kW):

$$W_{j=2,s} = \sum_i FF_{i,s}\, C_p \left(T_{out,s} - T_{mem}\right)$$

Single Stage

- Separation stage



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Permeate
- **1 bar**
- 298.15 K

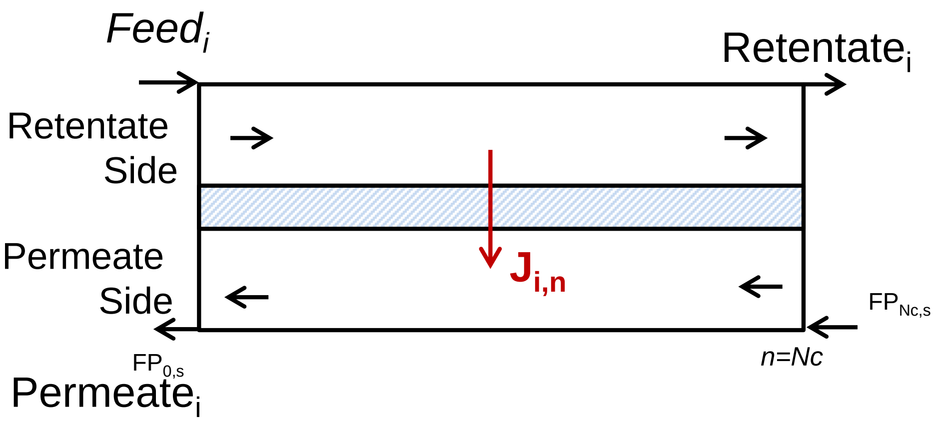
Units in stage:
- Compression system
- Heat exchanger
- Membrane
- Vacuum pump
- Expander

Vacuum pump (Hp):

$$W_{j=3,s} = \frac{1}{\eta}\sum_{i} FF_{i,s}\left(\frac{8314}{745.3}\right)T_{mem}\frac{\gamma}{\gamma-1}\left[\left(\frac{P_{atm}}{P_{2,s}}\right)^{(\gamma-1)/\gamma}-1\right]$$

Membrane model

Counter current flow



Material Balances:

$$0 = Fz_i|_x - Fz_i|_{x+1} + J_i|_x$$

$$0 = -\frac{\partial}{\partial x}\left(F_{c_i}\right) - J_i$$

Approximation:

$$\frac{\partial\left(F_{i,n} - F_{i,n-1}\right)}{h} = -J_{i,n}$$

$$h = \frac{L}{|Nc| - 1}$$

$$J_{i,n} = \boxed{2\pi r_{Fo} n_F}\,\boxed{\frac{P}{\delta}}\,\boxed{\left(P1xr_{i,n} - P2xp_{i,n}\right)}$$

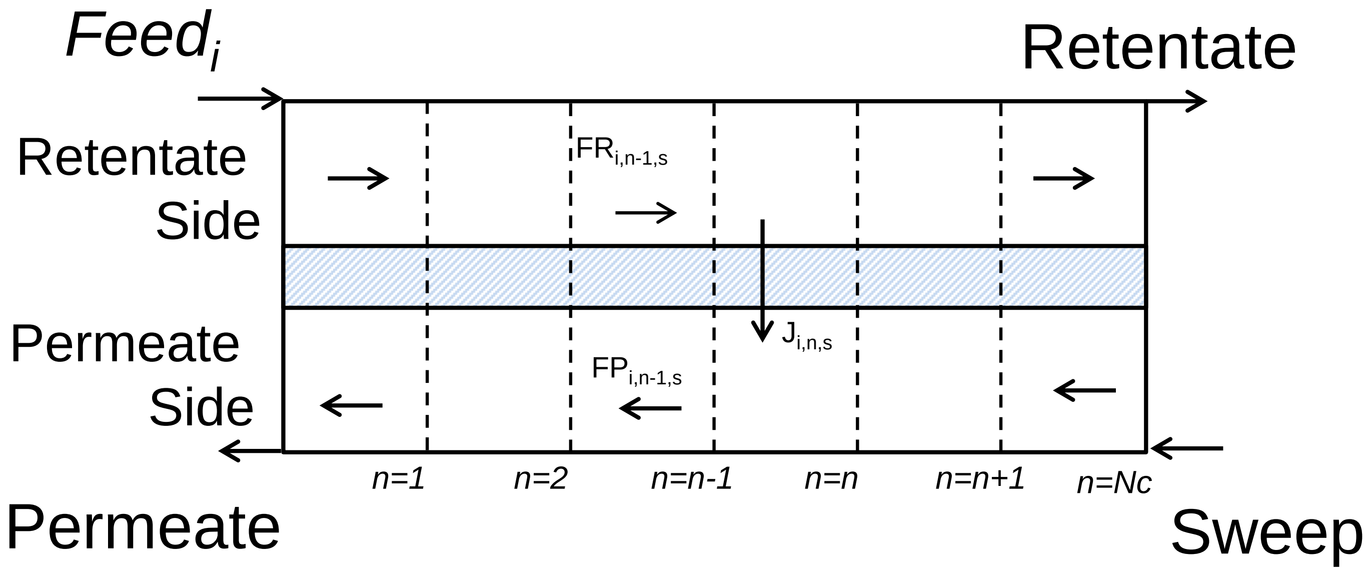
Membrane Area (section)

Permeance (kgmol/m^2 s bar)

Driving force (partial pressure difference)

Juan Morinelli, Kayode Ayaji, CCSI toolset

Membrane model



Main Assumptions:

- Counter current flow
- Finite differences method
- Sweep (possible)

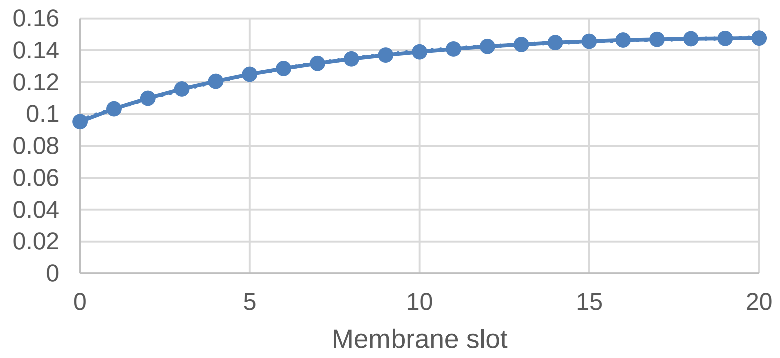
$$\mathrm{FR}_{\mathrm{i,n,s}} = \mathrm{FR}_{\mathrm{i,n-1,s}} - \mathrm{J}_{\mathrm{i,n,s}}\, h \qquad \forall i, n > 1, s$$

$$\mathrm{FP}_{\mathrm{i,n,s}} = \mathrm{F}P_{\mathrm{i,n-1,s}} - \mathrm{J}_{\mathrm{i,n,s}}\, h \qquad \forall i, n < |\mathrm{Nc}|, s$$

$$\mathrm{h} = \frac{\mathrm{L}}{|\mathrm{Nc}| - 1}$$

Membrane Pressure Drop

- Retentate side
  - – Linear regression
- Permeate side
  - – Rigorous model (Morinelly et al., 2012)


Permeate Pressure, Bars

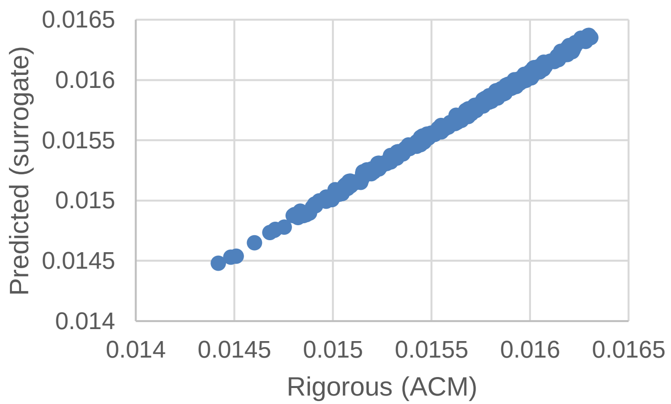
Surrogate model:

- ➢ Vapor viscosity (μ – cP) (3.6e11 cP = 1 bar*hr)
- ➢ μ*3.6e11 = μCP
- ➢ Input variables: F(x {molar fractions, T, P, F})
  - ▪ ACM (non-ideal calculations)
  - ▪ R2 = 0.999

$$P_{per}\frac{\partial P_{per}}{\partial x} = \frac{16RT\mu F_{per}}{\pi r_{FI}^{4} n_F}$$

$$V_{ret} = \frac{F_{ret}}{(SA\,\rho\,3600)}$$

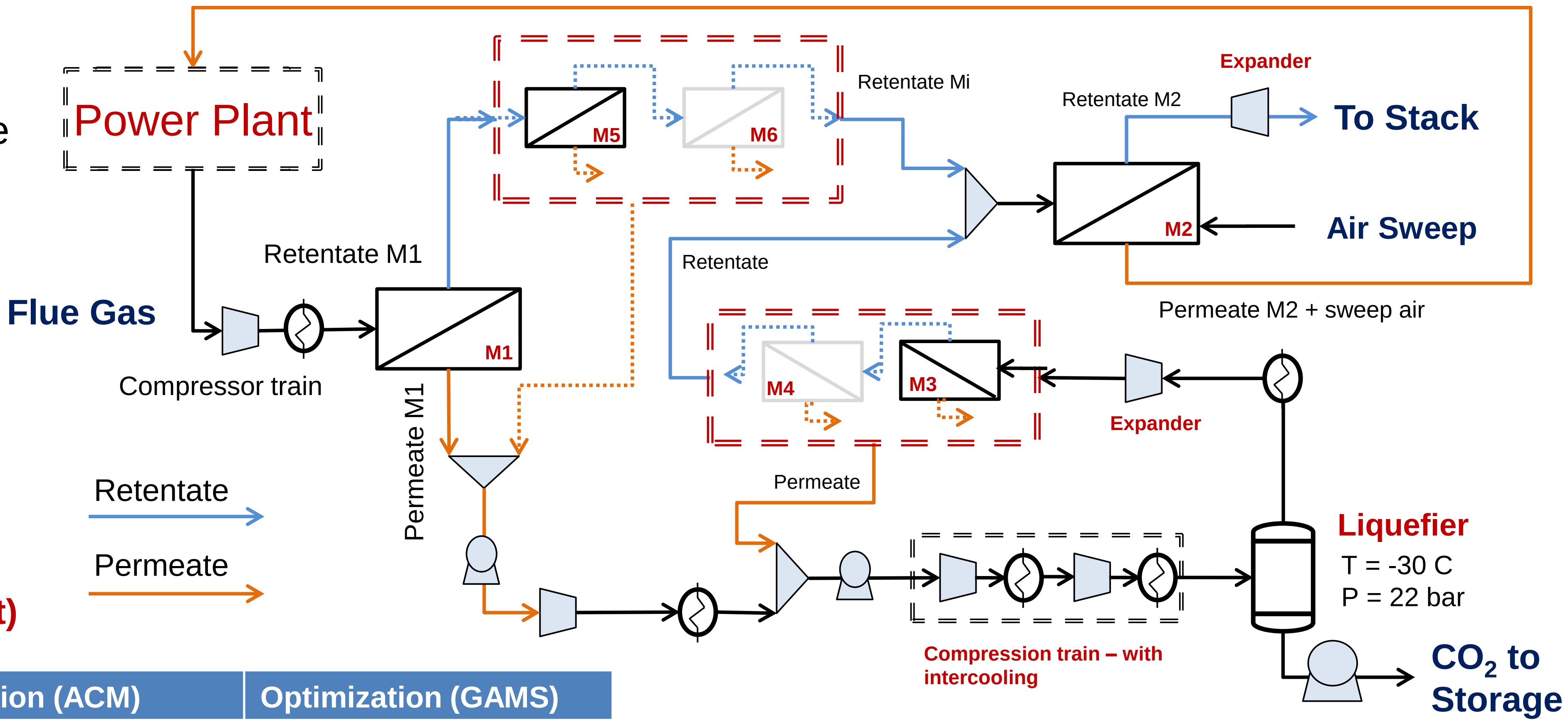
$$\rho = \frac{n}{V} = \frac{P}{RT} = \frac{bar}{\left(\frac{bar.m3}{kmol.K}\right)K} = \frac{kmol}{m3}$$


μ Permeate in CP

Case study (test example + model comparison)

Case study

- 650 MW power plant
- 90% Capture
- 99% CO_2 pure to storage
- 3 - 6 membranes
- α $CO_2/(Ar, O_2, N_2)=100$
- α $CO_2/H_2O=0.5$
- Permeance = 0.1204 ($kgmol/m^2$ s bar)



Test example

- ACM Simulation (CCSI toolset)

Model	Simulation (ACM)	Optimization (GAMS)
Compressor	Centrifugal compressor	Polytropic compressor
Flash calc.	Non-ideal	Ideal calculations
Liquefier	Non-ideal flash	Surrogate model

Flash Formulation

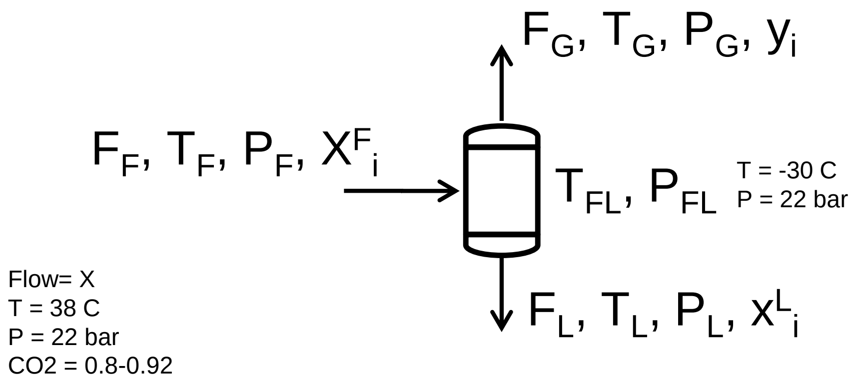
Flash Model (flash tank):

- **Non-Ideal calculations** are replaced by a **surrogate model**

Operating Conditions:

- Flue gas temp: 25-50 C
- Flue gas pressure: 15-30 bars
- Flue gas molar fractions (CO2): 0.5-0.89 kmol/kmol
- T_{FL}: -40 to -20 C
- Surrogate models for Gas outlet (ALAMO):
  - $r^2(F_G) = 0.978$, $r^2(F_{CO2}) = 0.992$, $r^2(F_{N2}\ F_{O2}\ F_{Ar}) = 0.999$

Liquefier (flash tank)



F_G, T_G, P_G, y_i

F_F, T_F, P_F, X^F_i

T_{FL}, P_{FL}

T = -30 C
P = 22 bar

F_L, T_L, P_L, x^L_i

Flow= X
T = 38 C
P = 22 bar
CO2 = 0.8-0.92

Variables:

- Flue Gas: F_F, T_F, P_F, X^F_i
- Gas: F_G, T_G, P_G, y_i
- Liquid: F_L, T_L, P_L, x^L_i
- Flash Tank: T_{FL}, P_{FL}, Q_{FL}
- 27 variables (i = 5)

Optimization Variables

Degrees of Freedom: 27 – 18 = 9 (8 Feed + T_{FL})

Equations:	# Eqns:
$P_F = P_{FL} = P_L = P_G$	3
$T_{FL} = T_G = T_L$	2
$F_G = f(F_F, T_F, P_F, x^F_i, T_{FL})$	1
$Fy_i = f(F_F, T_F, P_F, x^F_i, T_{FL})$	5
$Q_{FL} = f(F_F, T_F, P_F, x^F_i, T_{FL})$	1
$F_L = F_F – F_G$	1
$x^L_i = (x^F_i F_F – Fy_i)/F_L$	5
18 equations	18 eqns

Case study (test example + model comparison)

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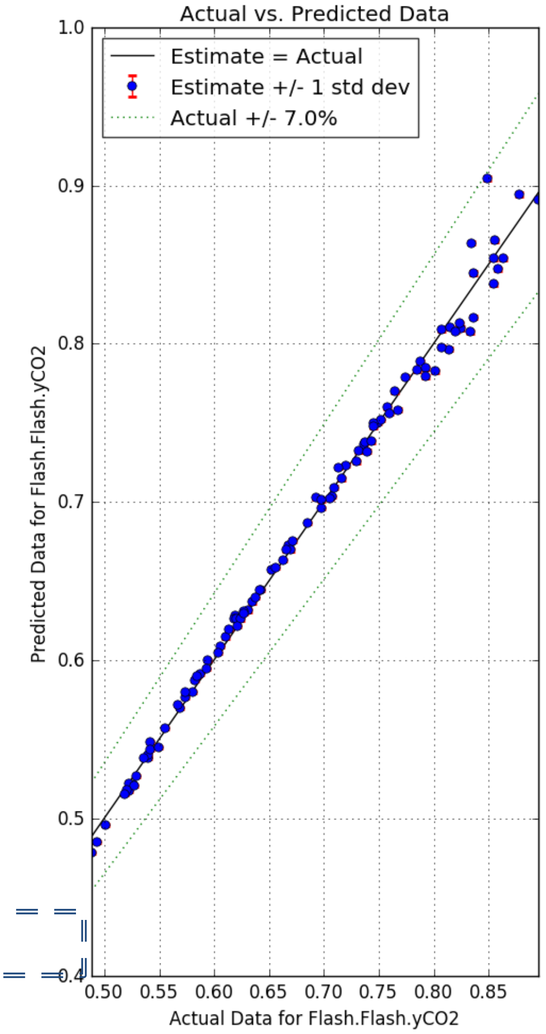
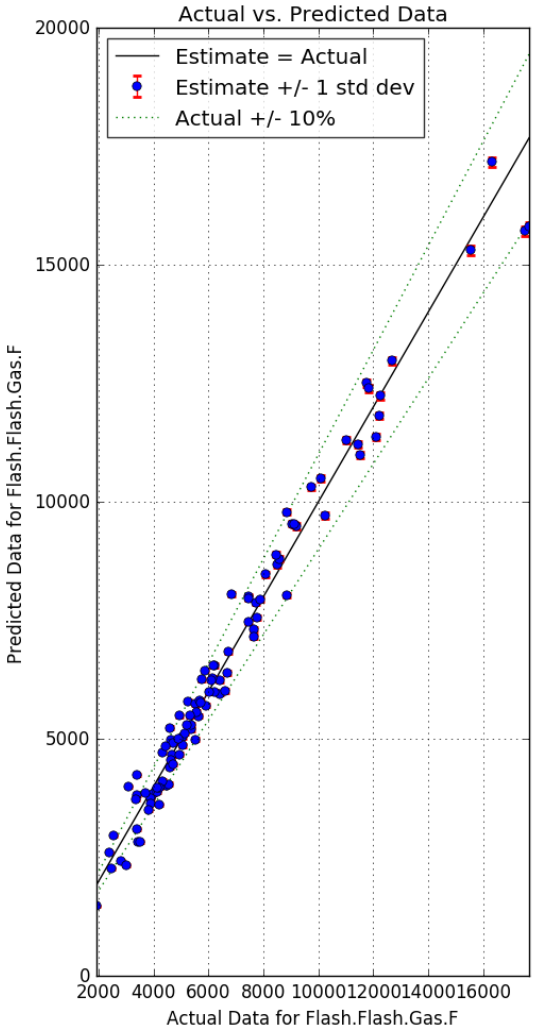
Optimization Variables





Degrees of Freedom: 27 – 18 = 9 (8 Feed + T_{FL})

Model Comparison

Case study

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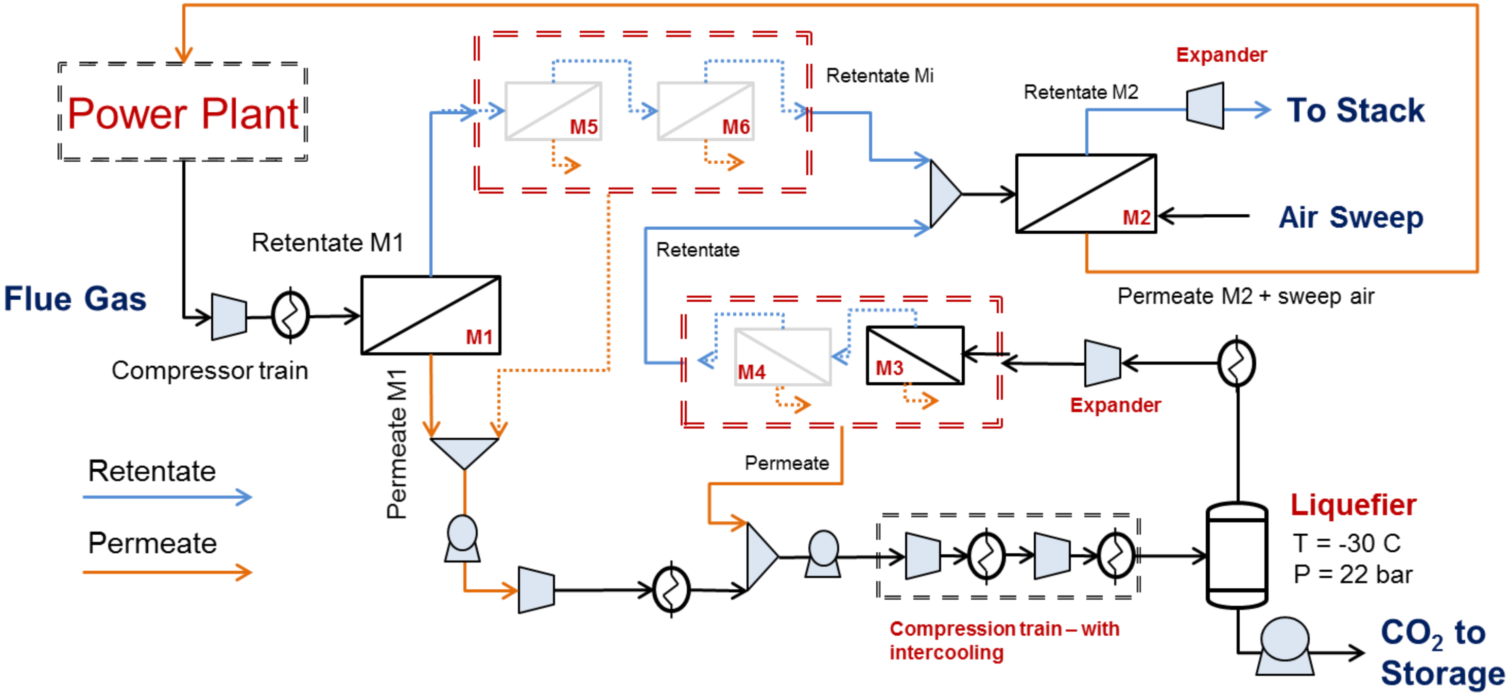
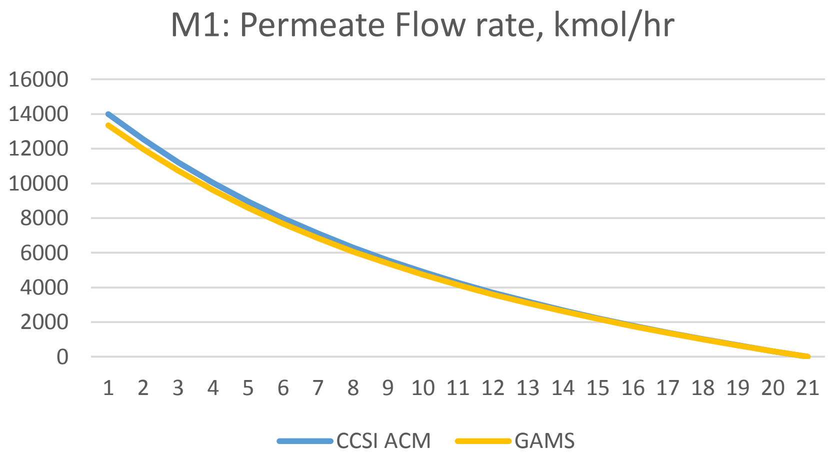
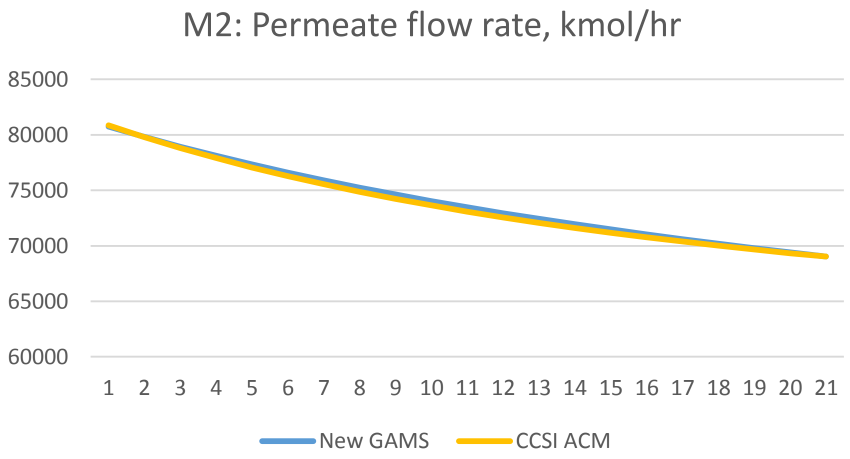
- 90% Capture
- 99% CO_2 pure to storage
- 3 membranes




M1: Permeate Flow rate, kmol/hr


M2: Permeate flow rate, kmol/hr

Model Comparison

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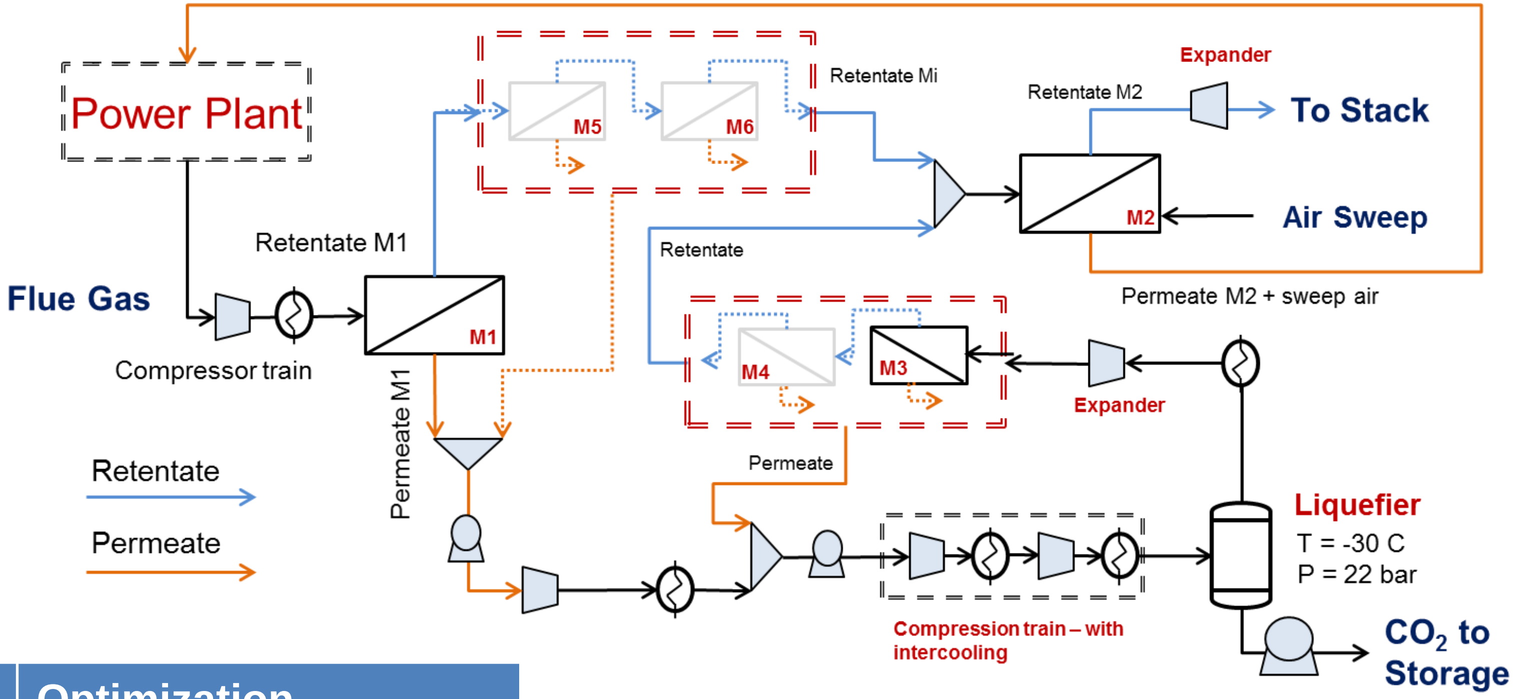
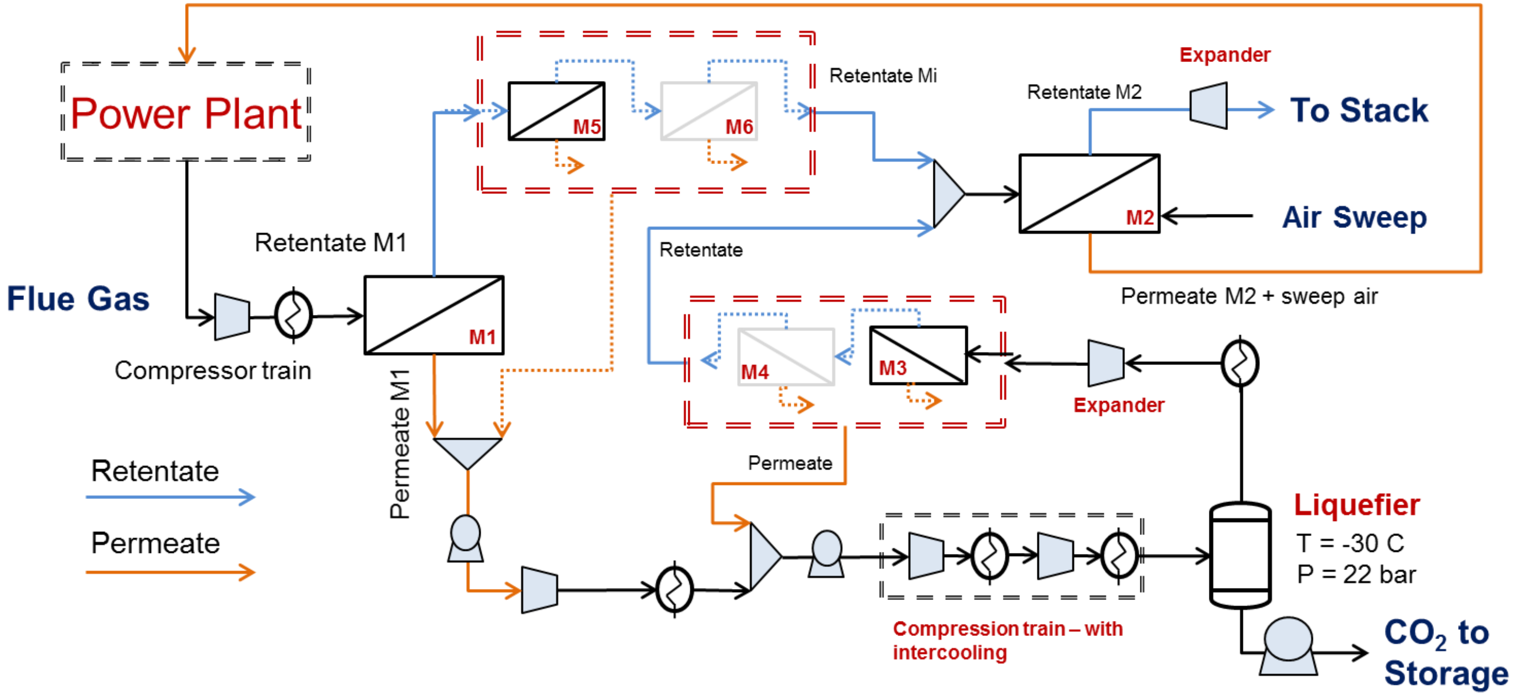


Model	Simulation (ACM)	Optimization GAMS (% change)
Relative COE ($/MWh)	-	-3.35
Net power (MW)		+2.85
Membrane (M$)		0.00
Compressors (M$)		+2.78
Expanders (M$)		+49.59
Pump (M$)		-4.25
Heat exchanger (M$)		-52.06

Model	Simulation	Optimization
Equations	5,285	2,631
Variables	5,494	2,801

Membrane System Optimization

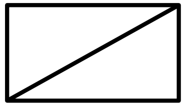


Design:

- # 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)



T$_{mem}$ = 50 C
Permeance = 0.1204 fixed (kgmol/m^2 s bar)

	Optimal (4 stages)	**Base case** (3 stages)
Relative COE ($/MWh)	-	**1.70**
Net power (MW)		-0.06
Membrane (M$)		0.07
Compressors (M$)		0.24
Expanders (M$)		0.10
Vacuum pump (M$)		0.57
Heat exchanger (M$)		0.16

Remarks

- Developed a superstructure optimization model.
  - Find the optimal plant layout and operating conditions (rigorous models).
  - Surrogate model generation, validation to avoid non-ideal calculations in critical regions.

- A robust mathematical optimization framework has been developed.
  - Simultaneous optimization of the process configuration, unit design and operating conditions.
- Integrated conceptual design and process synthesis tools.
    - Complements typical **flowsheet optimization**.
    - Facilitate the rapid development of PCC Technologies.

- Extensible to other membrane and process configurations.

Acknowledgments

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Thank you for your attention