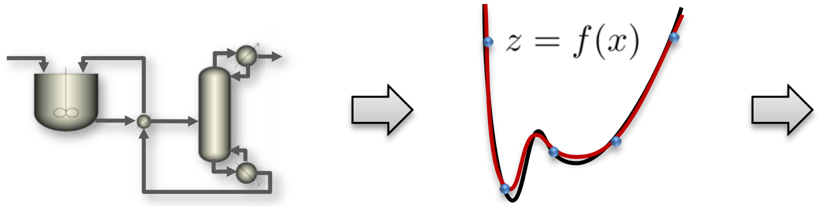

$$\min \; f(x) \quad \text{s.t.} \; g(x) = 0$$

Superstructure Formulation and Optimization for Carbon Capture Processes

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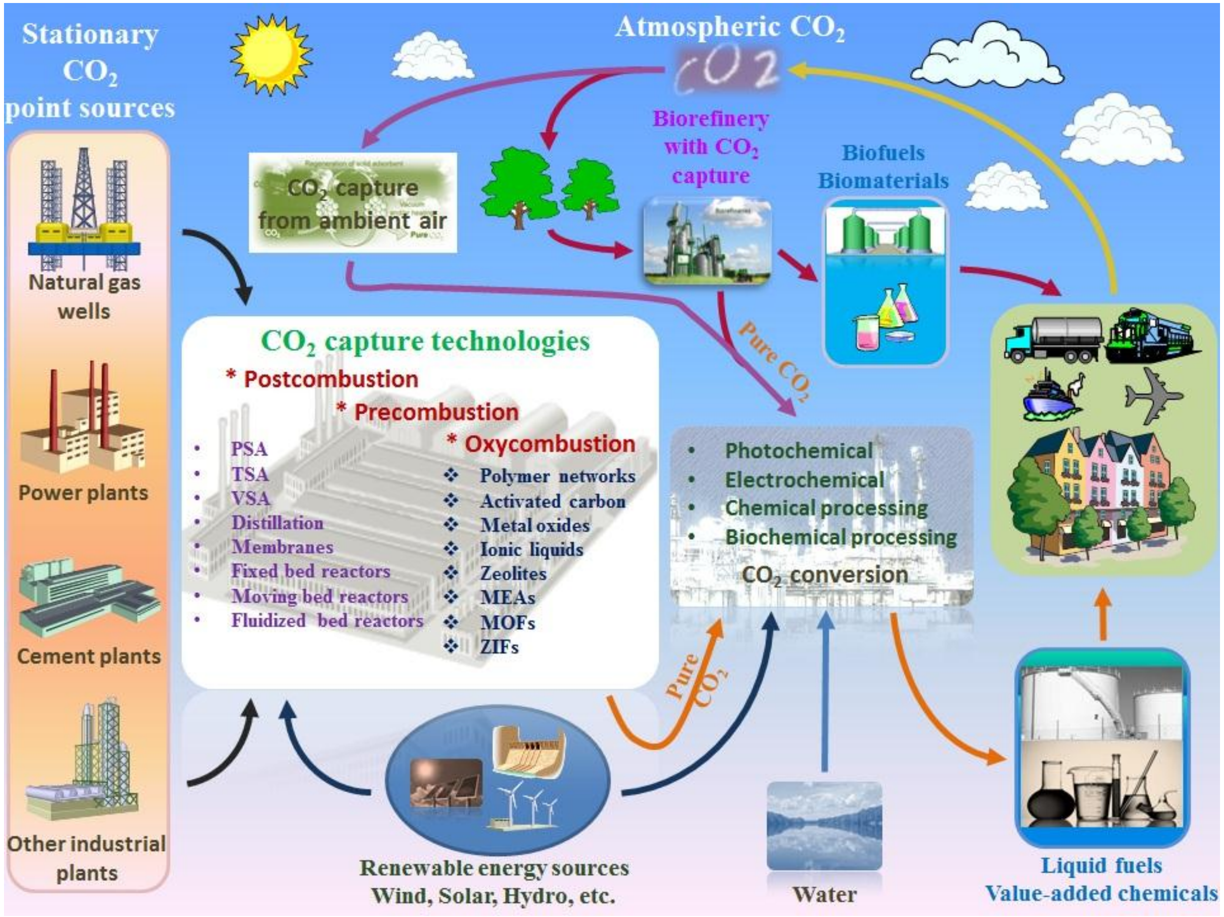
CAPD CENTER Carnegie Mellon University NETL CCSI

OUTLINE

- Motivation
- Carbon capture processes
- Superstructure optimization
- Surrogate models for optimization
- MINLP formulation
- Case study
- Conclusions

MOTIVATION



Backbone of energy supply

- *Petroleum*
- *Coal*
- *Natural Gas*

Huge amount of CO_2 emissions

- *One third from power plant*

Global warming issues

- *Ice melting*
- *Ocean level rising*

CO_2 emissions reduction

- *CO_2 capture, Utilization, & Storage (CCUS)*

Carbon capture technologies: Key of the CCUS

CO_2 CAPTURE PROCESSES

Most widely investigated capture technology: *MEA solvent based postcombustion*

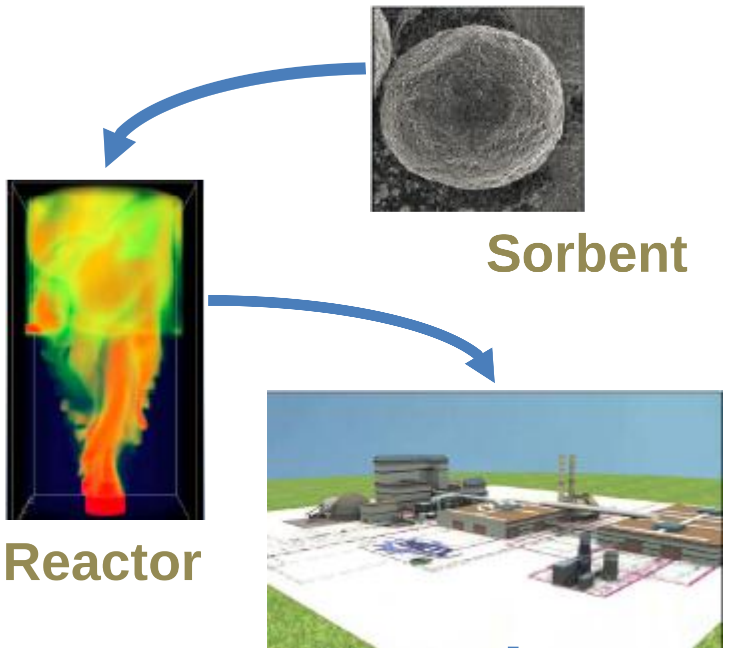
- **Cost & energy-intensive technology**
- **Thermal & oxidative degradation**

Innovative carbon capture technologies

- **High-efficient solvents/sorbents**
  - **Greater capacity and selectivity**
- **Cost-effective capture process**
  - **Reduced energy for regeneration**

DOE: Carbon Capture Simulation Initiative (CCSI)

- **5 National Labs and 6 Universities**
- **Solid sorbent technology: initial demonstration case**
- ***https://www.acceleratecarboncapture.org/drupal/***



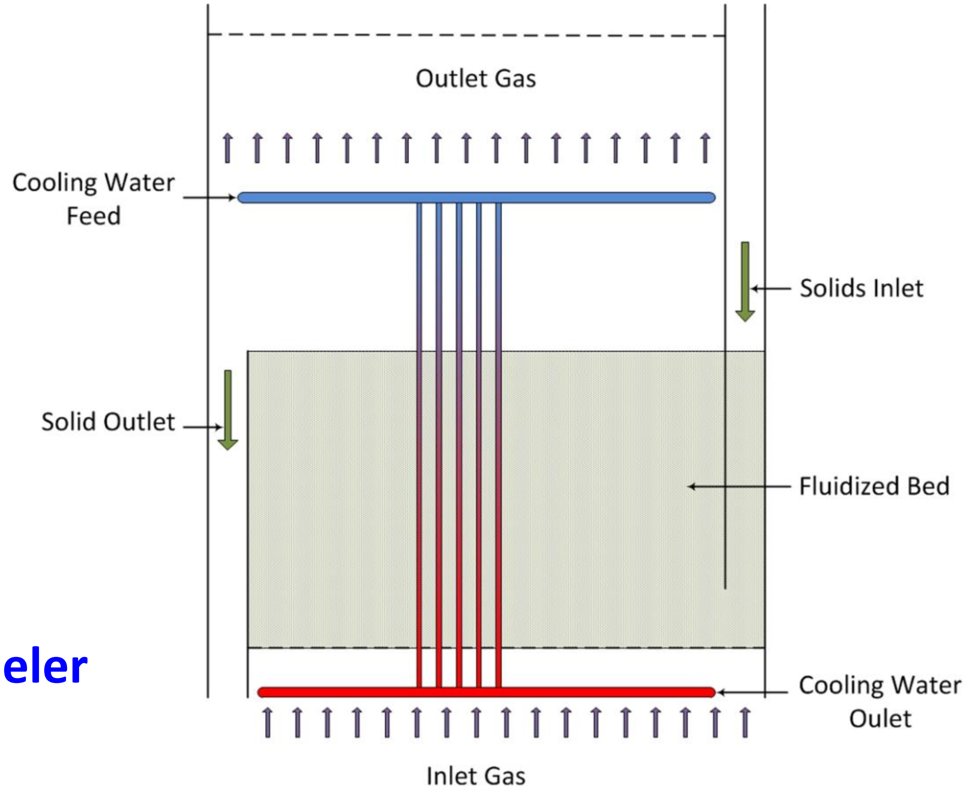
SOLID SORBENT CAPTURE PROCESS

Solid sorbent reactor

- ***Bubbling fluidized bed***
- **Fast fluidized bed**
- **Moving bed**
- **Fixed bed**

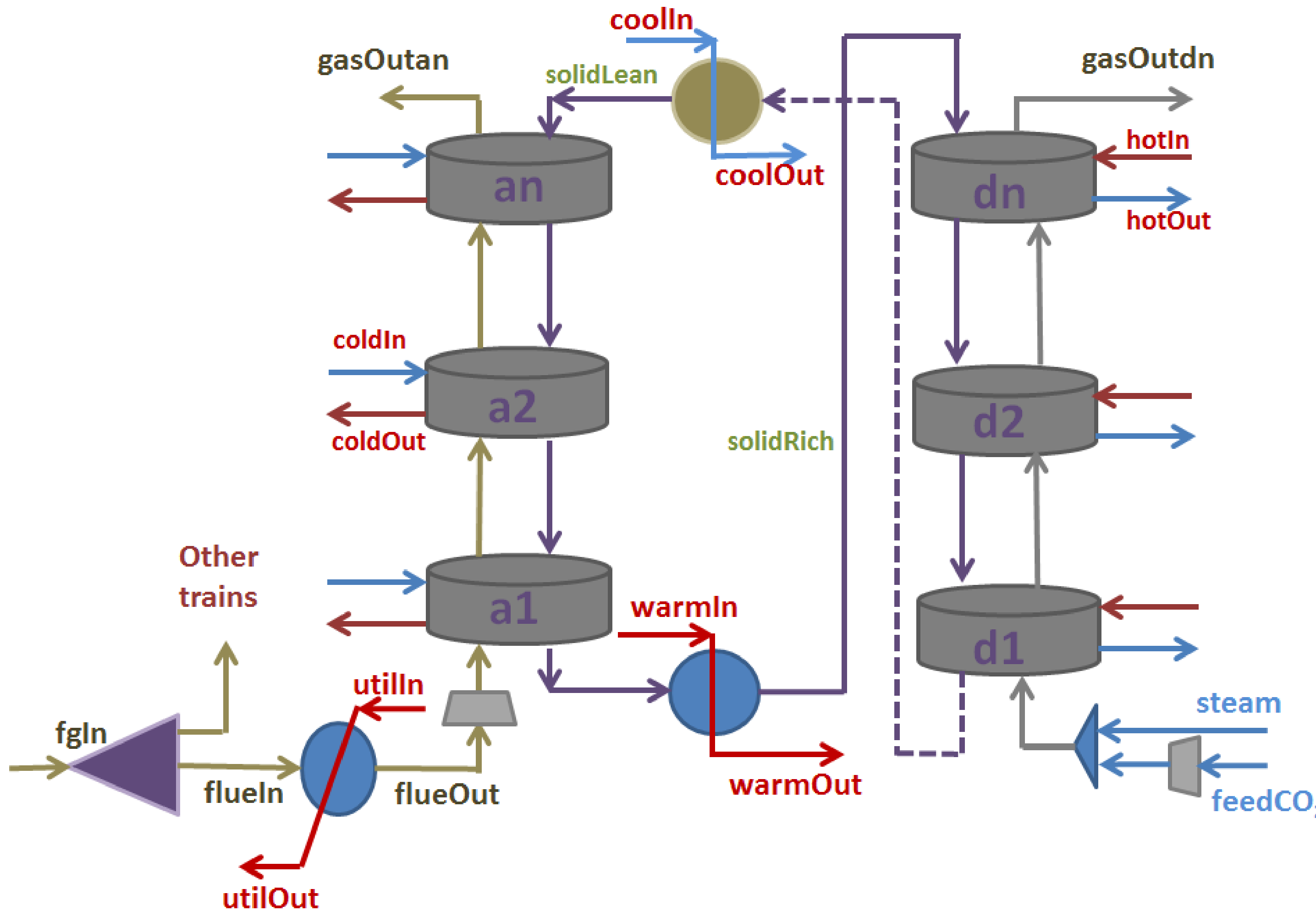
Bubbling fluidized bed

- **1D models**
- **Modeled in Aspen Custom Modeler**
- **Differential model**
- **Uses Aspen Properties package**



(A Lee, I&EC Research, 2013)

CO_2 CAPTURE PROCESS FLOWSHEET



General flow sheet for solid sorbent based carbon capture process

SUPERSTRUCTURE OPTIMIZATION

Objectives

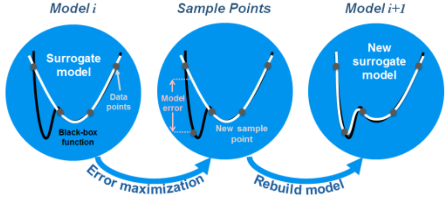
- Achieve the set carbon capture rate
- Minimize the cost of electricity (COE)
- Identify & develop the optimized bubbling fluidized bed process designs
    - — Optimal topology
    - — Optimal design conditions
    - — Optimal operating conditions

Hurdles

- Computationally intractable because of the detailed first principle models

Handles

- Generate the set of low complexity algebraic surrogate models
    - — Automated Learning of Algebraic Models for Optimization (ALAMO)

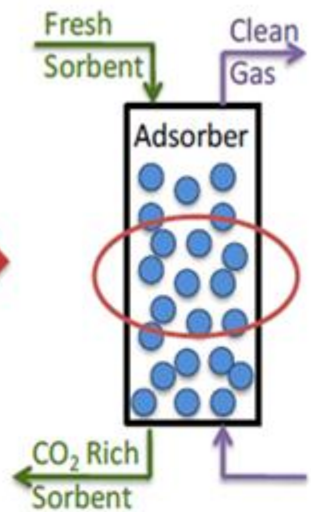


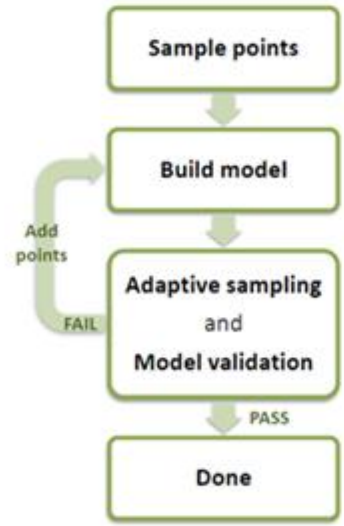
(http://archimedes.cheme.cmu.edu/?q=alamo)

SURROGATE MODEL GENERATION

Process models | **Aspen software** | **ALAMO** | **Surrogate models**

$$x \in \mathbb{R}^D \quad x^l \leq x \leq x^u \quad \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \\ \vdots \\ x_D \end{pmatrix}$$





$$\begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_k \\ \vdots \\ z_K \end{pmatrix} \quad z \in \mathbb{R}^K \quad z = f(x)$$

Independent variables *x*

- **Geometry**
- **Operating conditions**
- **Inlet flow conditions**

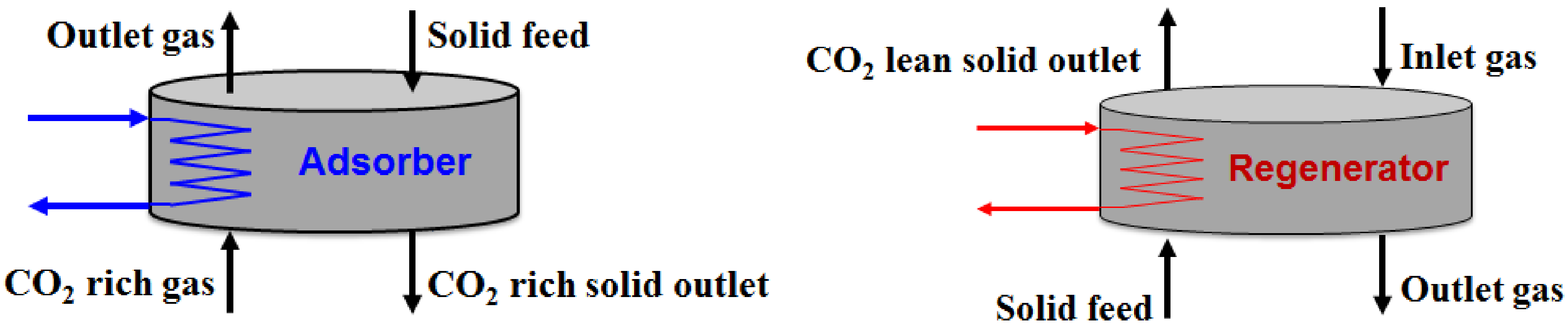
Dependent variables *z*

- **Geometry required**
- **Operating condition required**
- **Outlet flow conditions**
- **Design constraints**

(A. Cozad et al. ALAMO: Automatic learning of algebraic models for optimization.589b. Thursday, 8:50 AM, AIChE 2013)

BUBBLING FLUIDIZED BED

Bubbling fluidized bed reactor diagram



Model inputs

- Inlet pressure
- Inlet temperatures
- Inlet mass flow-rates
- Inlet gas mole fractions
- Inlet solid compositions
- Heat exchanger conditions

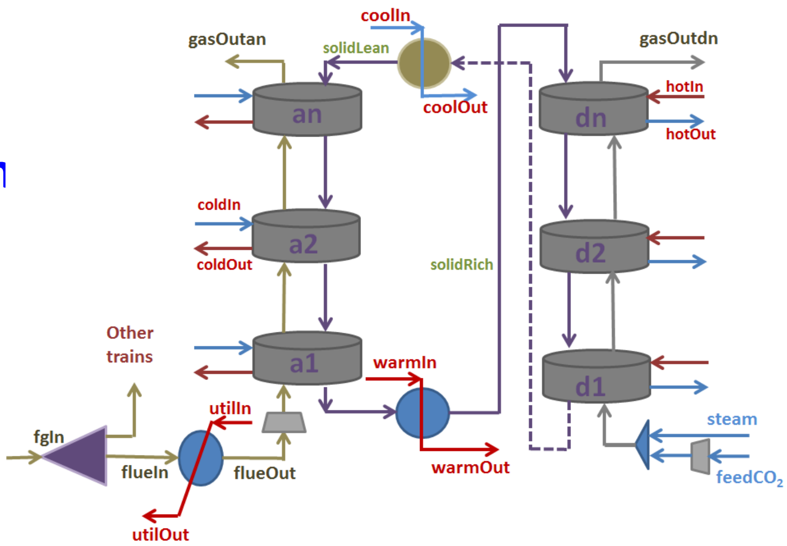
Model outputs

- Outlet pressure
- Outlet temperatures
- Outlet mass flow-rates
- Outlet gas mole fractions
- Outlet solid compositions

MINLP FORMULATION-ASSUMPTIONS

Assumptions for mixed integer nonlinear programming formulation

- Each stage is a single stage operation
- No pressure change for liquid and solid flow
- Each stage of adsorber/regenerator operation requires attached heat exchanger
- Surrogate models for fluidized bed adsorber and regenerator
- First principle models for SolidRich/SolidLean heat exchanger, blower, mixer



OBJECTIVE FUNCTION

Objective function

$$COE = \frac{(CCF)(TOC_{Sc} + TOC_{Cc}) + OC_{FIX} + (CF)(OC_{VAR})}{(CF)(MWh)} + COE_{TS\&M}$$

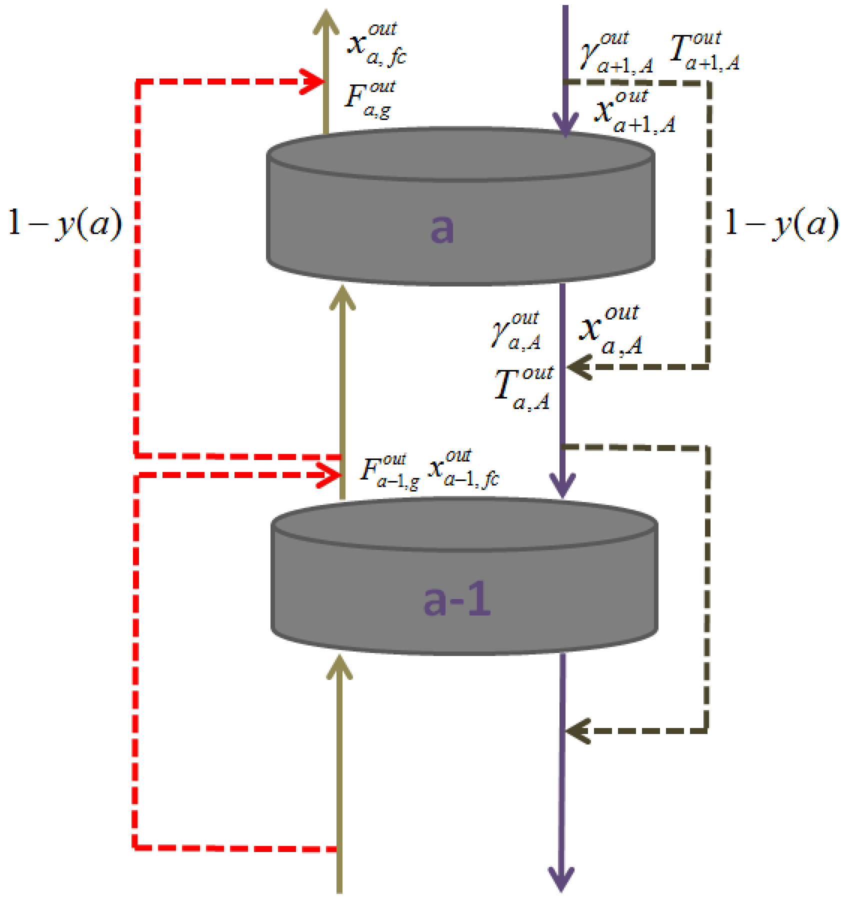
Where $$TOC_{Cc} = TOC_{Cs} + TOC_{rhx} + TOC_{lhx} + TOC_{flx}$$

$$TOCc_s = TOC_{ves} + TOC_{blow} + TOC_{HX} + TOC_{ele} + TOC_{pla} + TOC_{plat} + TOC_{elem}$$

- TOC_{Cc}: Capture system capital cost
- OC_{FIX}: Fixed operating & maintenance cost
- OC_{VAR}: Total variable cost
- MWh: Annual net megawatt-hours of power
- $COE_{TS\&M}$: COE increment
- TOC_{rhx}: Cost of Rich solid heat exchanger
- TOC_{lhx}: Cost of Lean solid heat exchanger
- TOC_{flx}: Cost of flue gas heat exchanger
- TOC_{Sc}: Sc plant capital cost
- TOC_{Cs}: Capital cost of reactors
- TOC_{ves}: Cost of vessel
- TOC_{blow}: Cost of blower
- TOC_{HX}: Cost of in-let heat exchanger
- TOC_{pla}: Cost of plate
- TOC_{plat}: Cost of platforms and ladders
- TOC_{elem}: Cost of elevator motor
- TOC_{ele}: Cost of elevator

MINLP FORMULATION

Adsorber series



- **Flue gas flow**

$$x_{a,fc}^{out} = F(surrogates)y(a) + x_{a-1,fc}^{out}(1-y(a))$$

$$F_{a,g}^{out} = F(surrogates)y(a) + F_{a-1,g}^{out}(1-y(a))$$

$$T_{a,g}^{out} = F(Surrogates)y(a) + T_{a-1,g}^{out}(1-y(a))$$

- **Solid sorbent flow**

$$\gamma_{a,A}^{out} = F(Surrogates)y(a) + \gamma_{a+1,A}^{out}(1-y(a))$$

$$x_{a,A}^{out} = F(Surrogates)y(a) + x_{a+1,A}^{out}(1-y(a))$$

$$T_{a,A}^{out} = F(Surrogates)y(a) + T_{a+1,A}^{out}(1-y(a))$$

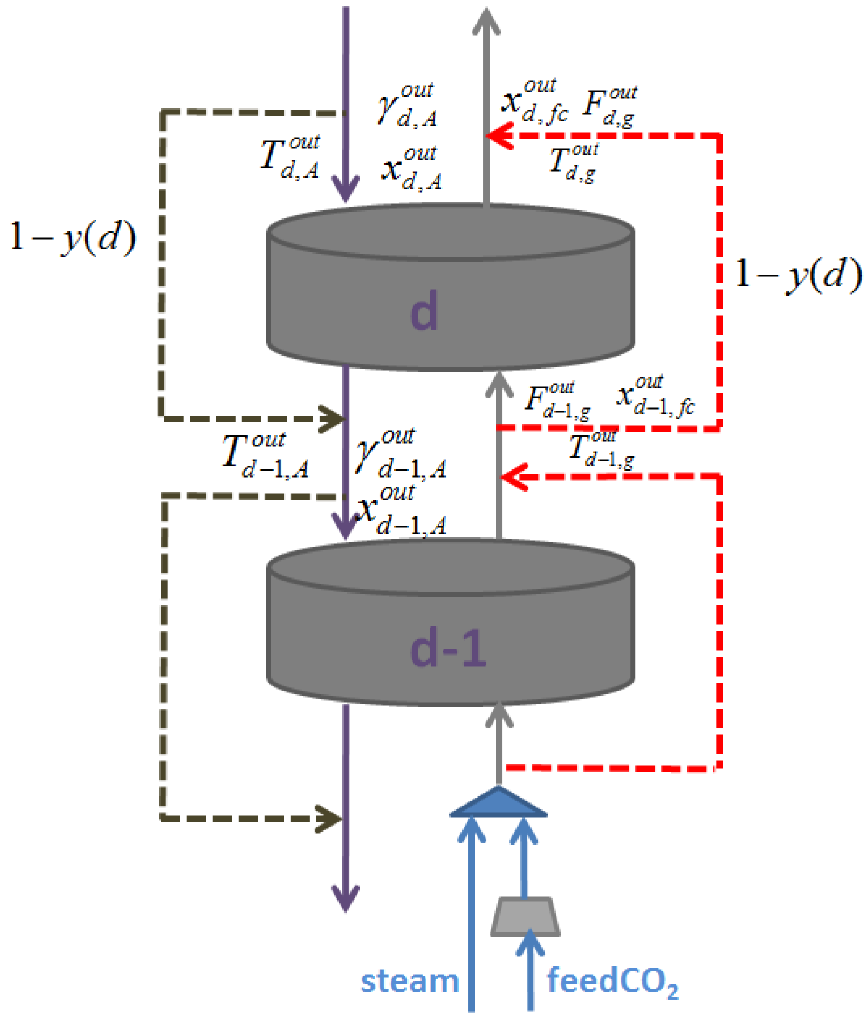
- **Logical constraints**

$$y(a) \geq y(a+1), \forall a \in a_{\max}$$

$$\sum_a y(a) \geq 1$$

MINLP FORMULATION-CONTINUED

Regenerator series



- **Clean gas flow**

$$x_{d,fc}^{out} = F(surrogates)y(d) + x_{d-1,fc}^{out}(1-y(d))$$

$$F_{d,g}^{out} = F(surrogates)y(d) + F_{d-1,g}^{out}(1-y(d))$$

$$T_{d,g}^{out} = F(Surrogates)y(d) + T_{d-1,g}^{out}(1-y(d))$$

- **Solid sorbent flow**

$$\gamma_{d,A}^{out} = F(Surrogates)y(d) + \gamma_{d+1,A}^{out}(1-y(d))$$

$$x_{d,A}^{out} = F(Surrogates)y(d) + x_{d+1,A}^{out}(1-y(d))$$

$$T_{d,A}^{out} = F(Surrogates)y(d) + T_{d+1,A}^{out}(1-y(d))$$

- **Logical constraints**

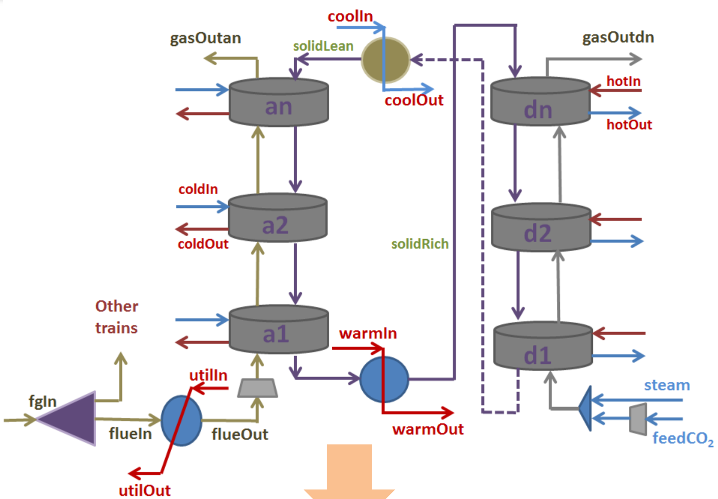
$$y(d) \geq y(d+1), \forall d \in d_{\max}$$

$$\sum_d y(d) \geq 1$$

CASE STUDY

Given conditions

- Conditions of flue gas
- Max number of adsorbers: 4
- Max number of regenerators: 4
- Max number of trains: 16
- Minimum capture rate: 90%



Objectives

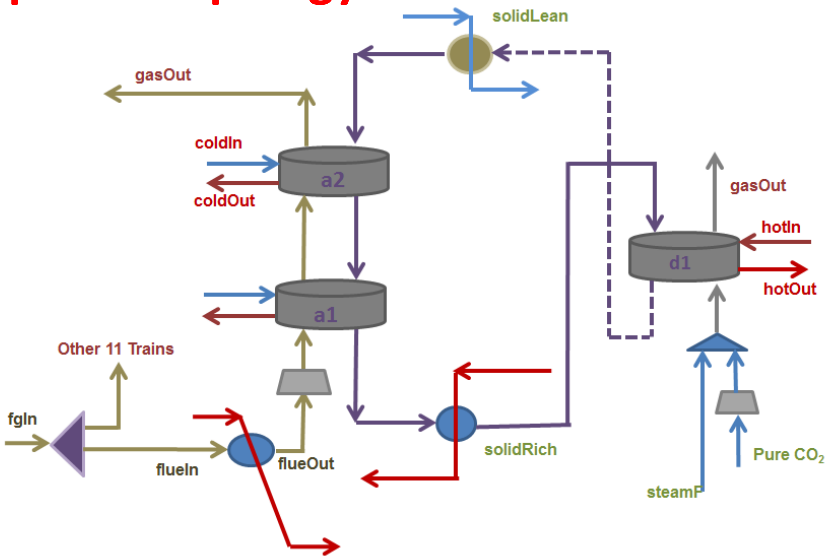
- Minimize cost of electricity
- Minimize total capital cost
- Decide the optimal number of trains in parallel
- Decide the optimal number of reactor in series
- Seek optimal operation conditions
- Seek an optimal geometry for each unit

Mixed-integer nonlinear programming model

- Parameters
- Variables
- Equations
  - Economic modules
  - Process modules
    - Material balances
    - Hydrodynamic/Energy balances
    - Reactor surrogate models
  - Link between economic modules and process modules
  - Binary variable constraints
  - Bounds for variables

RESULTS

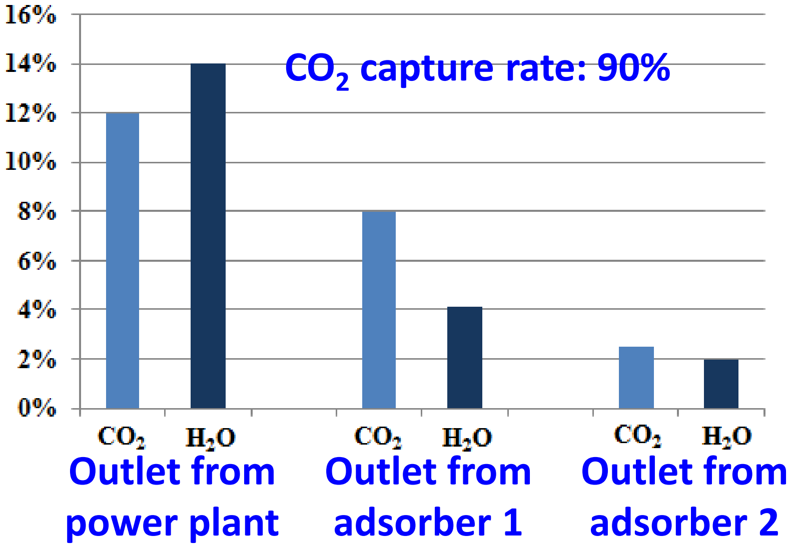
Optimal topology



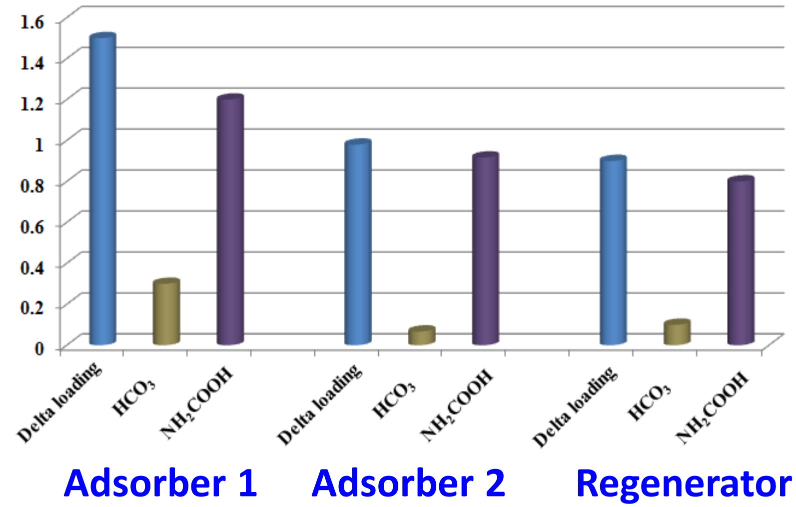
Variables	Lower	Value	Upper
COE($/MWh)*	0	137.3	1000
CapEX($M)	100	230.1	1000
steamFlow(kg/s)	~	108	~
Derate(MW)	0	103.7	650
sorbentF(kg/hr)	4E5	8.8E5	9E5
Nu (Number of trains)	12	12	16

- Cost of Electricity based on calculated capture system with base plant. + $48/MWh to account for compression, transport & storage

Molar composition of flue gas



Outlet sorbent composition (mol/kg)



CONCLUSIONS

- **We developed a surrogate model based framework to seek the optimal topology and the relevant optimal design/operating levels for carbon capture processes**

- **ALAMO provides simple surrogate models of adsorbers and regenerators and thus leads to a low-complexity optimization model**

- **Next steps:**
  - **—Extend MINLP to select simultaneously the reactor type for each stage**
  - **—Integrate heat integration across the capture and compression system with superstructure formulation**