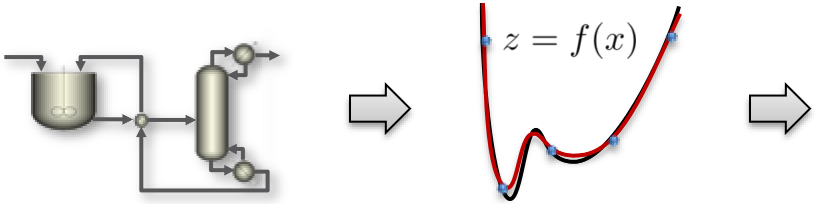

$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & g(x) = 0 \end{aligned}$$

Surrogate Model based Optimal Synthesis of Solid Sorbent Carbon Capture Processes

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OUTLINE

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

CO_2 CAPTURE PROCESSES

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

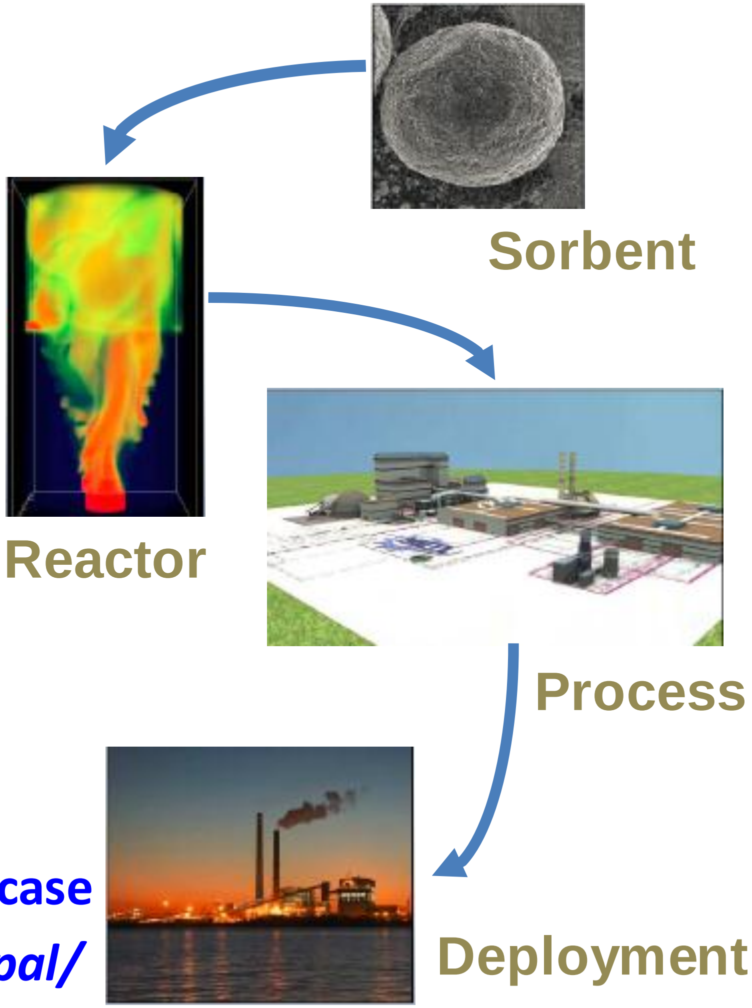
- Cost & energy-intensive technology
- Thermal & oxidative degradation

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)

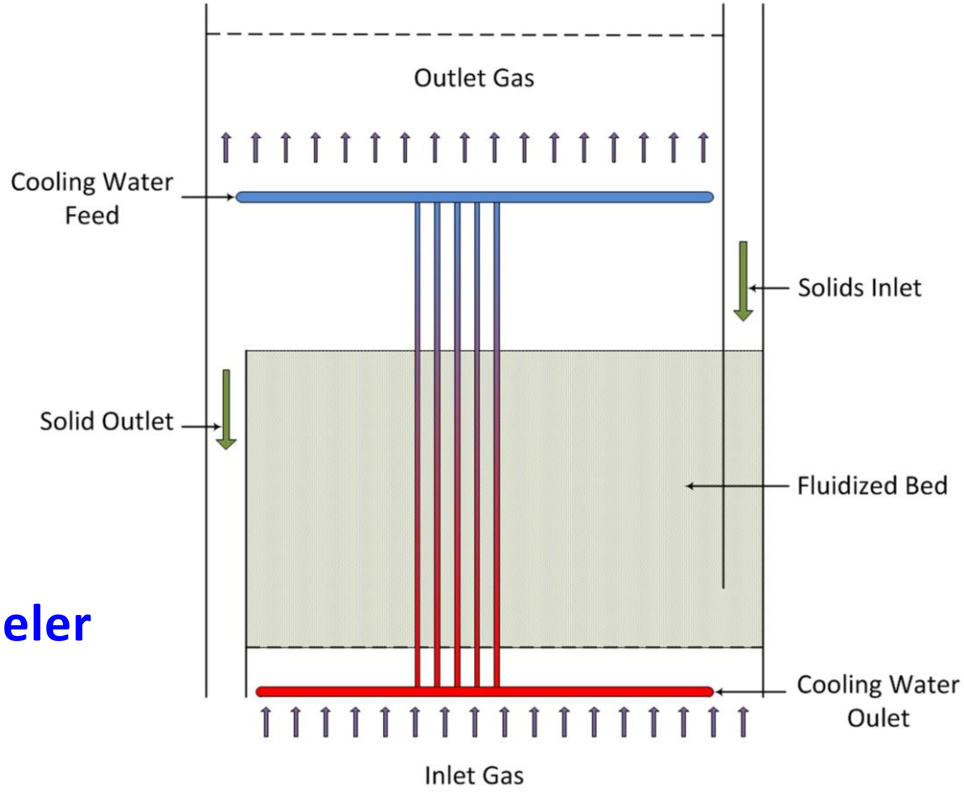
- 5 National Labs and 6 Universities
- Solid sorbent technology: initial demonstration case
- *https://www.acceleratecarboncapture.org/drupal/*



SOLID SORBENT CAPTURE PROCESS

Solid sorbent reactor

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

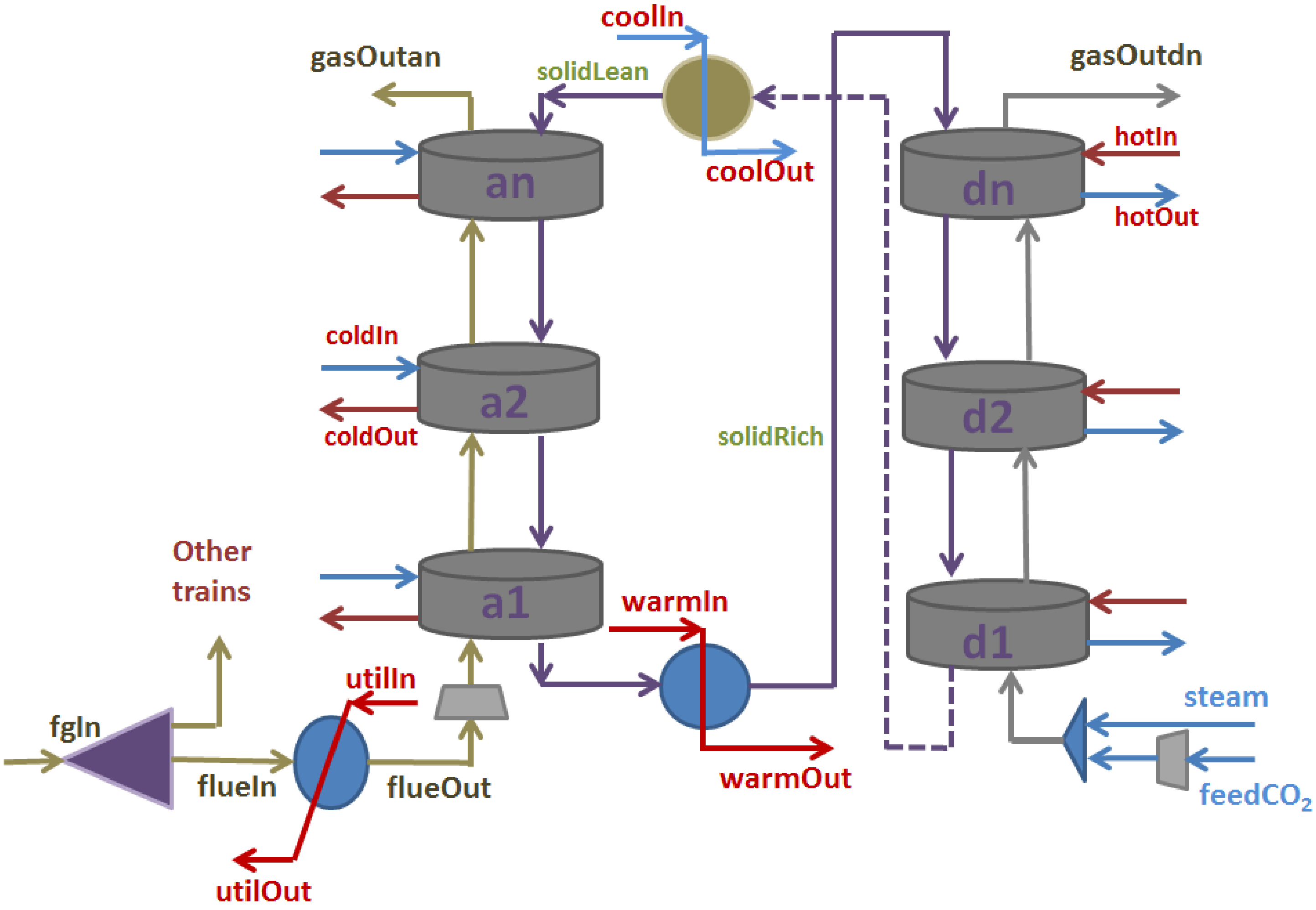


Bubbling fluidized bed

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

(A Lee, D Miller. A one-dimensional(1-D) three-region model for a bubbling fluidized-bed adsorber. I&EC Research, 2013)

CO_2 CAPTURE PROCESS FLOWSHEET



General flow sheet for solid sorbent based carbon capture process

SUPERSTRUCTURE OPTIMIZATION

Objectives

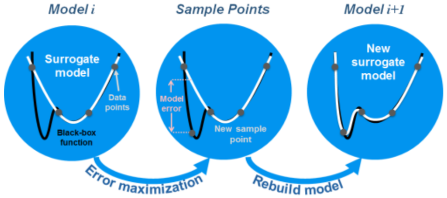
- **Achieve the set carbon capture rate**
- **Minimize the cost of electricity (COE)**
- **Identify & develop the optimized bubbling fluidized bed process designs**
  - **Optimal topology**
  - **Optimal design conditions**
  - **Optimal operating conditions**

Hurdles

- **Computationally intractable because of the detailed first principle models**

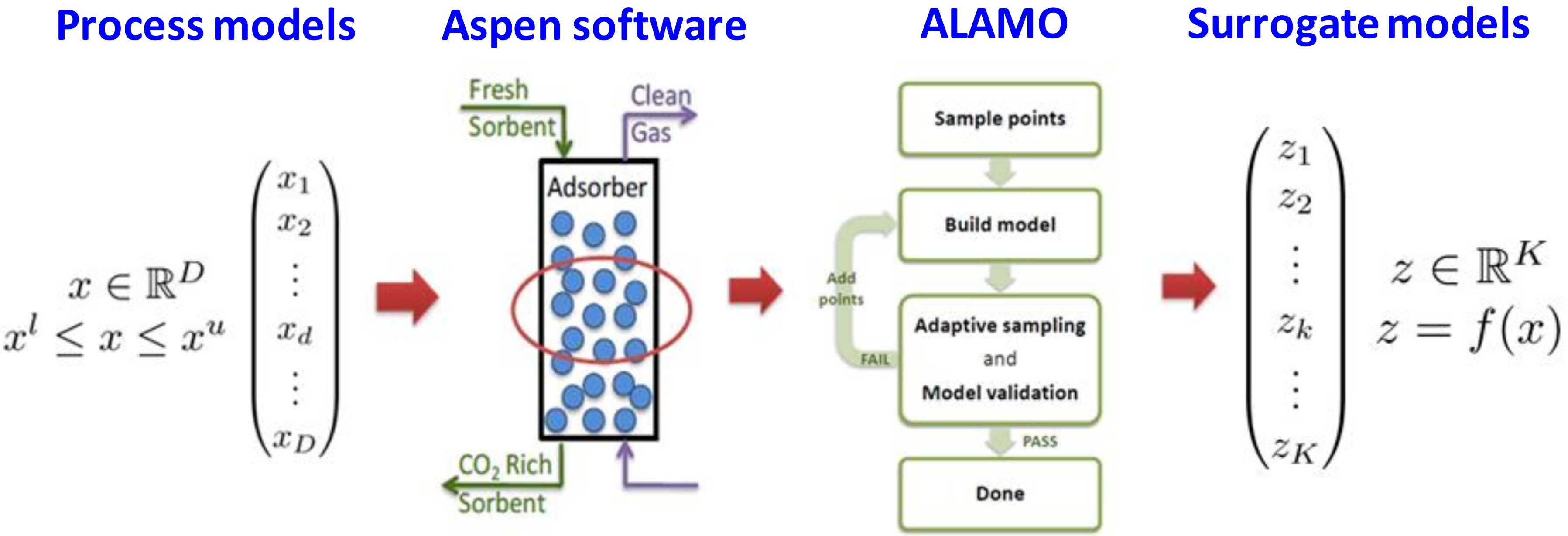
Handles

- **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



Independent variables *x*

- Geometry
- Operating conditions
- Inlet flow conditions

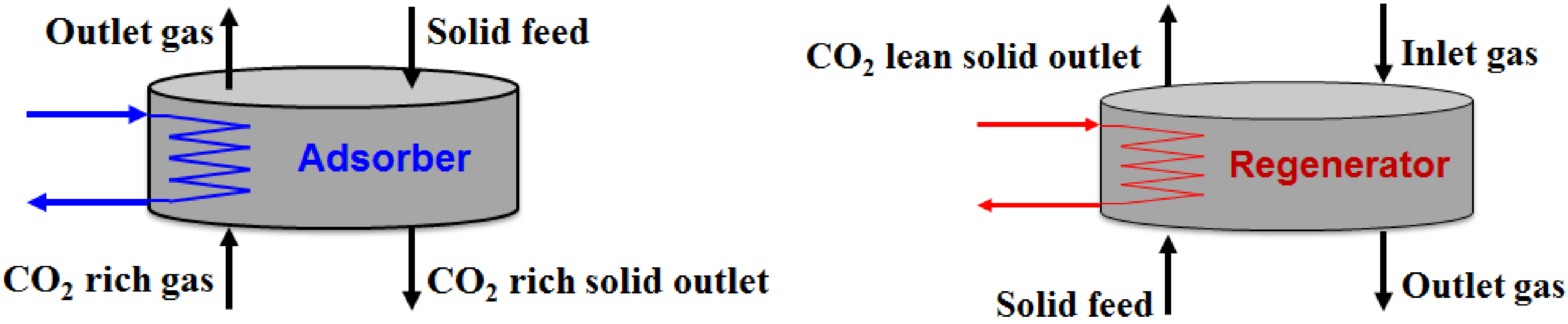
Dependent variables *z*

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

(A. Cozad et al. Automatic learning of algebraic models for optimization. AIChE Journal, 2014)

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

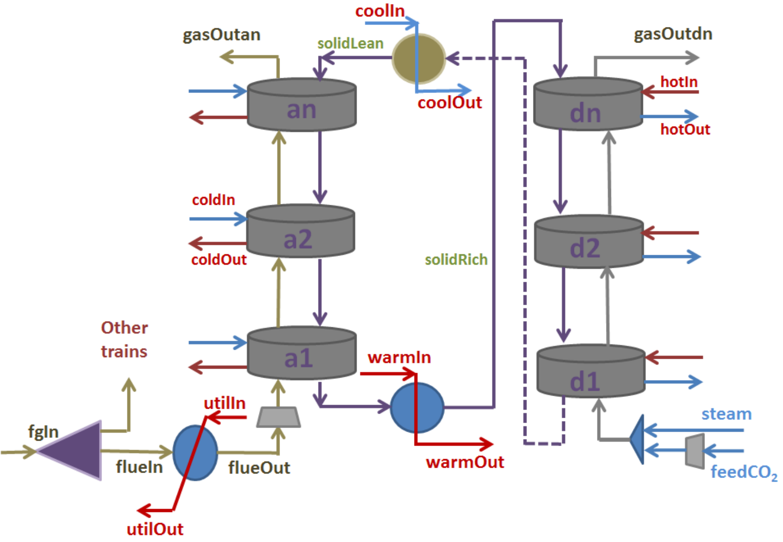
Model outputs

- 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:

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

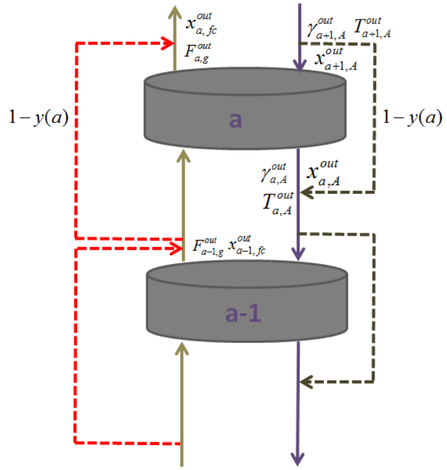
$$TOCc_{s} = TOC_{ves} + TOC_{blow} + TOC_{HX} + TOC_{ele} + TOC_{pla} + TOC_{plat} + TOC_{elem}$$

- 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**

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

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

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

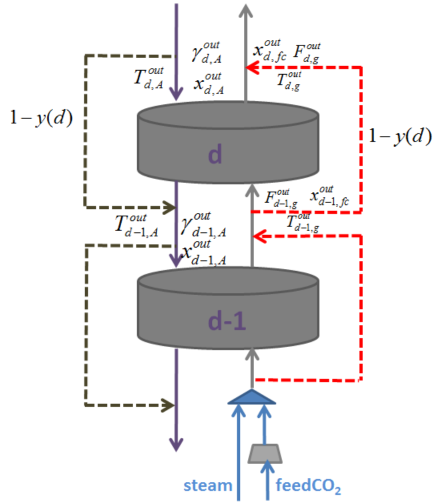
- **Solid sorbent flow**

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

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

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

Regenerator series



- **Clean gas flow**

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

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

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

- **Solid sorbent flow**

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

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

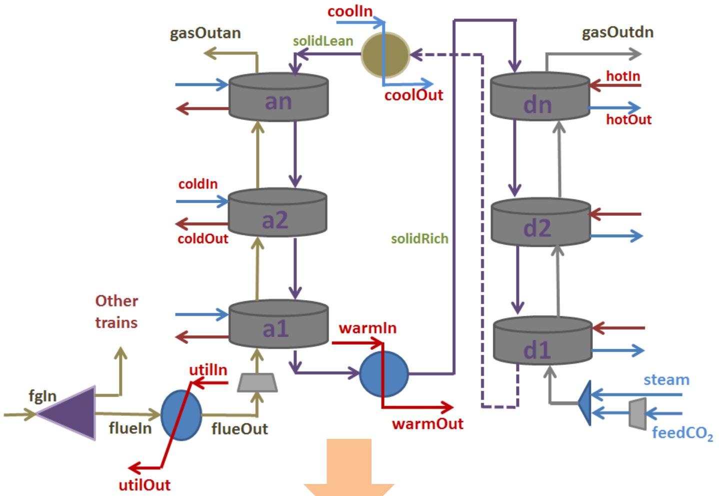
$$T^{out}_{d,A} = F(Surrogates)y(d) + T^{out}_{d+1,A}(1-y(d))$$

- **Logical constraints** $y(s) \ge y(s+1), \forall s \in s_{\max}$ $\quad \sum_{s} y(s) \ge 1 \quad \{a,d\} \in s$

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

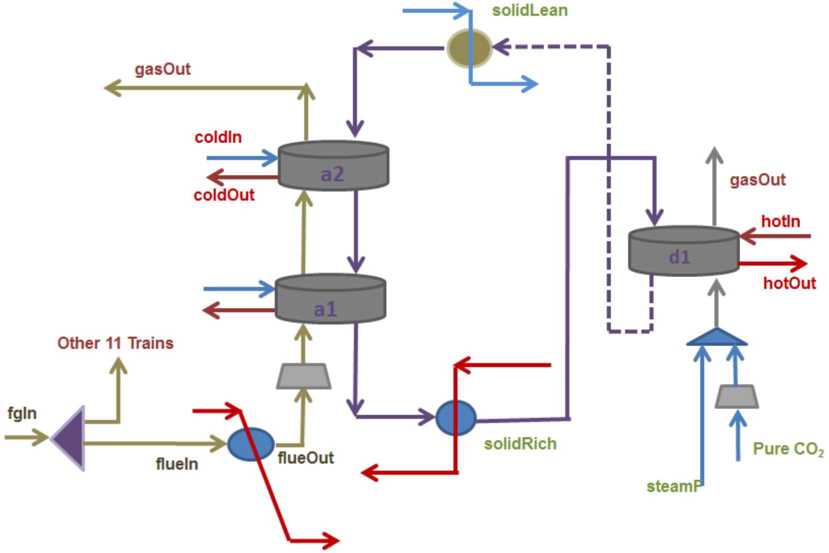
- Minimize cost of electricity
- Minimize total capital cost
- Decide the optimal number of trains in parallel
- Decide the optimal number of reactor in series
- Seek optimal operation conditions
- Seek an optimal geometry for each unit

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

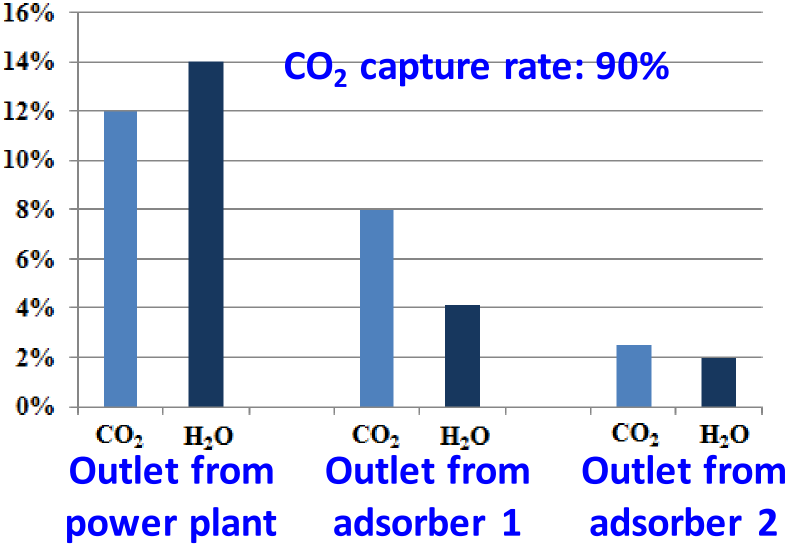
Optimal topology



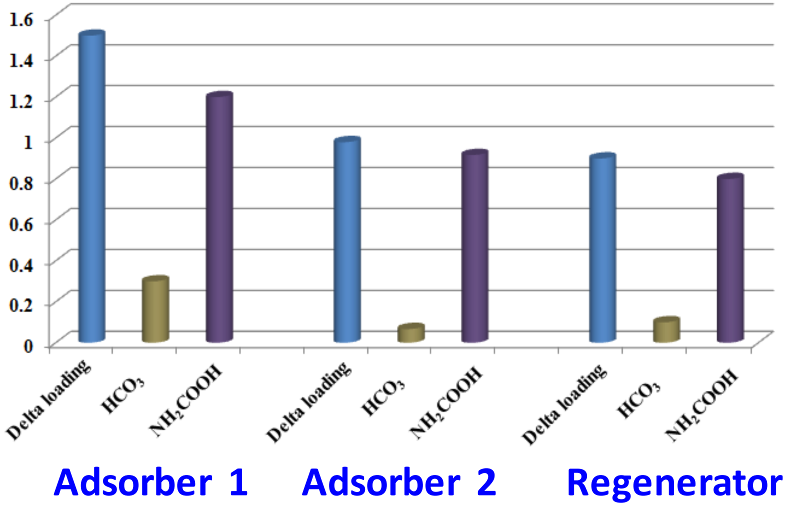
Variables	Lower	Value	Upper
COE($/MWh)*	0	137.3	1000
CapEX($M)	100	230.1	1000
steamFlow(kg/s)	~	108	~
Derate(MW)	0	103.7	650
sorbentF(kg/hr)	4E5	8.8E5	9E5
Nu (Number of trains)	12	12	16

* Cost of Electricity (COE) 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**