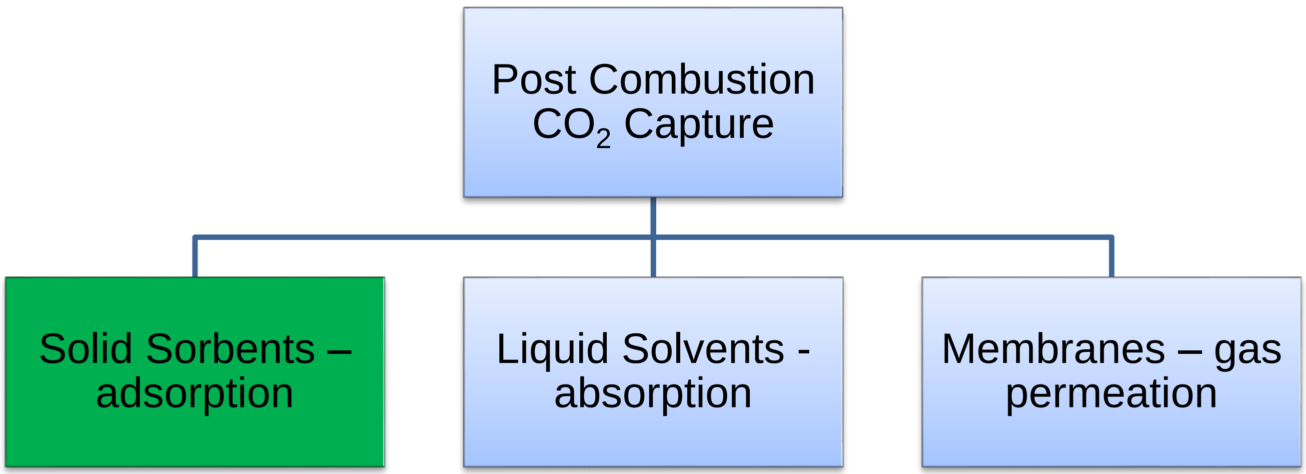
Optimal Synthesis of a Solid Sorbent-based CO_2 Capture Process

Miguel Zamarripa[*], John Eslick[*], Andrew Lee[*], Nick Sahinidis[+] and David Miller[*]
[*]National Energy Technology Laboratory, Pittsburgh, PA
[+]Carnegie Mellon University, Pittsburgh PA

Energy Systems Initiative (ESI) Meeting, Carnegie Mellon University.
March 12th, 2017.

Post Combustion Technologies



Process and modeling issues:

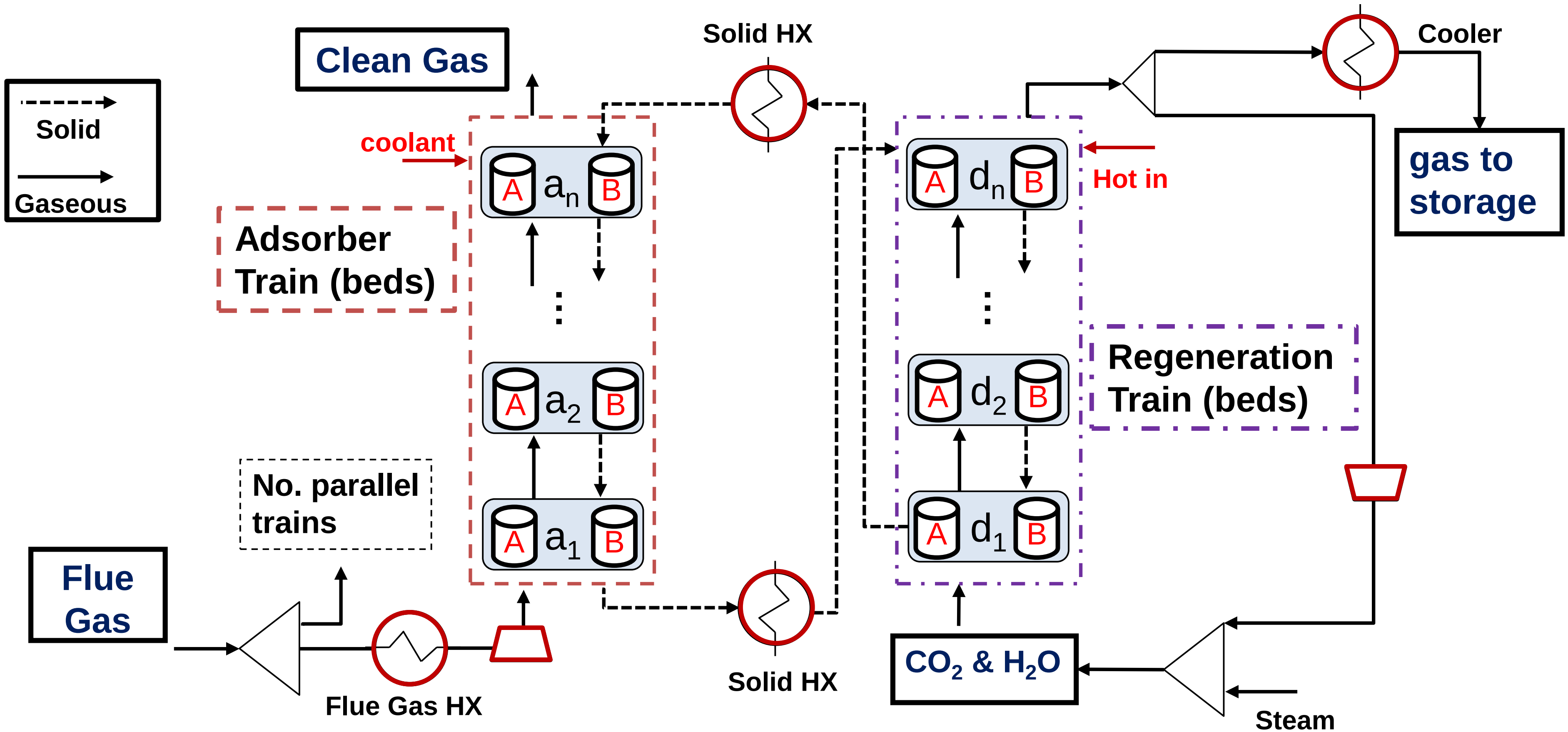
- Process complexity.
- Energy Intensive.
- Costing methodologies.

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

Goal:

- Minimize the cost of electricity due to CO_2 capture.
  - Establish a consistent framework to optimize the **cost, design** and **operating conditions** of carbon capture technologies.
  - Superstructure-based mathematical optimization framework.

Superstructure Optimization Framework



- Discrete Decisions:
- Continuous decisions:

Problem **Complexity** Increases with:
- # of technologies
- # of stages
- Non-linearities of the problem

MINLP

Fixed & Operating Cost

Cost of Electricity

$$\min COE = \frac{(Investment \cdot \varepsilon \; + Operating_{fix} + Operating_{var} \cdot \alpha_1)}{(Net\ Power \cdot \alpha_2 \cdot \beta \cdot \tau)}$$

$$s.t. \quad Material\ Balances$$
$$Energy\ Balances$$
$$Equipment\ Design$$
$$Process\ Configuration$$

Costing Methodology:

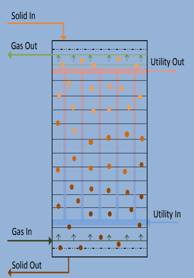
- **Investment cost**
  - Sorbent, Power Plant, Capture (ads, rgn, HX, cmp).
- **Operating cost:**
  - Fixed: labor, maintenance, others.
  - Variable: utilities "coolant & steam", waste water, others.
- **Net power**:
  - Power PP – (kW for compression, blowers, pumps, etc).

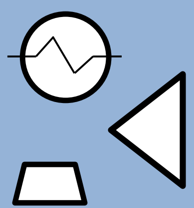
Benefits

- Superstructure-based optimization explores multiple technologies and process configurations to design the process.
- Mathematical tool to analyze new "potential" solid sorbents, fluidization regimes, etc.
- Scale up solid sorbent technologies.

Proposed Framework

Process Models

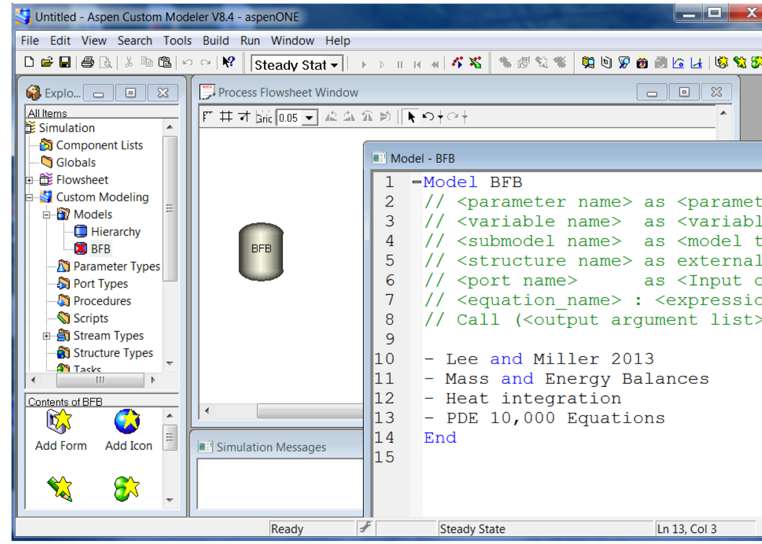




Adsorption & Regeneration process

- **Bubbling fluidized bed reactor**
  - Mass & energy balances[1]
  - PDEs + Algebraic Eqns.
  - 14,187 Equations (single unit)
  - Aspen Custom Modeler

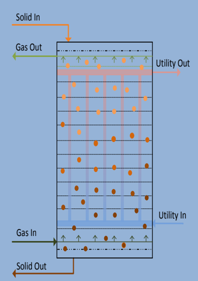
- Units: Heat exchangers, blowers, pumps, etc.

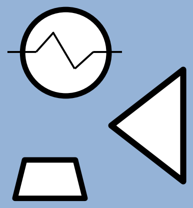


[1] Lee, A., & Miller, D. C. (2012). A one-dimensional (1-d) three-region model for a bubbling fluidized-bed adsorber. *Industrial & Engineering Chemistry Research*,*52*(1), 469-484.

Proposed Framework

Process Models





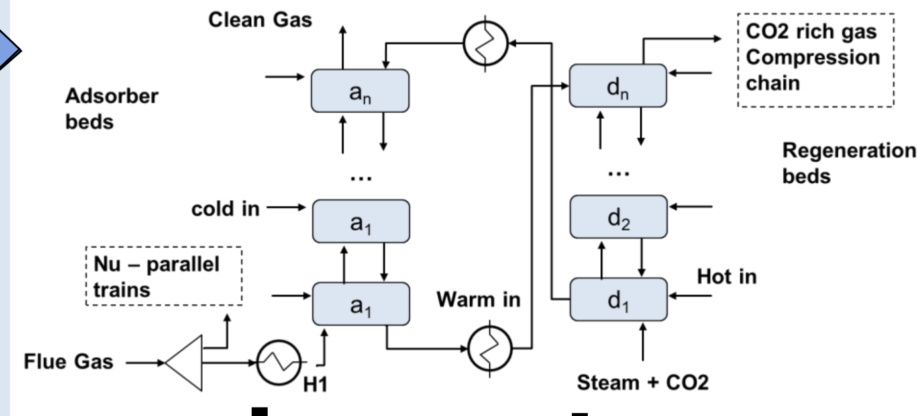
Rigorous Models

Surrogate Models
(black box, correlations, etc.)

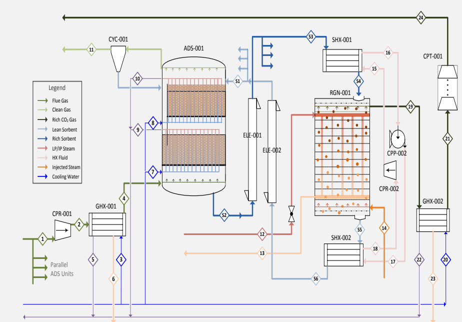
First Principle Models

- Nonlinear algebraic equations

Superstructure Opt. Model



Carbon Capture Process



Detailed Simulation

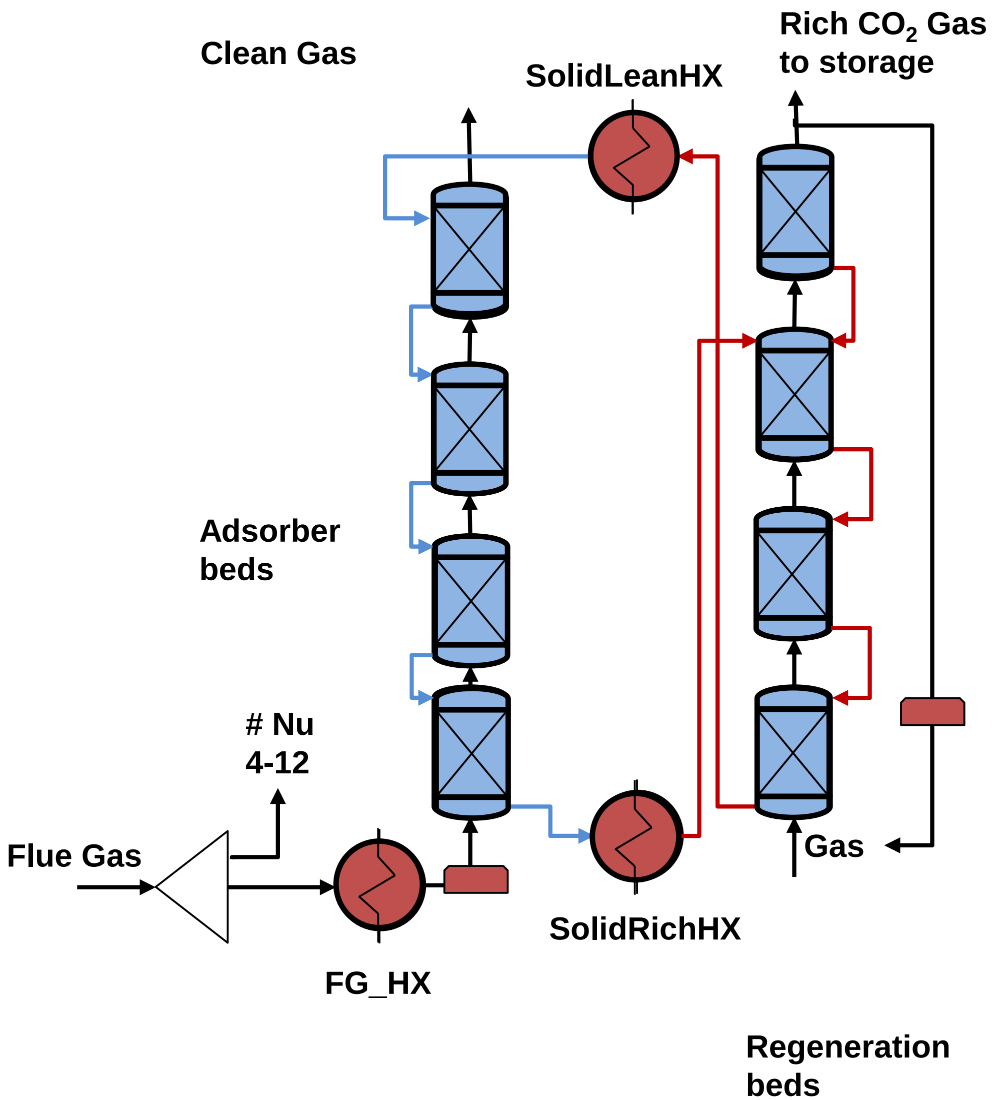
Optimized Process

Solid Sorbent System – Case Study

Adsorption system

Plant consists on:

- Flue gas (**650 MW power plant**)
- 90 % capture needed
- CO_2 ~12% (molar fraction)
- 4 adsorber & regeneration beds
  - 2 technologies (reactor configuration)
- 4 – 12 parallel units.



Mathematical Model

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

Surrogate Models: Framework for Optimization and Uncertainty Quantification and Surrogates - FOQUS

Carbon Capture Simulation Initiative tool set:

- 100 R&D award 2016.

Process Simulation
- Detailed model

Data Management
- Sampling
- Analysis
- Refining

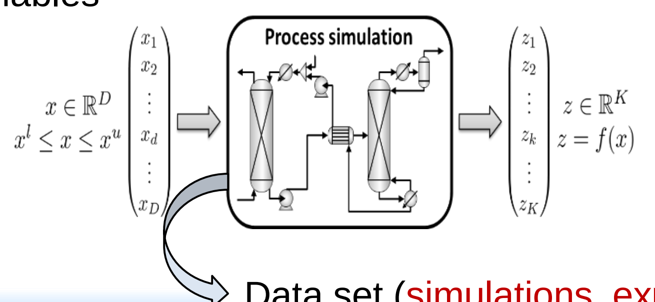
Surrogate model
- Generation
- Validation

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

ALAMO
a black-box modeling tool

Input variables

Output variables



Data set (simulations, experiments, etc.)

Automated Learning of Algebraic Models

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

Final surrogate Model:

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

CCSI Carbon Capture Simulation Initiative

National Energy Technology Laboratory · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory EST. 1943 · Pacific Northwest National Laboratory · U.S. Department of Energy

Surrogate Models: Framework for Optimization and Uncertainty Quantification and Surrogates - FOQUS

Carbon Capture Simulation Initiative tool set:

- 100 R&D award 2016.

Process Simulation
- Detailed model

Data Management
- Sampling
- Analysis
- Refining

Surrogate model
- Generation
- Validation

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

Surrogate model (simple example)

- Flue Gas Heat Exchanger (flash calc.)
  - Ideal Calculations (Antoine equation + Raoult's Law)
  - Non-ideal calculations with ACM
  - Surrogate model

Ideal Calc (Antoine eqn. + Raoult's law):

$$lnP_{Sat}^{i} = C_{1i} + \frac{C_{2i}}{T + C_{3i}} + C_{4i}T + C_{5i}lnT + C_{6i}T^{C_{7i}}$$

$$y_{H2O}P = x_{H2O}P_{Sat}^{H2O}$$

$$GasOut = GasIn\left(\frac{x_{CO2} + x_{N2}}{1 - y_{H2O}}\right)$$

Or

Non-Ideal Calc:

Equation of state used by aspen:

Call(y) = pFlash(Tout, Pout, Zin);

Highly non linear

Or

Surrogate Model:

- **Input variable:** outlet Temperature
- **Output variable:** yH2O

Data set:

- T_u = 54 C, upper bound
- T_l = 40 C, lower bound
- i = $(t_u - t_l)/200$

For i
Tout = T_l + I
Call(y) = **pFlash**(Tout, Pout, Zin);
Print(y_{H2O})
end

$$y_{H2O} = \alpha T + \beta T^2$$

Surrogate model (simple example)

- Flue Gas Heat Exchanger (flash calc.)
  - Ideal Calculations (Antoine equation + Raoult's Law)
  - Non-ideal calculations with ACM
  - Surrogate model

$$\%\ \text{error} = \frac{(Aspen\ - other)100}{Aspen}$$

Gas Outlet	ASPEN	Ideal	% error	Surrogate Model	% error
Flow rate, kmol/hr	15613	15794	**1.1**	15642	**0.1**
Temperature, C	43.72	43.72	0	43.72	0
Pressure, bar	1.009	1.009	0	1.009	0
y CO2, mol frac.	0.128	0.127	1.1	0.128	0.1
y H2O, mol frac.	0.078	0.089	13.3	0.080	1.9
y N2, mol frac.	0.794	0.784	1.1	0.792	0.1

Surrogate Models: Framework for Optimization and Uncertainty Quantification and Surrogates - FOQUS

Carbon Capture Simulation Initiative tool set:

- 100 R&D award 2016.

Process Simulation
- Detailed model

Data Management
- Sampling
- Analysis
- Refining

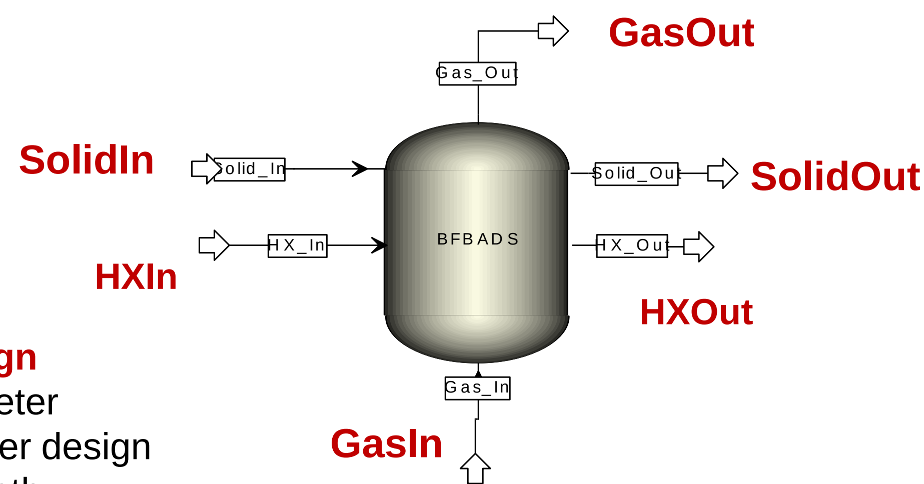
Surrogate model
- Generation
- Validation

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

Adsorption system

- BFB for Adsorption & Regeneration
- Detailed ACM simulation.

17 inputs vars
20 outputs vars



Reactor Design
Dt – unit diameter
Heat Exchanger design
Solids bed depth

CCSI Carbon Capture Simulation Initiative

Surrogate Models: Framework for Optimization and Uncertainty Quantification and Surrogates - FOQUS

Carbon Capture Simulation Initiative tool set:

- ➢ 100 R&D award 2016.

Process Simulation
- Detailed model

Data Management
- Sampling
- Analysis
- Refining

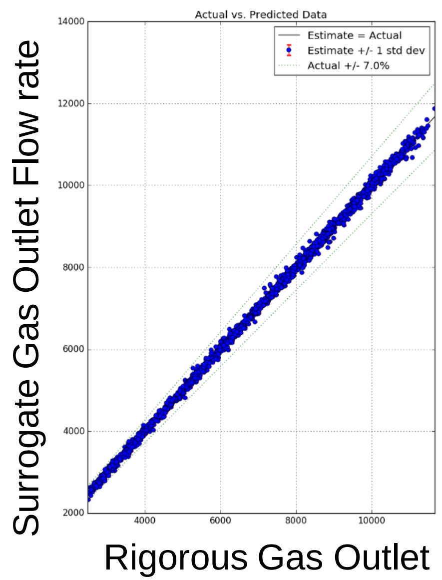
Surrogate model
- Generation
- Validation

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

Adsorption system

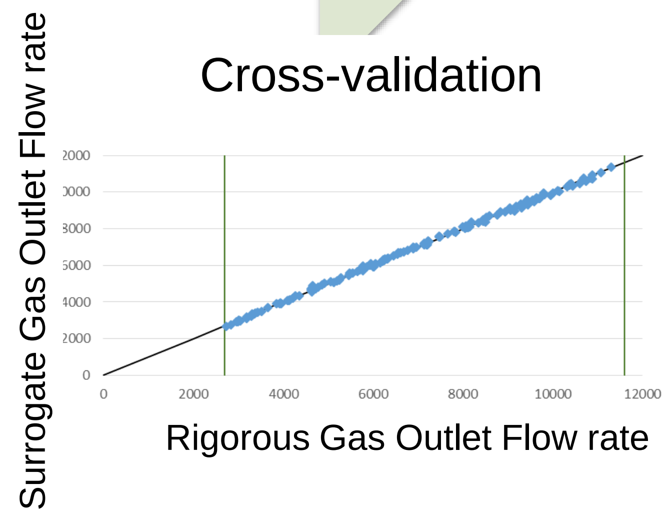
- Data Set:
  - 2000 samples
  - Latin Hypercube Sampling method
- Cross-Validation
  - 200 samples
  - LHS method

Fit data



R^2= 0.99

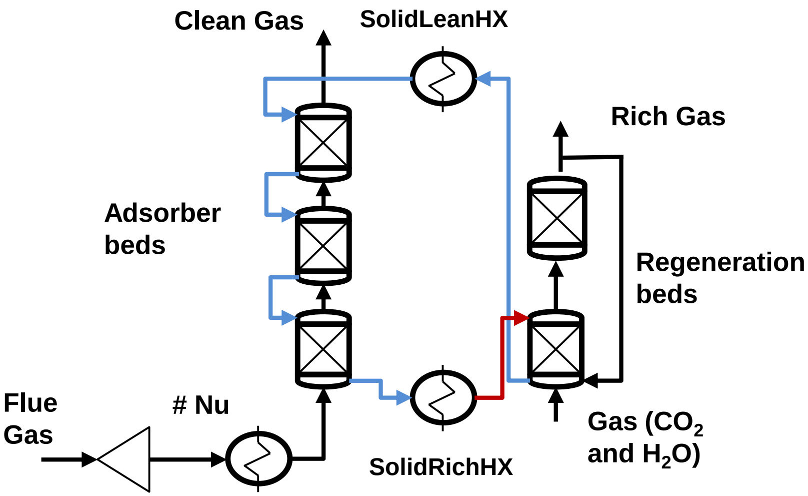
Cross-validation



R^2= 0.99

CCSI Carbon Capture Simulation Initiative · National Energy Technology Laboratory · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · Pacific Northwest National Laboratory · U.S. Department of Energy

Base Case



Summary:

- Base case (Fixed Layout: 3 ads, 2rgn)
- Optimization model (GAMS/Dicopt):
  - 383 equations
  - 588 variables
- Rigorous model (Aspen, ACM)
  - 118323 equations
  - 118679 variables
- 90% CO_2 Capture.

Optimization vs Rigorous Simulation

	% error
COE, &/MWh	0.9
Net Power, MW	1.1
Steam Flow, kg/hr	0.8
CPU time, s	-
Adsorber cost, $	
A1	0.9
A2	3.2
A3	0.1
A4	-
Regenerator Cost, $	
D1	0.4
D2	5.8
D3	-
D4	-

Optimization model provides a valid estimation of the COE

Optimal Solutions

Summary:

- Superstructure optimization allow us to explore all the possible plant layouts.
- Optimization model (GAMS/Dicopt):
  - 383 equations
  - 588 variables (24 Discrete)
- Rigorous model (ASPEN)
  - 118323 equations
  - 118679 variables
- 90% CO_2 Capture.

	Different initialization			Fixed layout			
	Optimal	Case 1	Case 2	Case 4	Case 5	Case 6	Case 7
% COE increase	-	0.347	0.766	3.689	3.68	4.536	6.23
Adsorber beds		3	3	3	2	3	3
Regeneration beds		3	2	1	3	2	2
Ads parallel units		6	6	6	6	6	7
Rgn parallel units		6	6	6	5	4	7

Remarks

- Solving a superstructure optimization problem using rigorous models is challenging problem.
  - Rigorous models have been replaced by carefully tuned surrogate models.
  - Surrogate model generation, validation and cross-validation have been simplified with **FOQUS** (**F**ramework for **O**ptimization and **U**ncertainty **Q**uantification and **S**urrogates).
  - A Mix of first principle and surrogate models provide a valid estimation of the cost.

- Integrated conceptual design and process synthesis tools facilitate the rapid development of Post Carbon Capture Technologies.
  - A robust mathematical optimization framework has been developed to optimize the cost, design and operating conditions of a CO_2 capture plant.
  - Establishing a consistent basis for analyzing the cost of electricity due to capture is a critical issue to analyze different Post Combustion Capture Technologies.
  - The methodology presented could be extended to incorporate multiple post combustion technologies.

Acknowledgments

National Energy Technology Laboratory, Center for Advanced Process Decision Making and Oak Ridge Institute for Science and Education.

Want to use **FOQUS**?

Ask for our testing and evaluation license.

Thank you for your attention

CCSI Carbon Capture Simulation Initiative · National Energy Technology Laboratory · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · Pacific Northwest National Laboratory · U.S. Department of Energy