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Carbon Capture Simulation Initiative

Synthesis of optimal capture processes using advanced optimization

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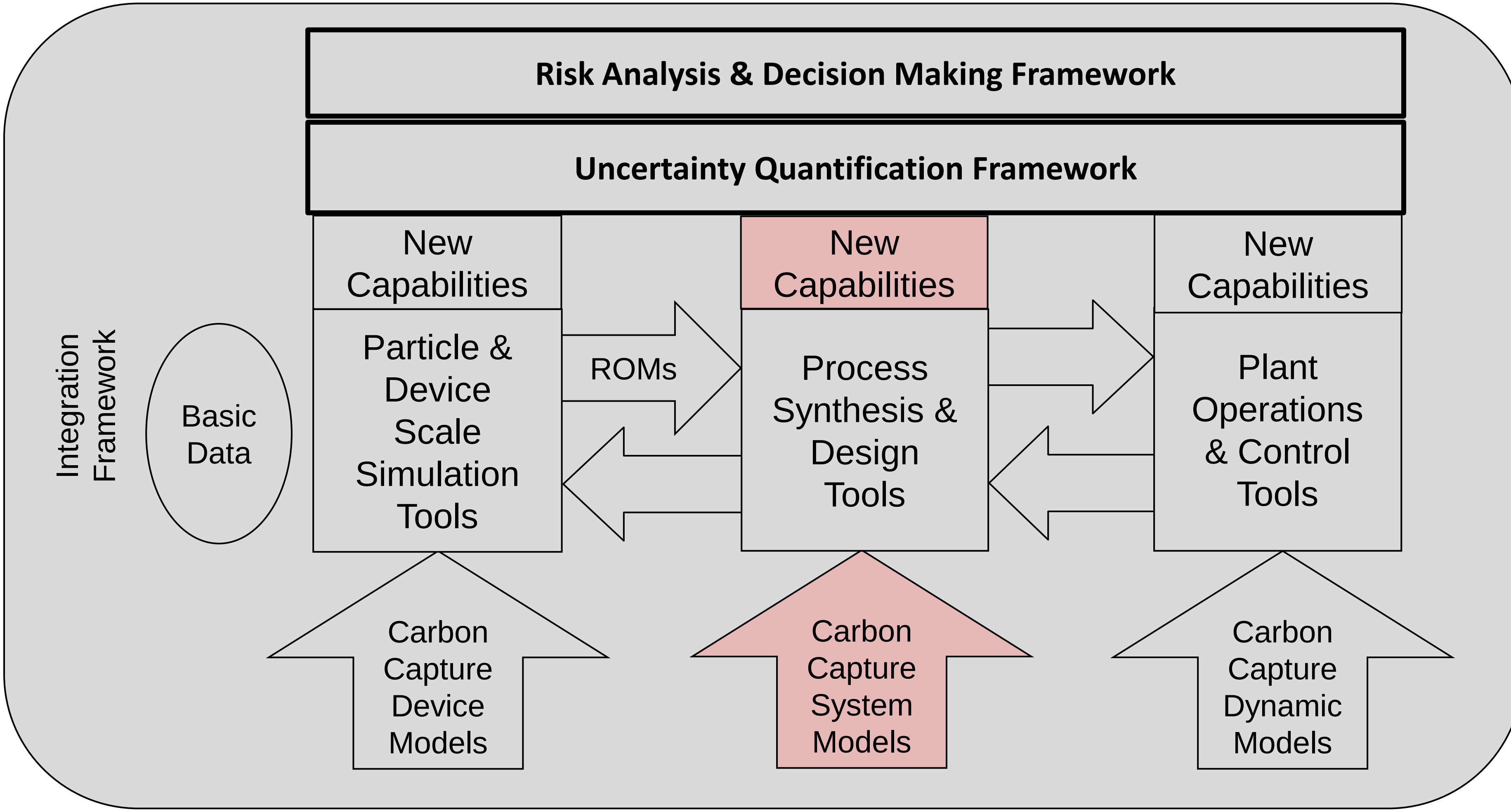
Synthesis of optimal capture processes using advanced optimization



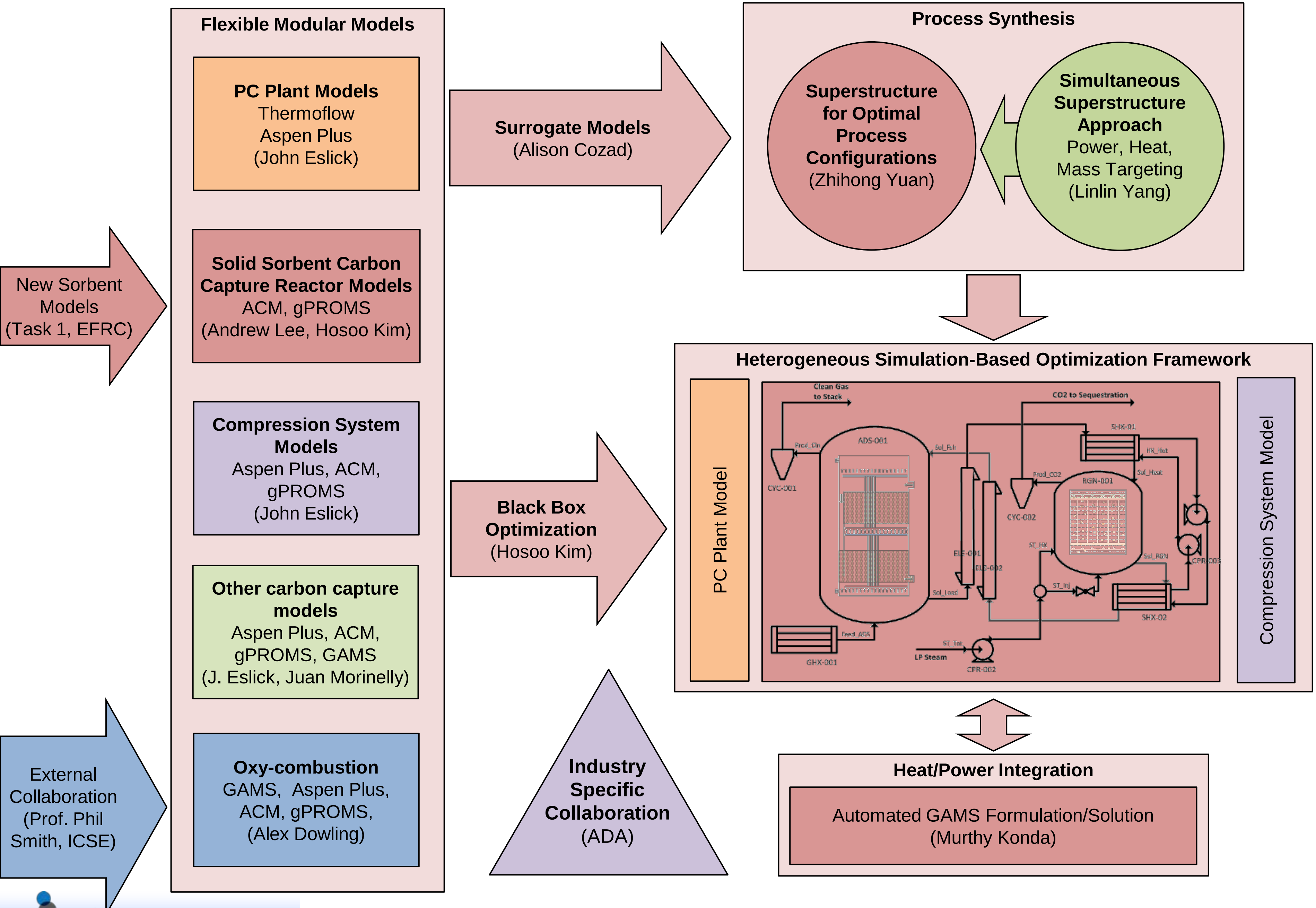
CCSI Process Synthesis & Design

Facilitate the rapid screening of new concepts and technologies

Enable identification & development of optimized process designs

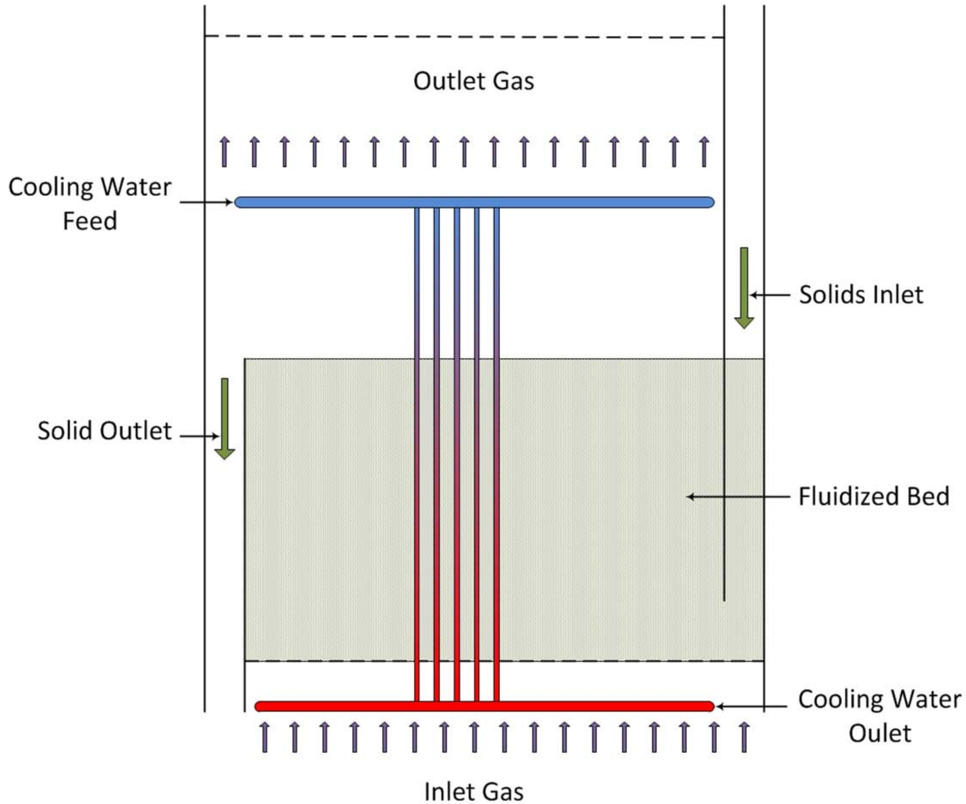
- Multiple potential technologies for carbon capture
  - Different reactors types
  - Different sorbent materials
  - Different regimes (high T, low T, PSA, TSA)
- Need systematic way to evaluate candidate processes, materials
  - Need to consider <u>best process</u> for <u>different materials</u>

- Identify configurations for more detailed simulation (i.e., CFD)
- Integrate and optimize the entire process system
  - PC plant, carbon capture process, and compression system

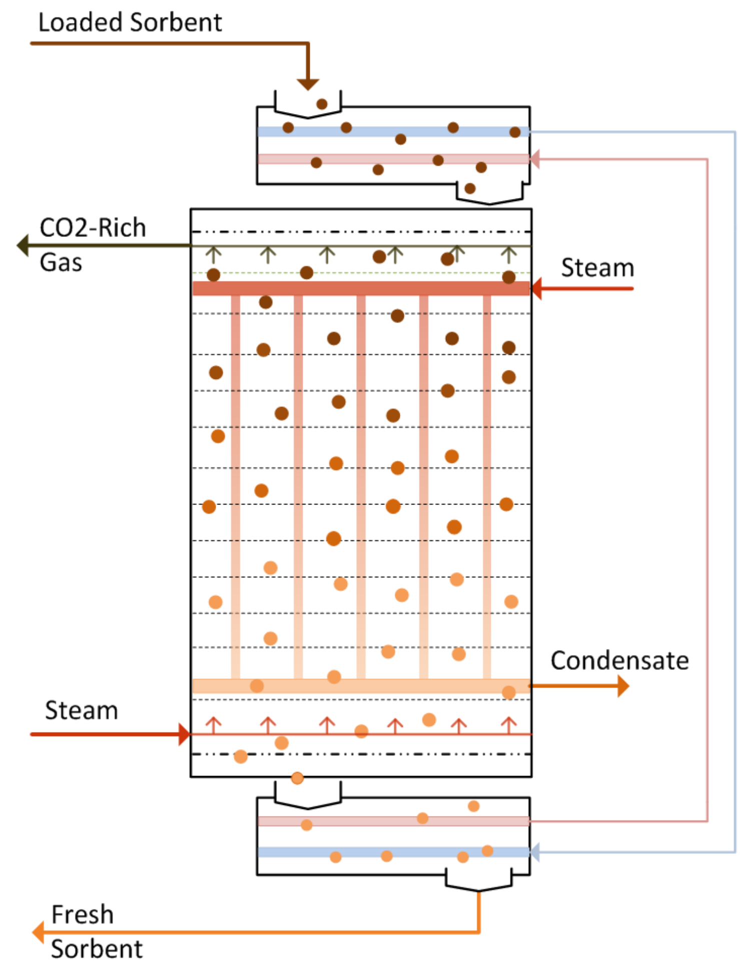

Flexible Modular Models
PC Plant Models
Thermoflow
Aspen Plus
(John Eslick)
Solid Sorbent Carbon Capture Reactor Models
ACM, gPROMS
(Andrew Lee, Hosoo Kim)
Compression System Models
Aspen Plus, ACM, gPROMS
(John Eslick)
Other carbon capture models
Aspen Plus, ACM, gPROMS, GAMS
(J. Eslick, Juan Morinelly)
Oxy-combustion
GAMS, Aspen Plus, ACM, gPROMS,
(Alex Dowling)
New Sorbent Models
(Task 1, EFRC)
External Collaboration
(Prof. Phil Smith, ICSE)
Surrogate Models
(Alison Cozad)
Process Synthesis
Superstructure for Optimal Process Configurations
(Zhihong Yuan)
Simultaneous Superstructure Approach
Power, Heat, Mass Targeting
(Linlin Yang)
Black Box Optimization
(Hosoo Kim)
Heterogeneous Simulation-Based Optimization Framework
PC Plant Model
Compression System Model
Clean Gas to Stack
CO2 to Sequestration
ADS-001
RGN-001
SHX-01
SHX-02
CYC-001
CYC-002
GHX-001
CPR-002
LP Steam
Industry Specific Collaboration
(ADA)
Heat/Power Integration
Automated GAMS Formulation/Solution
(Murthy Konda)

Solid Sorbent Adsorber/Regenerator

Bubbling Fluidized Bed Adsorber



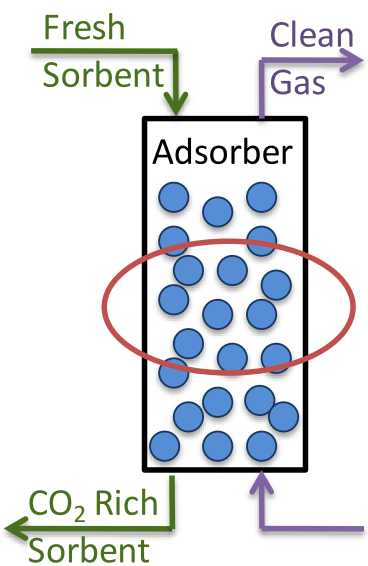
Moving Bed Regenerator



- Models function as adsorber or regenerator
- Predictive, 1-D models
- Implemented in AspenTech software

Methodology for Determining Optimal Process Configurations

Detailed model developed in commercial process simulation tool

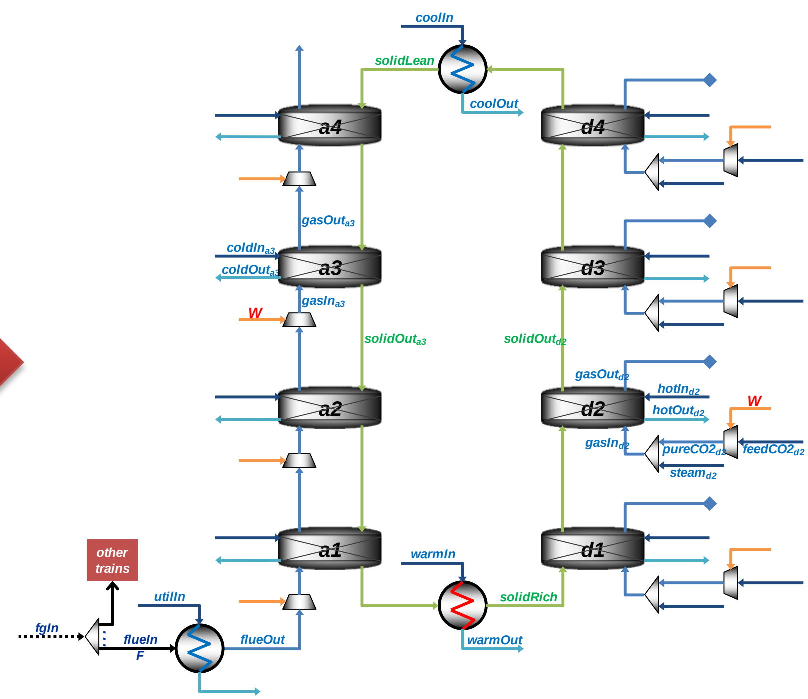


Develop Algebraic ROM

- **Sample points**
- **Build model**
- **Adaptive sampling** and **Model validation**
- **Done**

$$f(x)$$

Formulate and solve superstructure to determine optimal process configuration



YoungJung Chang, Alison Cozad, Hosoo Kim, Andrew Lee, Panagiotis Vouzis, N.V.S.N. Murthy Konda, A.J. Simon, Nick Sahinidis and David C. Miller, "Synthesis of Optimal Adsorptive Carbon Capture Processes." Paper 287c presented at *2011 AIChE Annual Meeting*, Minneapolis, MN, October 16-21, 2011.

Alison Cozad, YoungJung Chang, Nick Sahinidis and David C. Miller, "Optimization of Carbon Capture Systems Using Surrogate Models of Simulated Processes." Paper 134b presented at *2011 AIChE Annual Meeting*, Minneapolis, MN, October 16-21, 2011.

Alison Cozad, Nick Sahinidis and David C. Miller, "A Computational Methodology for Learning Low-Complexity Surrogate Models of Processes From Experiments or Simulations." Paper 679a presented at *2011 AIChE Annual Meeting*, Minneapolis, MN, October 16-21, 2011.

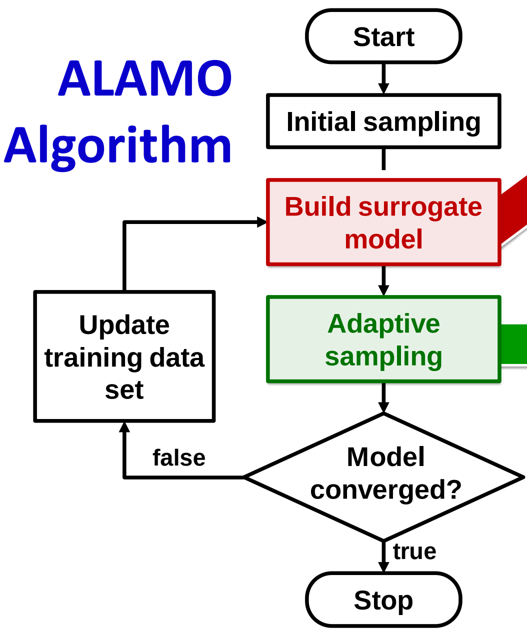
ALAMO Algorithm for Surrogate Model

ALAMO

Algebraic Model Checklist

- ✓ Accurate
- ✓ Tractable in algebraic optimization: Simple functional forms
- ✓ Generated from a minimal data set

ALAMO Algorithm



Build Surrogate Model

Goal: Build a model $\hat{z}(x)$ for each output $z(x)$.

Inputs: $x \in [x^l, x^u]^D$

Process block

Outputs: $z \in \mathbb{R}^K$

Model functional form

Step 1: Define a large set of potential basis functions

$$\hat{z}(x_1) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \beta_4 \frac{x_1}{x_2} + \beta_5 \frac{x_2}{x_1} + \beta_6 e^{x_1} + \beta_7 e^{x_2} + \dots$$

Step 2: Model reduction

$$\hat{z}(x) = \beta_0 + \beta_2 x_2 + \beta_5 \frac{x_2}{x_1} + \beta_7 e^{x_2}$$

Step 3: Determine model complexity

Information criterion = Accuracy + Complexity

Adaptive Sampling

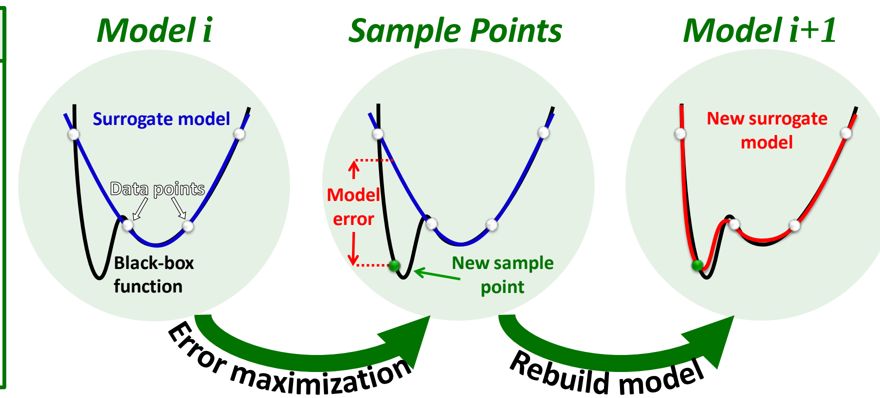
New samples

Error maximization

$$\max_x \left(\frac{z(x) - \hat{z}(x)}{z(x)} \right)^2$$

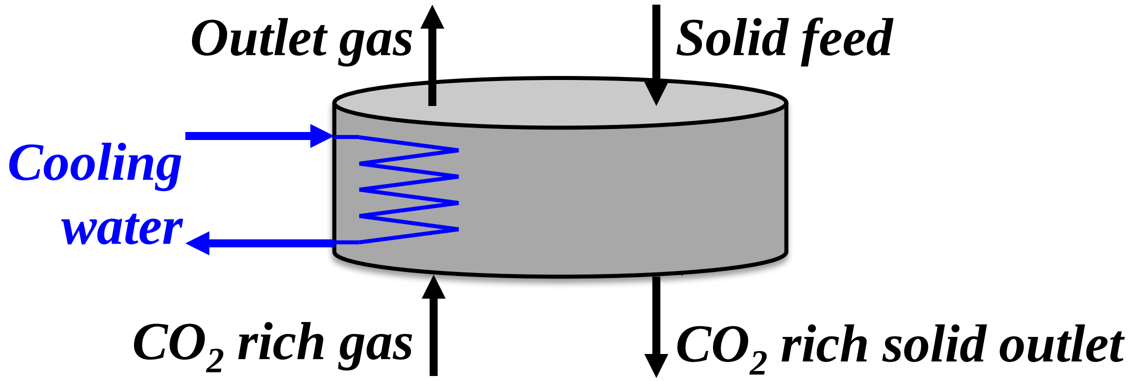
Simulation — Surrogate model

Search the problem space for areas of model inconsistency or model mismatch



BUBBLING FLUIDIZED BED

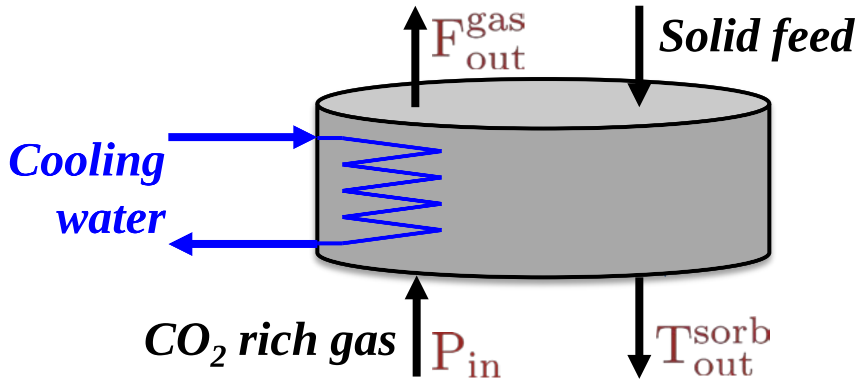
Bubbling fluidized bed adsorber diagram



- Model inputs (14 total)
  - Geometry (3)
  - Operating conditions (4)
  - Gas mole fractions (2)
  - Solid compositions (2)
  - Flow rates (4)

- *Model outputs (13 total)*
  - *Geometry required (2)*
  - *Operating condition required (1)*
  - *Gas mole fractions (2)*
  - *Solid compositions (2)*
  - *Flow rates (2)*
  - *Outlet temperatures (3)*
  - *Design constraint (1)*

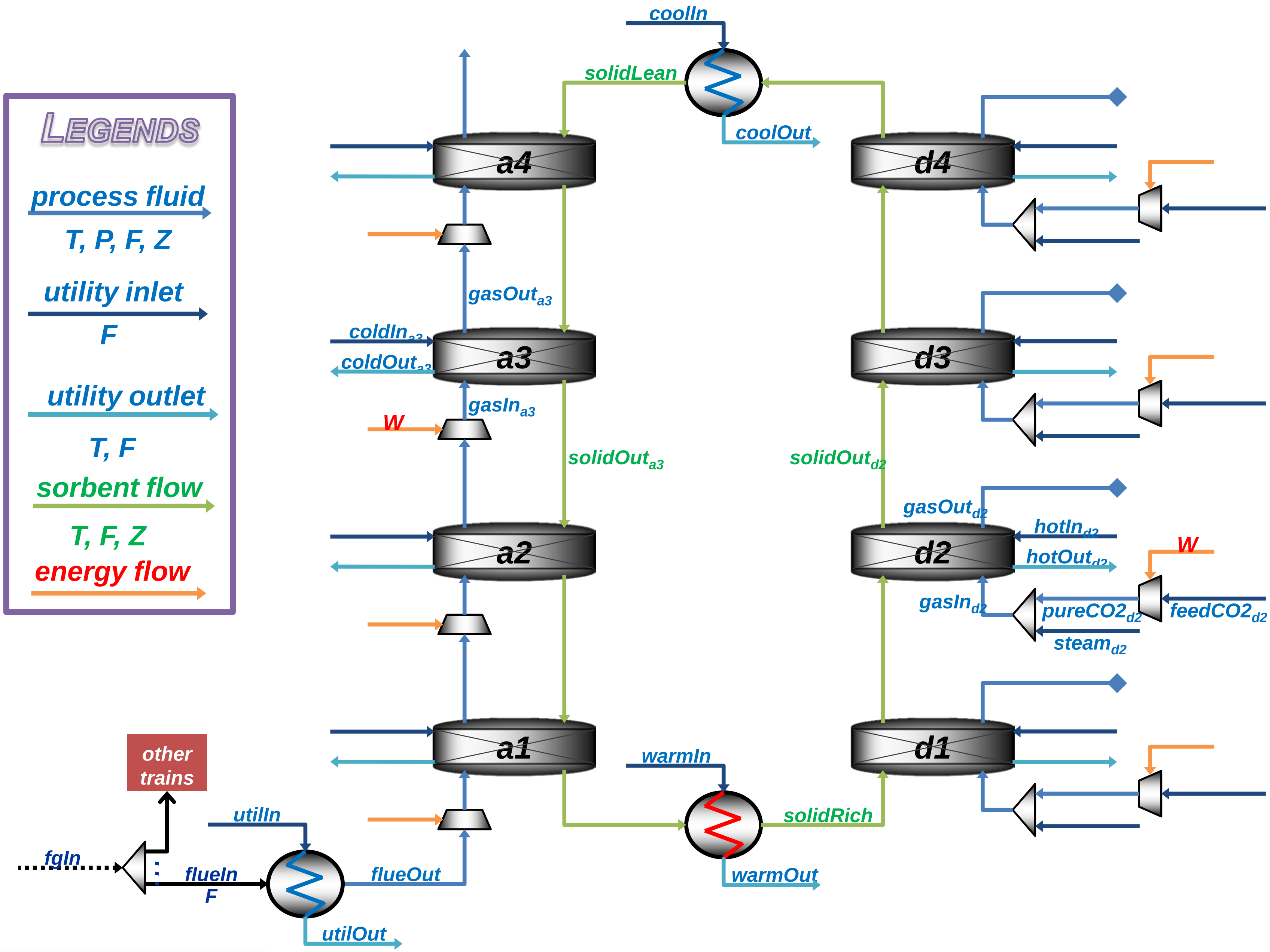
Example models



$$P_{in} = 1.0\,P_{out} + 0.0231\,L_b - 0.0187\,\ln(0.167\,L_b) - 0.00626\,\ln(0.667\,v_{gi}) - \frac{51.1\,xHCO3^{ads}_{in}}{F^{gas}_{in}}$$

$$T^{sorb}_{out} = 1.0\,T^{gas}_{in} - \frac{(1.77 \cdot 10^{-10})\;NX^2}{\gamma^2} - \frac{3.46}{NX\,T^{gas}_{in}\,T^{sorb}_{in}} + \frac{1.17 \cdot 10^4}{F^{sorb}\,NX\,xH2O^{ads}_{in}}$$

$$F^{gas}_{out} = 0.797\,F^{gas}_{in} - \frac{9.75\,T^{sorb}_{in}}{\gamma} - 0.77\,F^{gas}_{in}\,xCO2^{gas}_{in} + 0.00465\,F^{gas}_{in}\,T^{sorb}_{in} - 0.0181\,F^{gas}_{in}\,T^{sorb}_{in}\,xH2O^{gas}_{in}$$



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Optimization Formulation

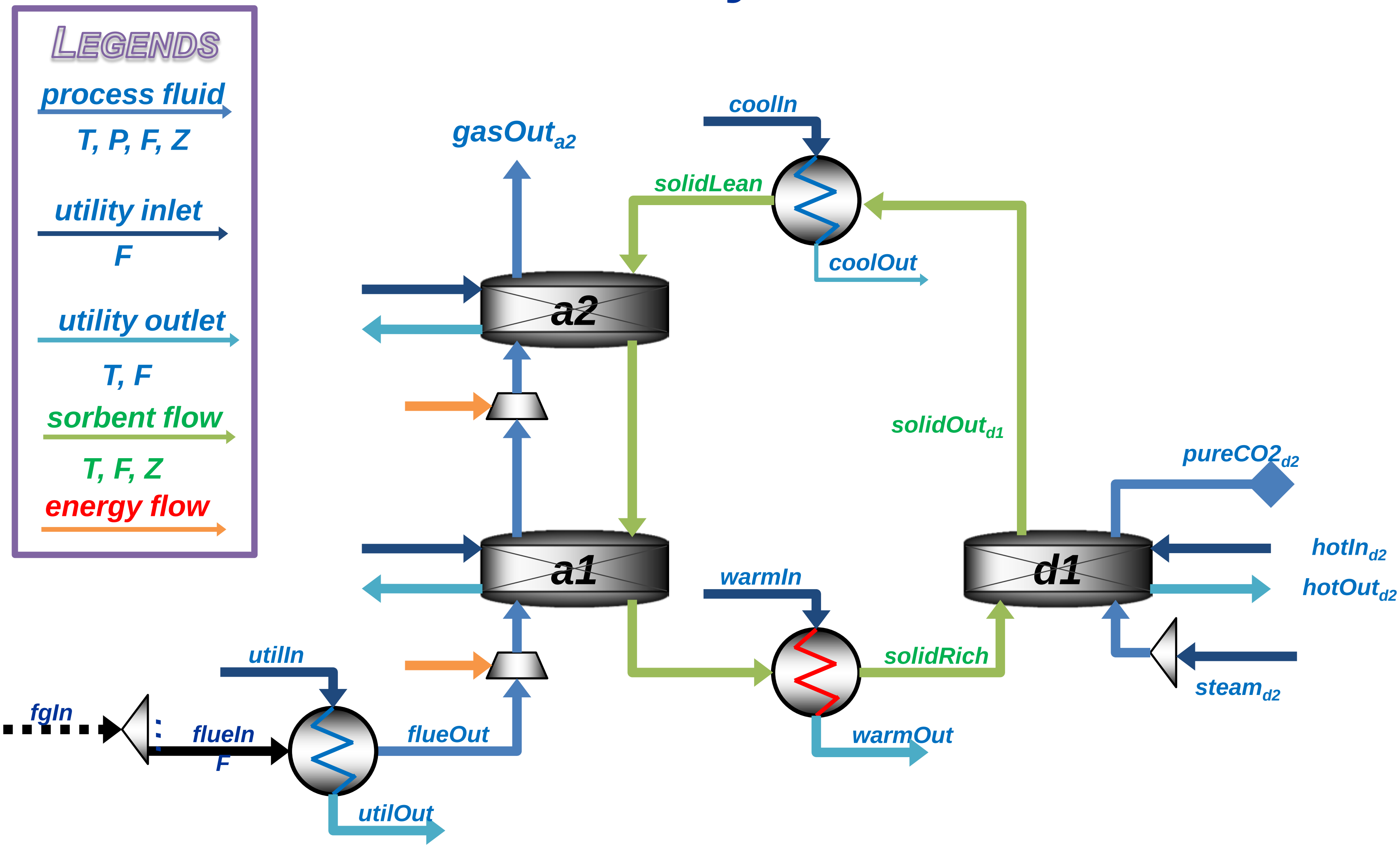
- Scenario:
  - Retrofit of new 650 MWe supercritical PC plant

- Requirement: 90% capture

- Objective: minimize Cost of Electricity
  - Function of
    - Parasitic energy requirements for capture & compression
      - Direct electricity use
      - Parasitic steam extraction
    - Capital cost of capture and compression systems
      - Literature correlations, hooks for proprietary data
    - Operating costs (fuel, labor, materials)
  - Assumes PC plant is fixed

- Formulated in GAMS, solved with BARON

Preliminary Results



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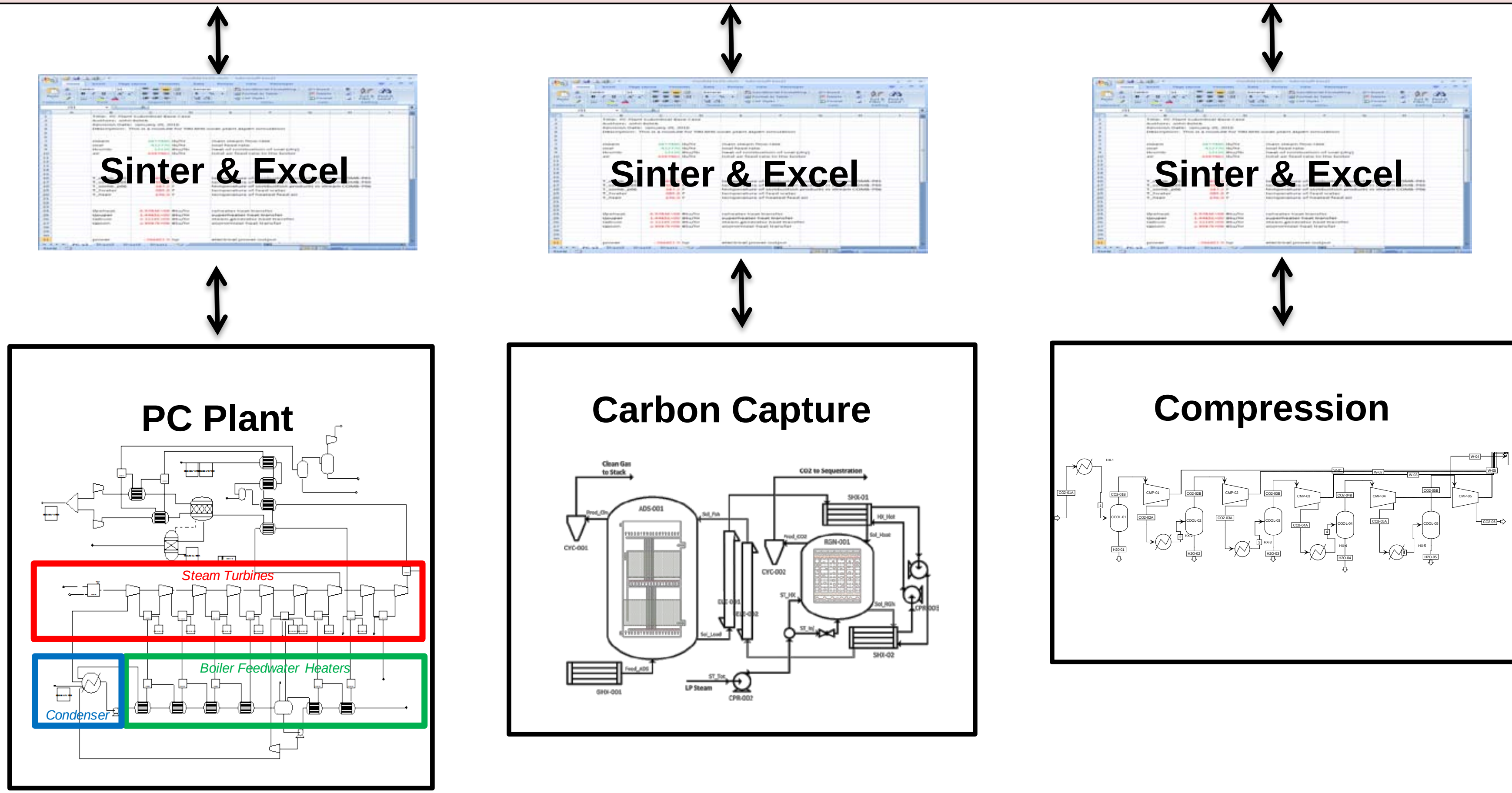
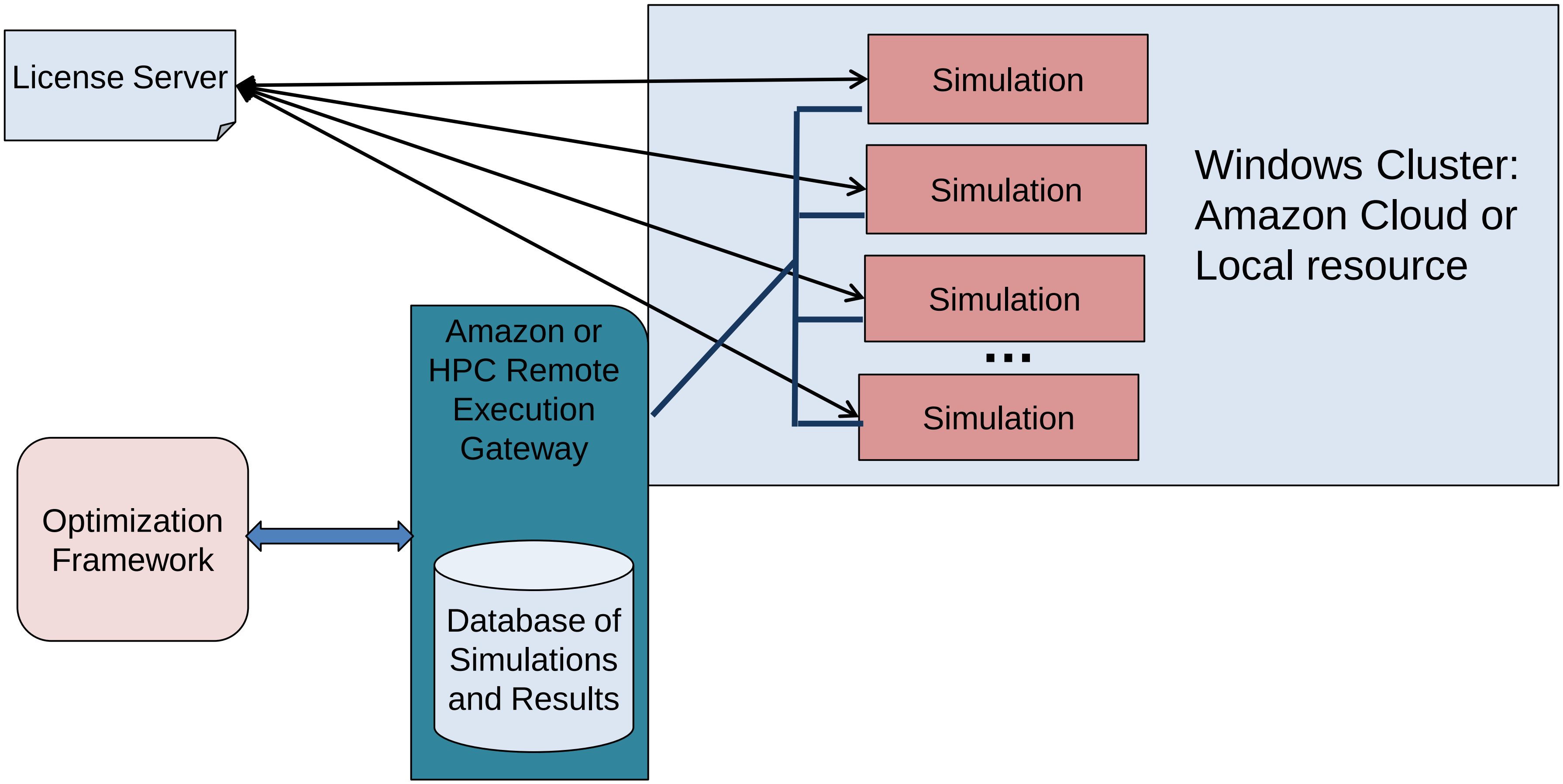
Heterogeneous Simulation-Based Optimization Framework

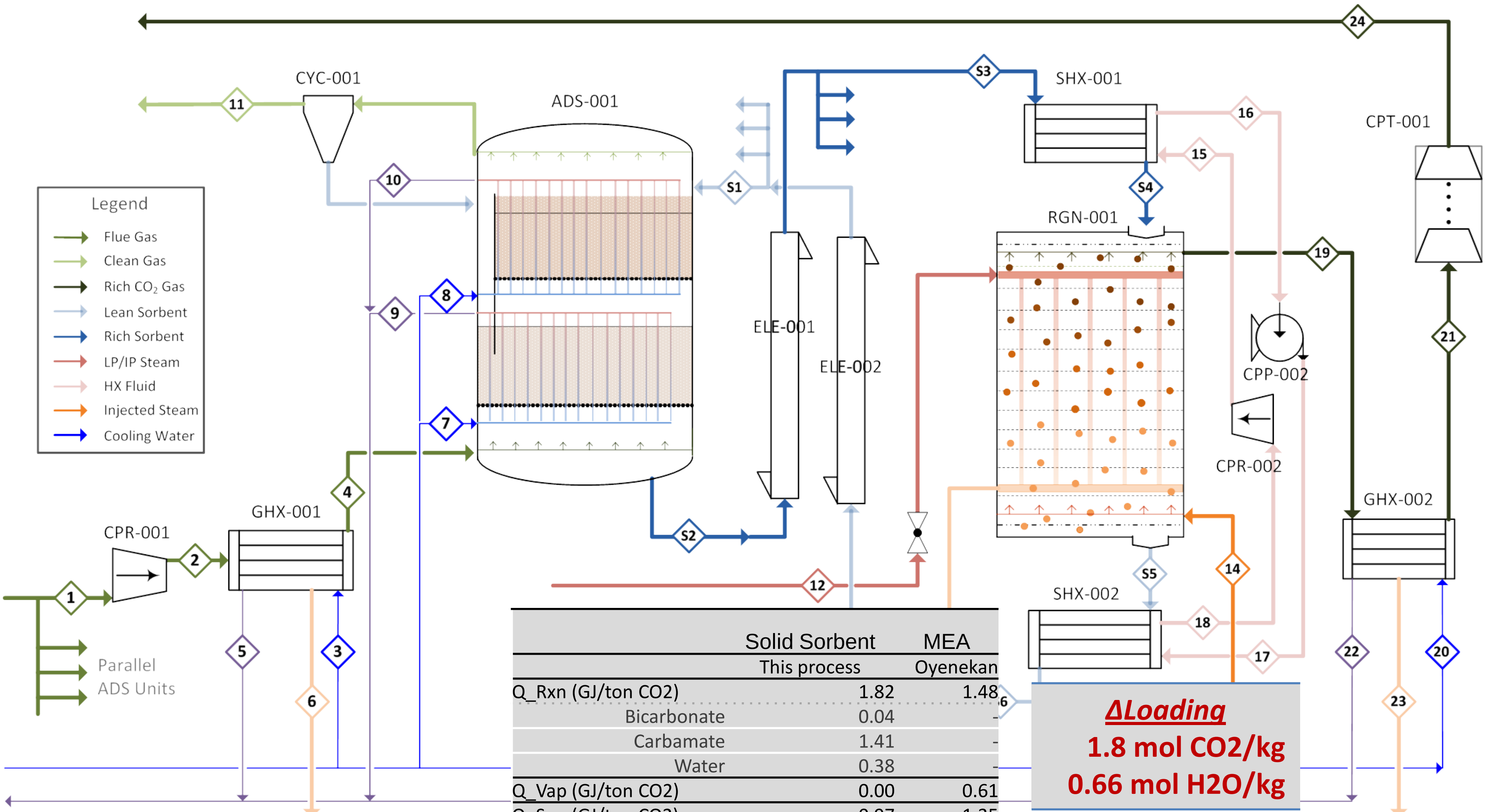


Enabling a Distributed Execution Environment



Hybrid Carbon Capture Process System (A650.1)

2 stage, counter-currently connected bubbling fluidized bed adsorber + moving bed regenerator



	Solid Sorbent This process	MEA Oyenekan
Q_Rxn (GJ/ton CO2)	1.82	1.48
Bicarbonate	0.04	-
Carbamate	1.41	-
Water	0.38	-
Q_Vap (GJ/ton CO2)	0.00	0.61
Q_Sen (GJ/ton CO2)	0.97	1.35
Total Q	2.79	3.44

ΔLoading

1.8 mol CO2/kg

0.66 mol H2O/kg

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Conclusions

- Approach for combining
  - Simulator-based models
  - Advanced optimization tools
    - ALAMO
    - Superstructure for determining optimal configuration
    - Derivative-free optimization (DFO)
- Resulting framework for optimal design
- Developed initial design for further demonstration of CCSI Toolset

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