CCSI
Carbon Capture Simulation Initiative

Computational Tools for Accelerating Carbon Capture Process Development

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4 June 2013

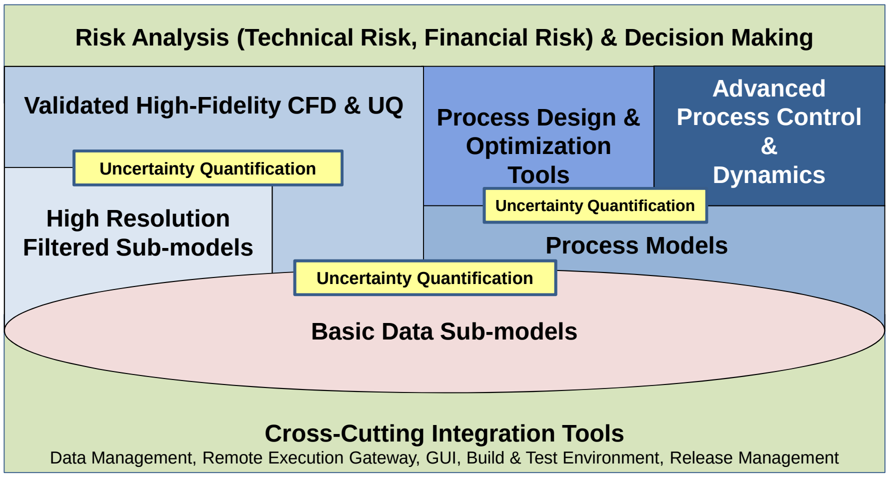
U.S. DEPARTMENT OF ENERGY

CCSI For Accelerating Technology Development

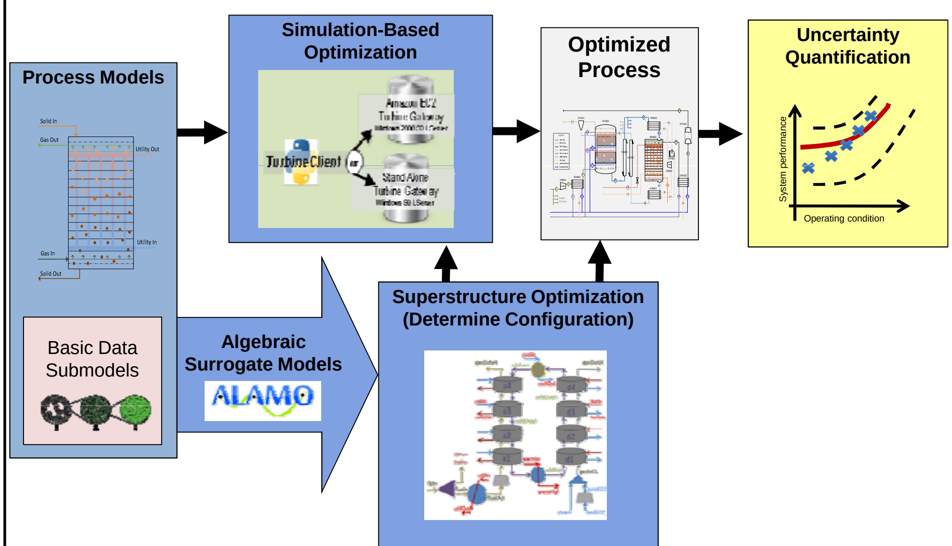
Identify promising concepts → Reduce the time for design & troubleshooting → Quantify the technical risk, to enable reaching larger scales, earlier → Stabilize the cost during commercial deployment

National Labs	Academia	Industry
Berkeley Lab, Pacific Northwest National Laboratory, NETL, Los Alamos National Laboratory, Lawrence Livermore National Laboratory	Carnegie Mellon, Princeton University, West Virginia University, Boston University, The University of Texas at Austin, The University of Utah Institute for Clean and Secure Energy	ADA, Alstom, B&W, GE, EPRI, Fluor, Southern Company, Phillips 66, AEP American Electric Power, Chevron, Edison, ExxonMobil, URS, Air Products, Eastman, ANSYS, AspenTech, Invensys, PSE

Advanced Computational Tools to Accelerate Next Generation Technology Development



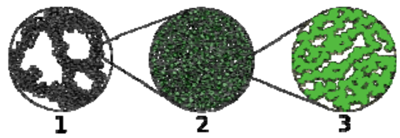
Tools to develop an optimized process using rigorous models

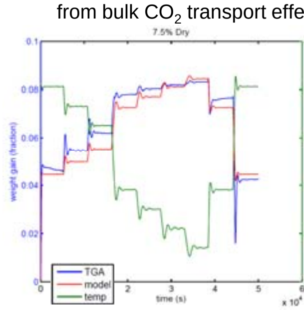


PEI-Impregnated Silica Sorbent Reaction Model

- A general lumped kinetic model, quantitatively fit to TDA data, needed for initial CFD and process simulations
- High-fidelity model:
  - Sorbent microstructure broken down into three length scales
  - Separate treatment of gas-phase and polymer-phase transport
  - Accurately describes TGA features arising from bulk CO_2 transport effects

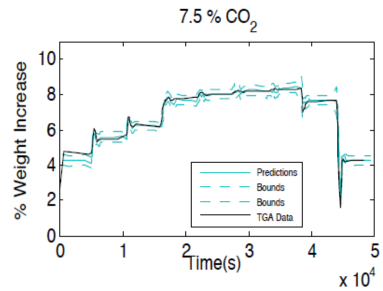
$$2R_2NH + CO_2(gas) \rightleftharpoons R_2NCO_2^- + R_2NH_2^+$$
$$R_2NH + H_2O(phys) + CO_2(gas) \rightleftharpoons HCO_3^- + R_2NH_2^+$$
$$H_2O(gas) \rightleftharpoons H_2O(phys)$$





(left) lumped kinetic fit to experimental TGA for NETL-32D sorbent

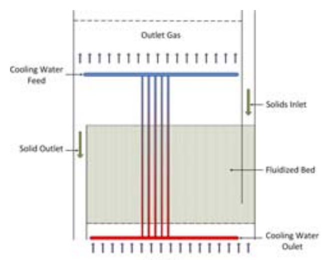
(right) calibrated model with discrepancy and error bounds



Solid Sorbent System Models

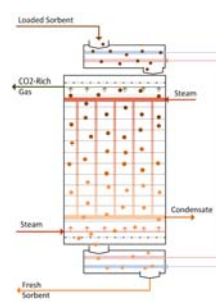
Bubbling Fluidized Bed (BFB) Models

- Flexible BFB models with immersed heat exchangers have been developed to be used as adsorber or regenerator, as needed, with varying locations for solids inlet and outlet streams
- Any number of BFB adsorbers and/or regenerators can be connected in series and/or in parallel depending on the user requirements
- A 2-stage adsorption model with customized variables suitable for incorporating UQ has been developed

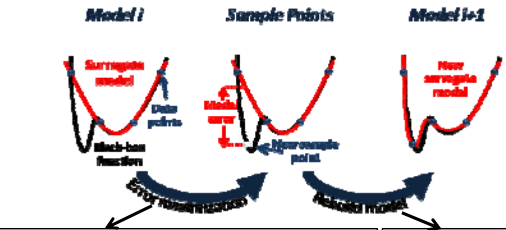


Moving Bed (MB) Models

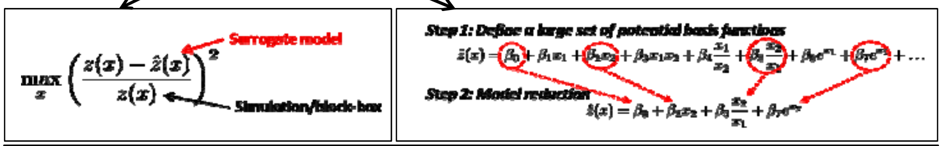
- External resistance to mass transfer has been modeled. This is particularly important in the regenerator model due to the high operating temperature.
- Heat exchanger model, mass and heat transfer coefficients, boundary conditions, temperature specifications, and properties models are revisited for better model accuracy.



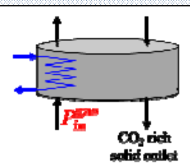
Automated Learning of Algebraic Models for Optimization



For building accurate, simple algebraic surrogate models of simulated processes



Example Model: BFB Adsorber Inlet Gas Pressure



- ACM Simulation
- >900 terms possible
- 14 input variables
- 0.13% error

$$\hat{P}_{in}^{gas} = P_{out}^{gas} + 0.019\, L_b + 0.0055\sqrt{D_T}$$

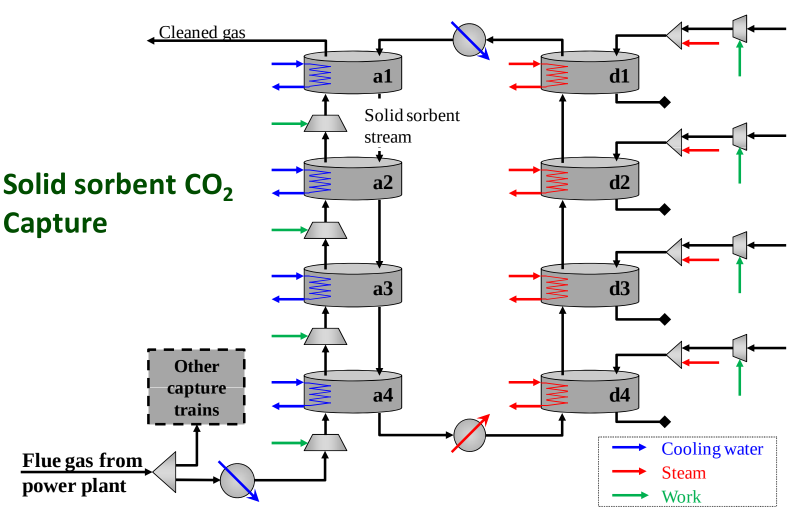
Pressure drop across length of bed

Proportional to outlet pressure

Pressure drop due to bed diameter

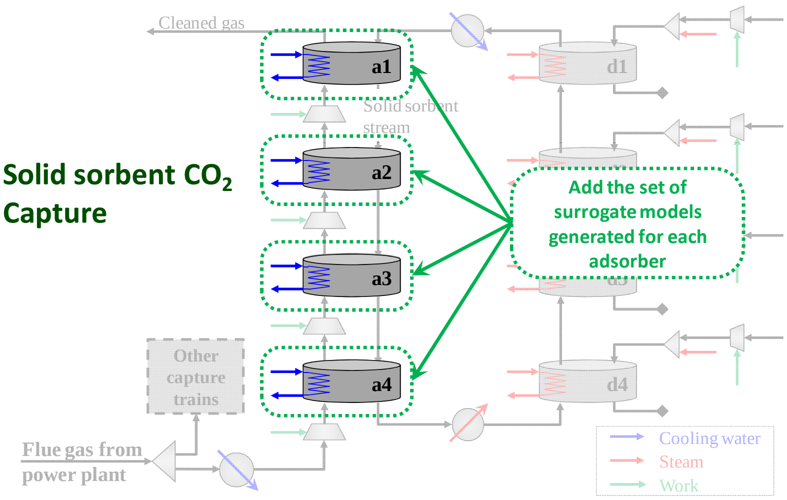
Superstructure Formulation & Optimization

Solid sorbent CO_2 Capture

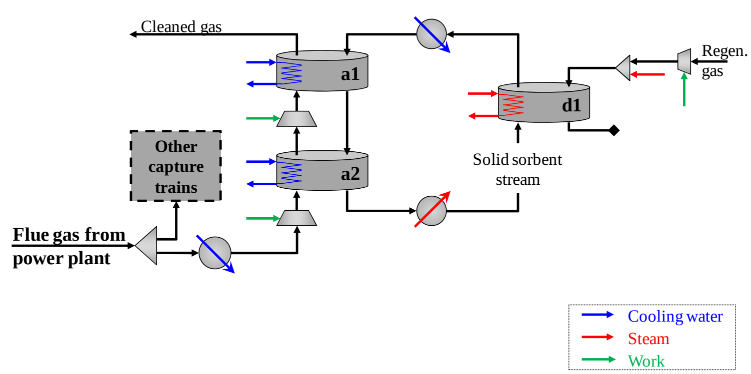


Insert Algebraic Surrogates into Superstructure

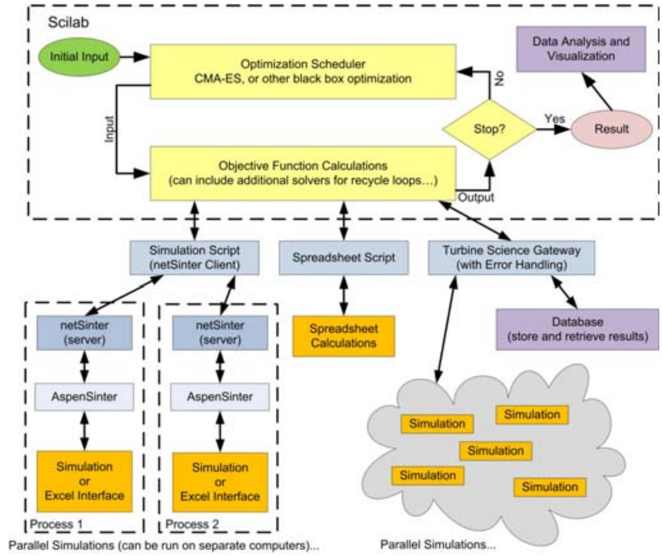
Solid sorbent CO_2 Capture



Initial Superstructure Solution



Simulation-Based Optimization: Verify Solution



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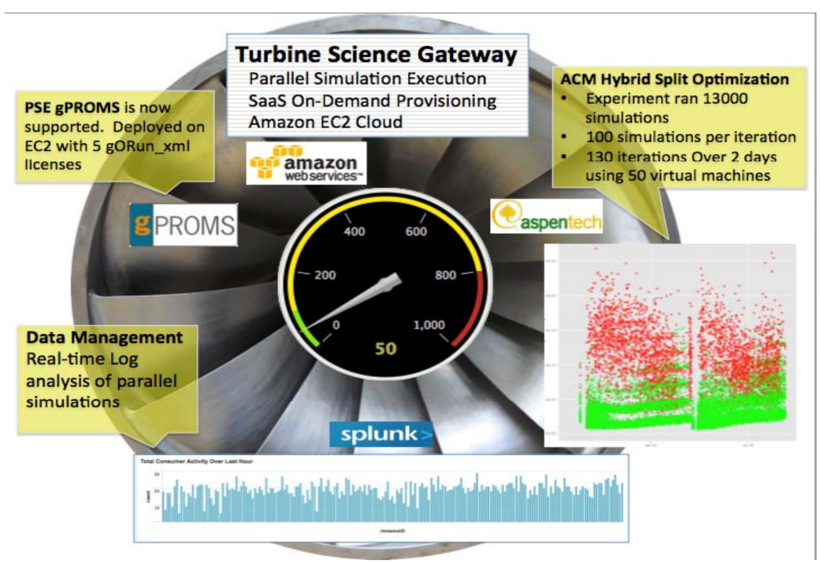
Turbine Science Gateway



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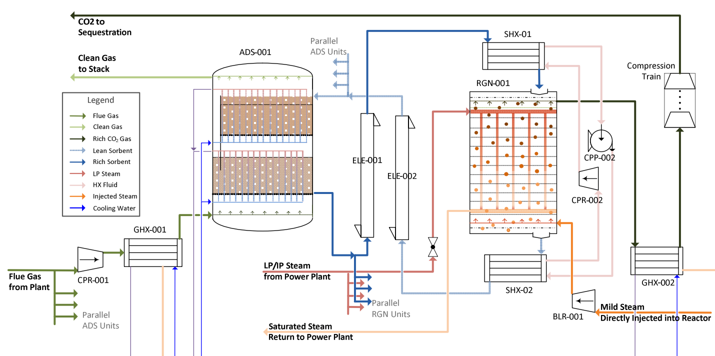
Decision Variables

Input Variable	Lower Bound	Upper Bound
Adsorber Diameter (m)	7	10
Top & Bottom Adsorber Bed Depth (m)	4	10
Top & Bottom Adsorber Heat Exchanger Tube Diameter (m)	0.01	0.05
Top & Bottom Adsorber Heat Exchanger Tube Pitch (m)	0.1	0.2
Top & Bottom Adsorber Cooling Water Flowrate (kmol/hr)	30,000	60,000
Sorbent Flowrate per Adsorber (kg/hr)	350,000	600,000
Gas Pre-Cooler Temperature (^{o}C)	40	60
Regenerator Height (m)	3	7
Regenerator Diameter (m)	6	10
Regenerator Heat Exchanger Tube Diameter (m)	0.01	0.05
Regenerator Direct Steam Injection Rate (kmol/hr)	900	1400
Regenerator Heat Exchanger Steam Flowrate (kmol/hr)	2,500	5,000

Optimized Process Developed using CCSI Toolset



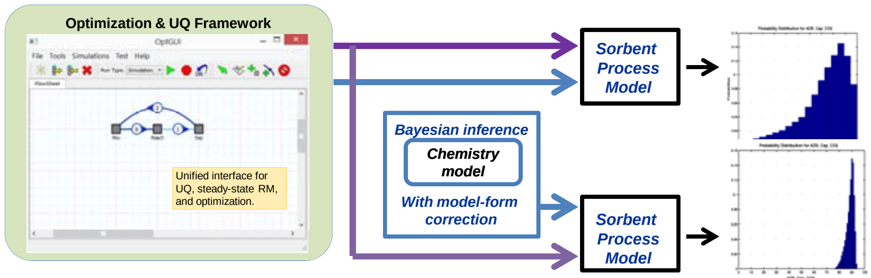
ΔLoading
1.8 mol CO2/kg
0.66 mol H2O/kg

	ADS-001A	ADS-001B
Diameter (m)	9.748	
Bed Depth (m)	7.232	4.854
Total HX Area (m^2)	1733.7	941.3

	RGN-001
Diameter (m)	7.147
Height (m)	4.592
Total HX Area (m^2)	1573.1

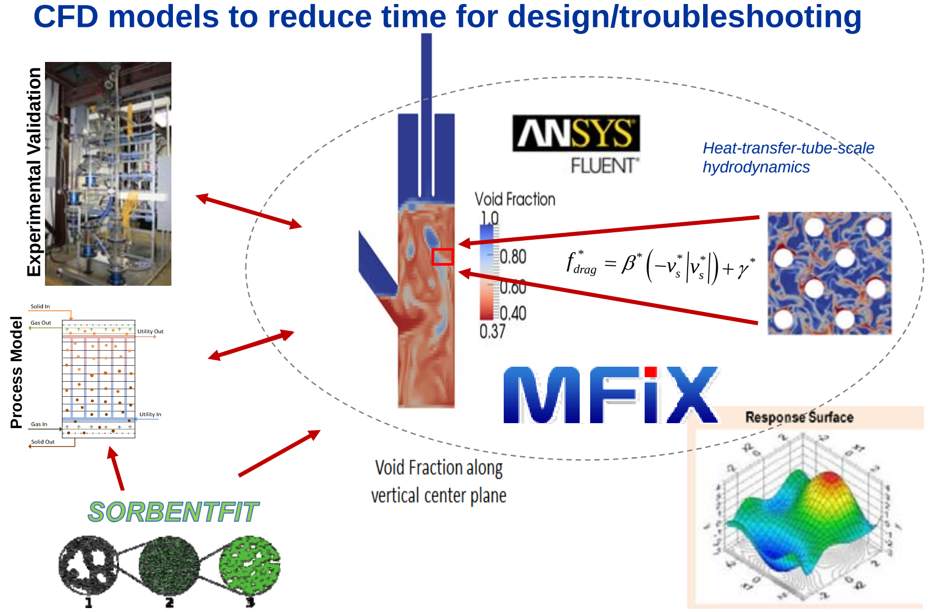
	Solid Sorbent	MEA[27] (Δ10°C HX)	MEA[27] (Δ5°C HX)
Q_Rxn (GJ/tonne CO2)	1.82	1.48	1.48
Q_Vap (GJ/tonne CO2)	0	0.61	0.74
Q_Sen (GJ/tonne CO2)	0.97	1.35	0.68
Total Q	2.79	3.44	2.90

Multi-Scale Uncertainty Quantification Framework



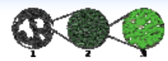
- **UQ for basic data models**
  - Bayesian UQ methodology
  - Integration of model form discrepancy into process & CFD models
- **UQ for CFD models**
  - Adaptive sampling capability for RM/UQ
  - Bayesian calibration capability
  - UQ of discrepancy between CFD/process models
- **UQ for process models**
  - Integration with optimization platform
  - Optimization under uncertainty

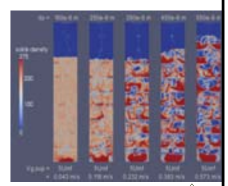
CFD models to reduce time for design/troubleshooting



CCSI Deploys Initial Computational Toolset

- Initial toolset released Oct. 2012, 1 year ahead of schedule due to industry request for early access
  - 3 companies have already licensed
  - Other companies pursing license
- Additional releases planned for Fall 2013, 2014, 2015.
- Final release planned for Jan. 2016





Risk Analysis (Technical Risk, Financial Risk) & Decision Making

Validated High-Fidelity CFD & UQ

Uncertainty Quantification

High Resolution Filtered Sub-models

Process Design & Optimization Tools

Advanced Process Control & Dynamics

Uncertainty Quantification

Process Models

Uncertainty Quantification

Basic Data Sub-models

Cross-Cutting Integration Tools

Data Management, Remote Execution Gateway, GUI, Build & Test Environment, Release Management