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Carbon Capture Simulation Initiative

US Department of Energy's Carbon Capture Simulation Initiative: Computational Tools for Accelerating Process Development

Debangsu Bhattacharyya
Department of Chemical Engineering
West Virginia University
Process Modeling Team Lead, CCSI

David C. Miller
U.S. Department of Energy
National Energy Technology Laboratory
Technical Lead, CCSI

WestVirginiaUniversity

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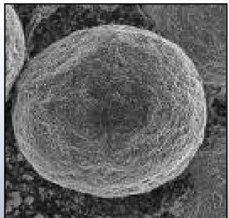
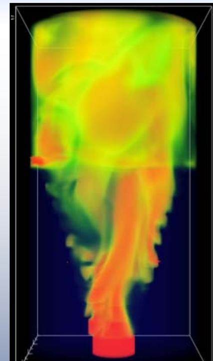
U.S. DEPARTMENT OF ENERGY

CCSI For Accelerating Technology Development

Carbon Capture Simulation Initiative






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

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Academia

Carnegie Mellon
Princeton University
West Virginia University
Boston University
The University of Texas at Austin
Institute for Clean and Secure Energy, The University of Utah

Industry

ADA Environmental Solutions
ALSTOM
B&W thebabcock&wilcoxcompany
GE
EPRI Electric Power Research Institute
Fluor
Southern Company
Phillips 66
AEP American Electric Power
Chevron
Southern California Edison
An EDISON INTERNATIONAL Company
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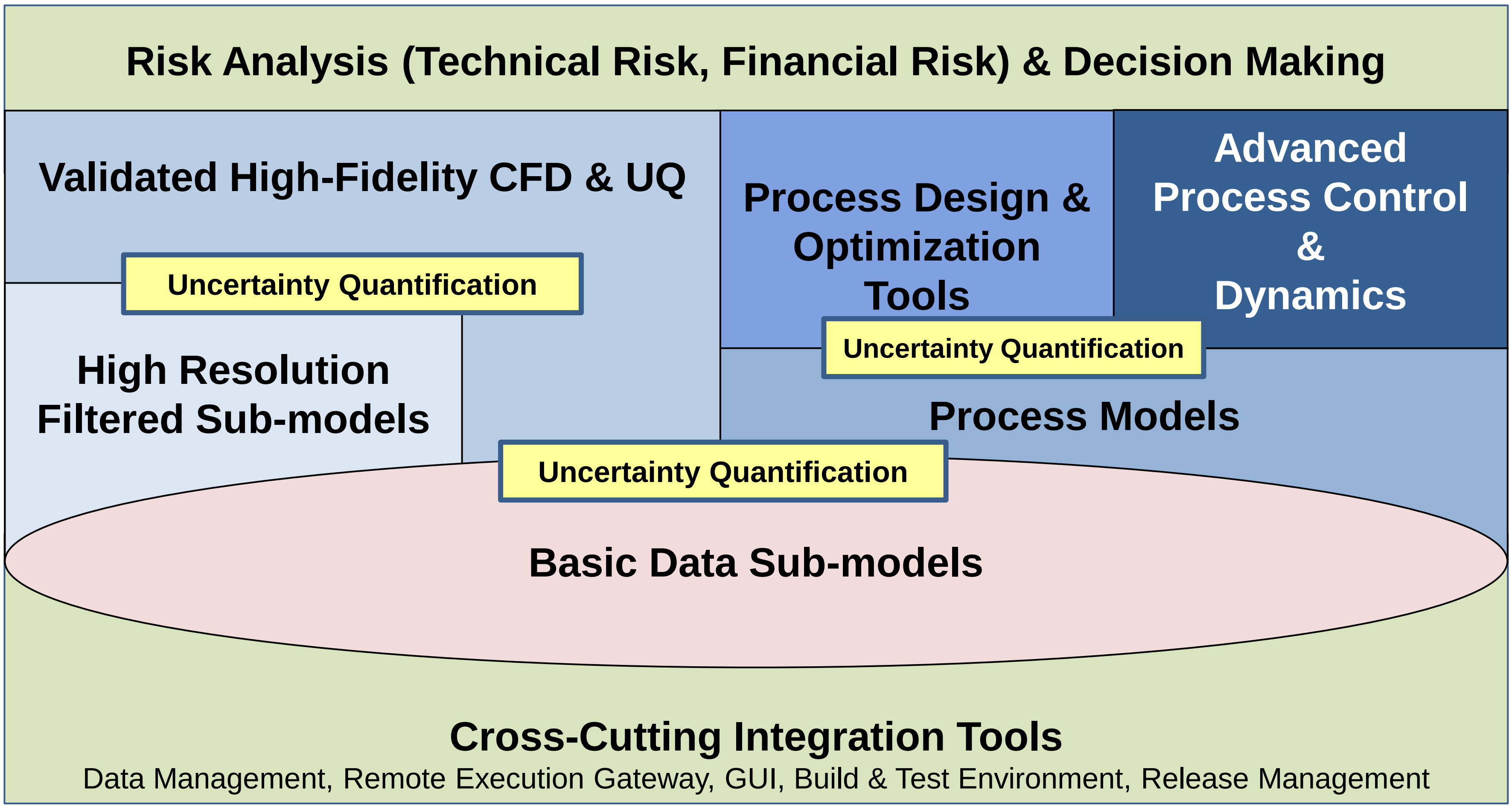
Advanced Computational Tools to Accelerate Next Generation Technology Development



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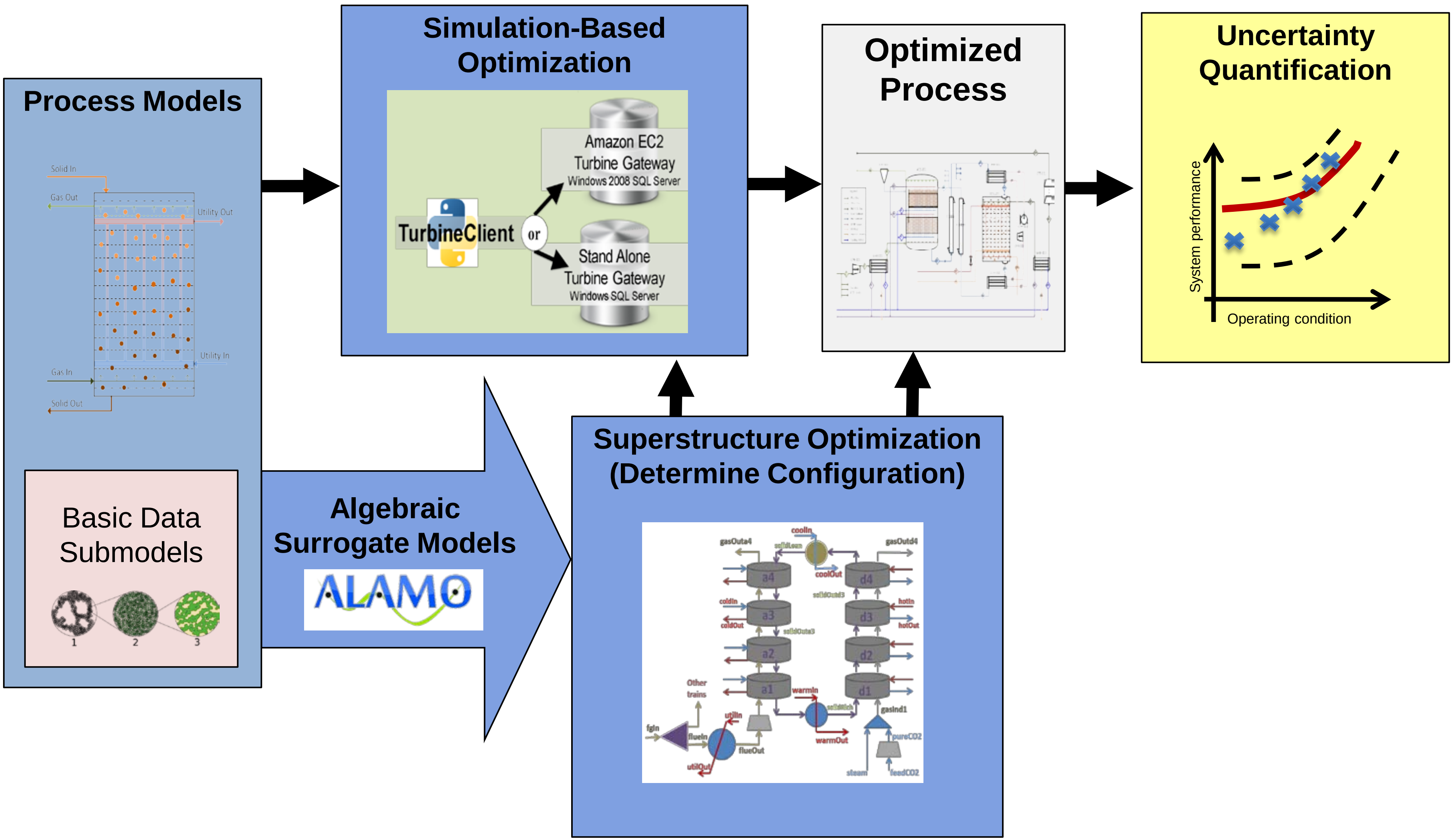
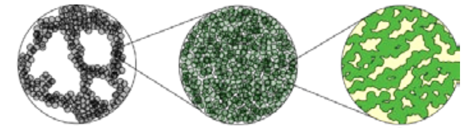
Tools to develop an optimized process using rigorous models



Basic Data Submodel

SORBENTFIT



$$H_2O_{(g)} \leftrightarrow H_2O_{(phys)}$$

$$2R_2NH + CO_{2,(g)} \leftrightarrow R_2NH_2^+ + 2R_2NCO_2^-$$

$$R_2NH + CO_{2,(g)} + H_2O_{(phys)} \leftrightarrow R_2NH_2^+ + HCO_3^-$$

$$r_{1,r,i} = k_{1,r,i}\left(\frac{P_i C_{r,H_2O,i}}{C_{r,t,i}} - \frac{n_{r,H_2O,i}}{K_{1,r,i}}\right)$$

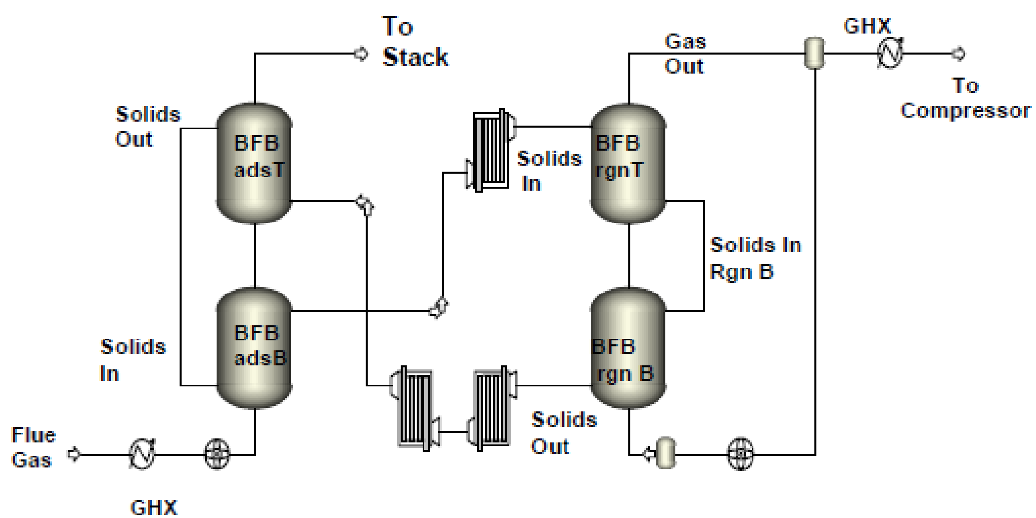
$$r_{2,r,i} = k_{2,r,i}\left(\left[1 - 2\frac{n_{r,carb,i}}{n_v} - \frac{n_{r,bicarb,i}}{n_v}\right] n_{r,H_2O,i}\left[\frac{P_i C_{r,CO_2,i}}{C_{r,t,i}}\right] - \left[\frac{\left\{\frac{n_{r,carb,i}}{n_v} + \frac{n_{r,bicarb,i}}{n_v}\right\} n_{r,bicarb,i}}{K_{2,r,i}}\right]\right)$$

$$r_{3,r,i} = k_{3,r,i}\left(\left[1 - 2\frac{n_{r,carb,i}}{n_v} - \frac{n_{r,bicarb,i}}{n_v}\right]^2 \left[\frac{P_i C_{r,CO_2,i}}{C_{r,t,i}}\right] - \left[\frac{\left\{\frac{n_{r,carb,i}}{n_v} + \frac{n_{r,bicarb,i}}{n_v}\right\} n_{r,carb,i}}{K_{3,r,i}}\right]\right)$$

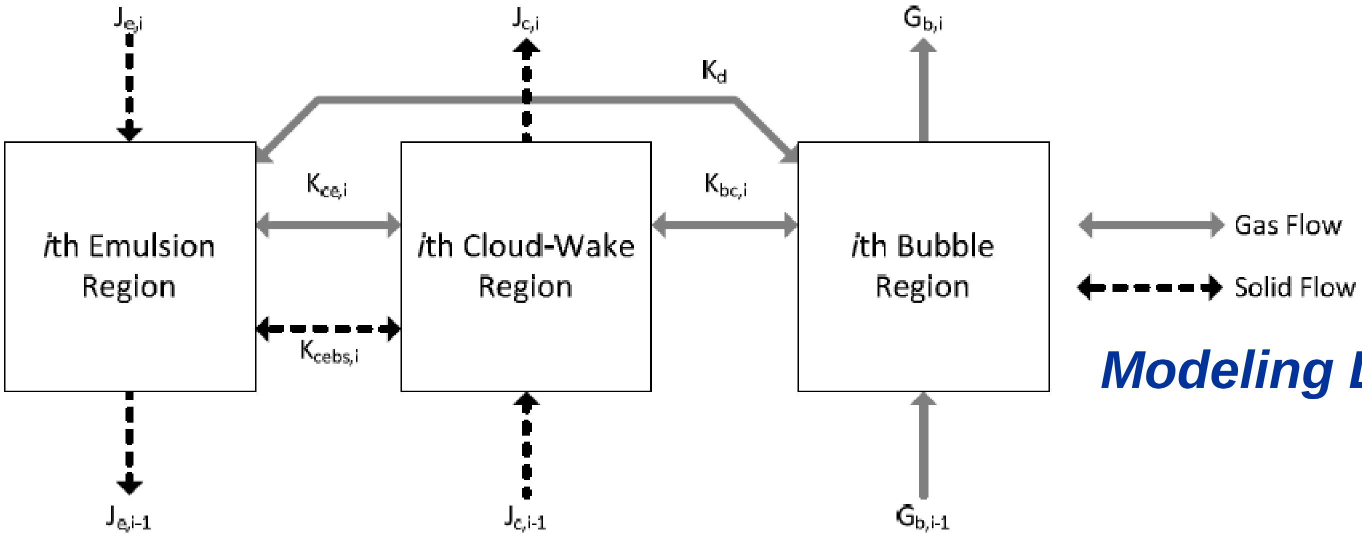
Lee et al. A model for the Adsorption Kinetics of CO_2 on Amine-Impregnated Mesoporous Sorbents in the Presence of Water, 28th International Pittsburgh Coal Conference 2011, Pittsburgh, PA, USA.

Development of Bubbling Fluidized Bed Model

- 1-D two-phase pressure-driven non-isothermal dynamic model of a solid-sorbent CO_2 capture in a two-stage bubbling fluidized bed reactor system.
- Models are flexible such that it can be used as an adsorber or regenerator
- Embedded cooler/heater depending on the application
- Flexible configuration- solids can enter/leave at/from the top or bottom
- A 2-stage adsorption model with customized variables suitable for incorporating UQ has been developed



MODEL DEVELOPMENT



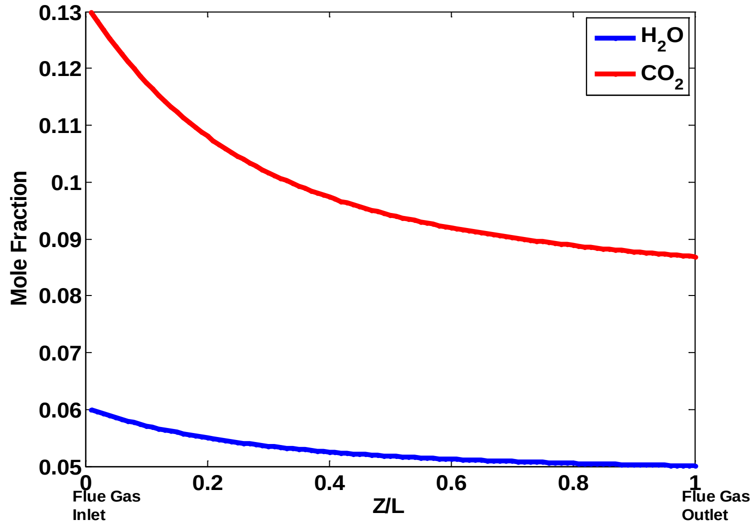
Modeling Domain*

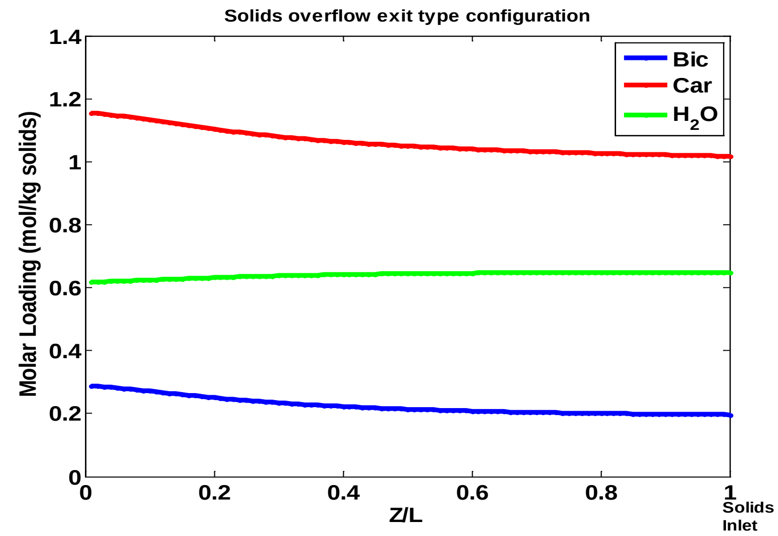
- Gaseous species : CO_2, N_2, H_2O
- Solid phase components: bicarbonate, carbamate, and physisorbed water.
- Transient species conservation and energy balance equations for both gas and solid phases in all three regions.

**Lee, A.; Miller, D. A One-Dimensional (1-D) Three Region Model for a Bubbling Fluidized Bed Adsorber. Ind. Eng. Chem. Res. 52, 469-484, 2013*

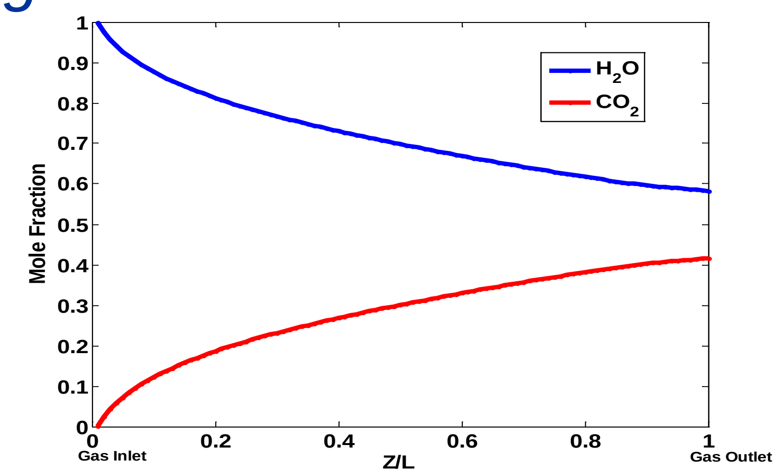
Bubbling Bed Model : Results

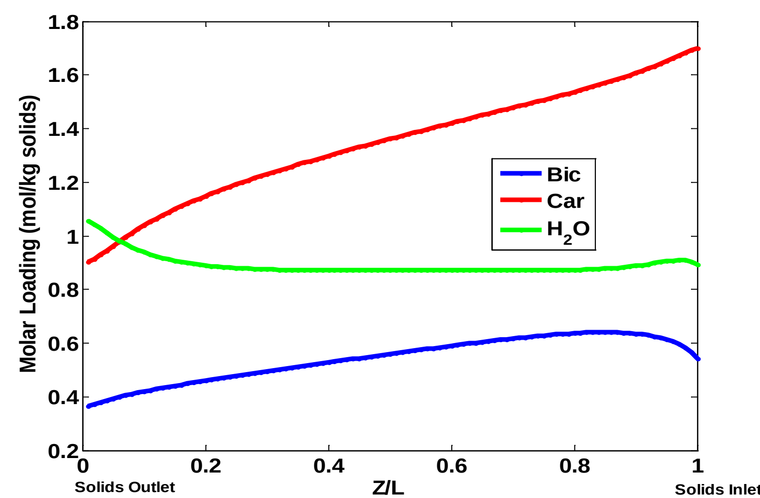
Adsorber





Regenerator





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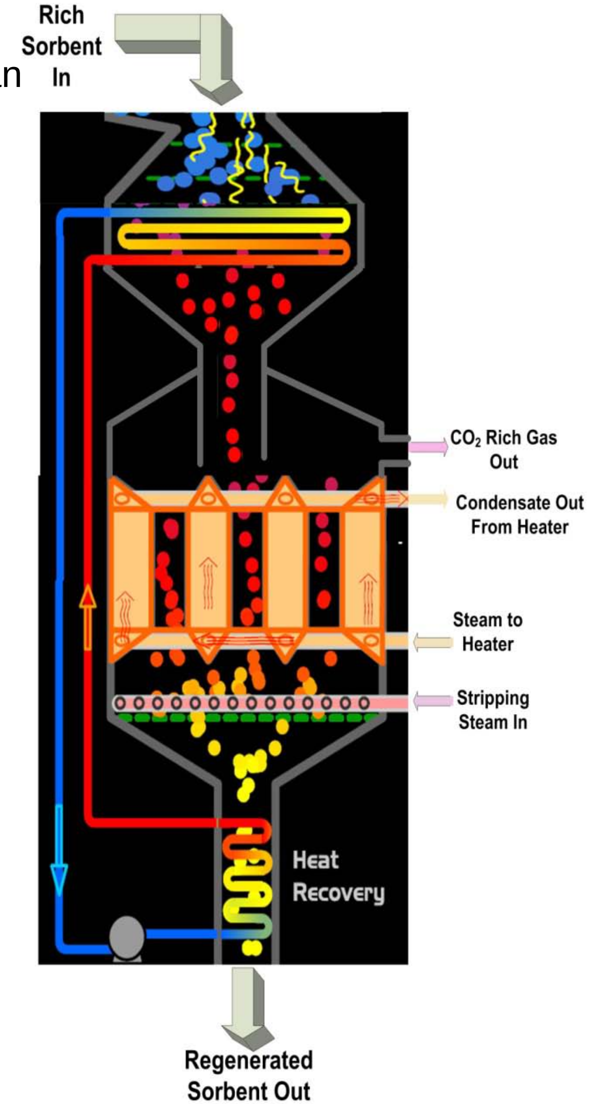
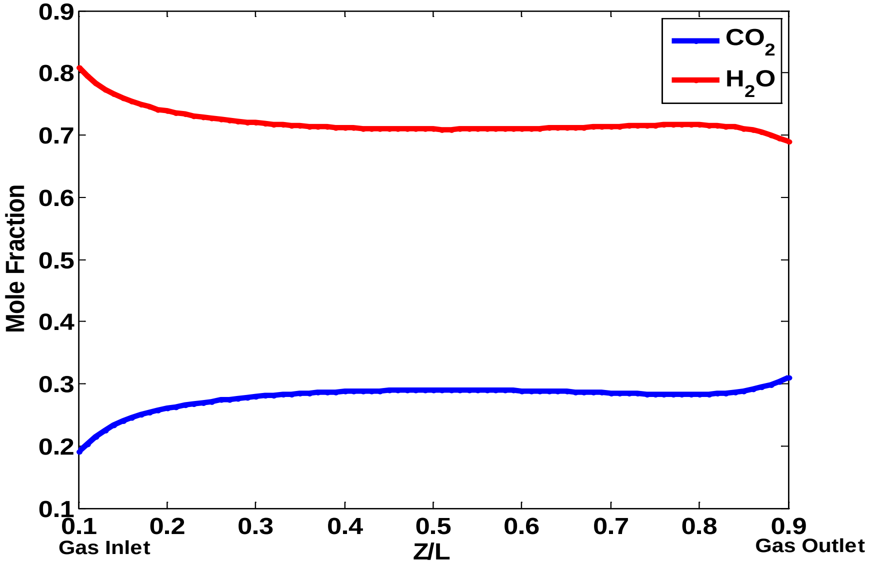
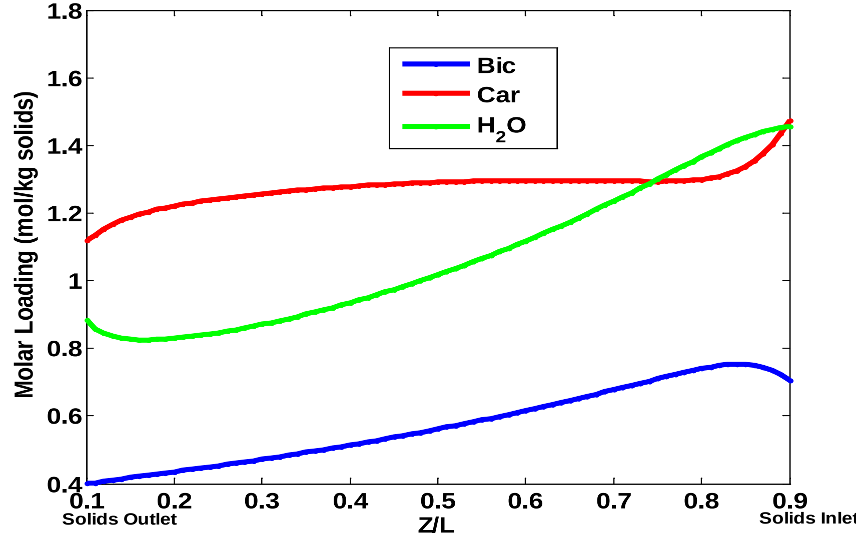
Development of Moving Bed Model

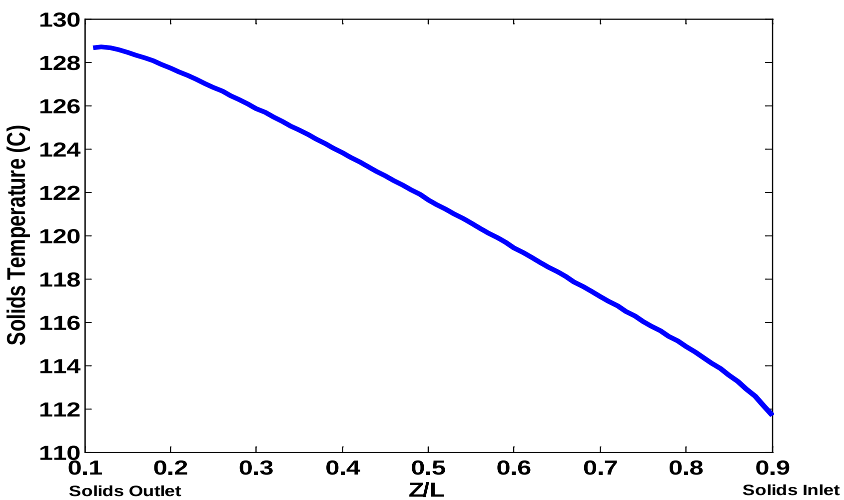
- A 1-d two-phase model of the moving bed model with embedded heat exchan mainly for regenerator
- Integrated pre and post-heat exchangers are considered for heat recovery
- Gas and solids flows are modeled by plug flow model with axial dispersion
- For pressure drop calculation, a modified Ergun equation by using the slip velocity between the solids and gas is used instead of the superficial fluid velocity
- Energy balance equations consider heat transfer between solid and gas and tube wall and the mixed phase
- Heat transfer coefficient between the mixed phase and the tube wall is calculated by a modified packet-renewal theory
- Bed hydrodynamics are described by analogy to fixed bed and fluidized bed systems
- Reaction kinetics are similar to the bubbling bed model

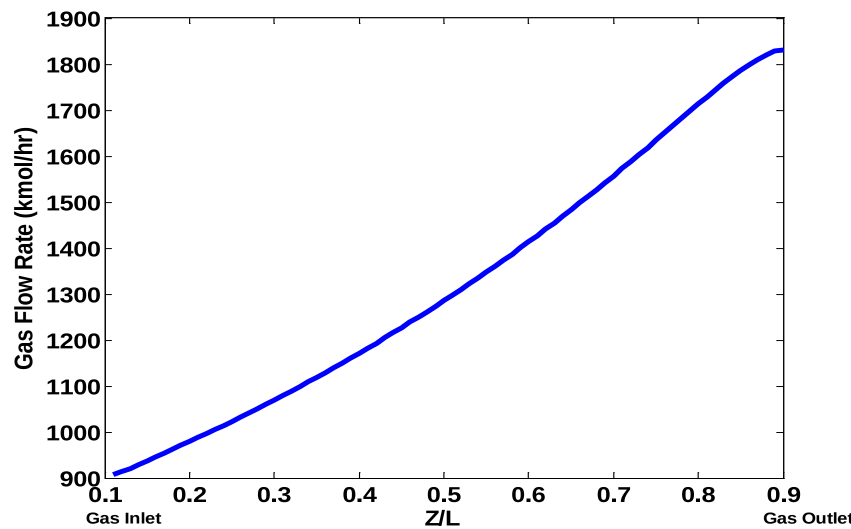


Moving Bed Regenerator: Results









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Solid Sorbent Models: Balance of the Plant

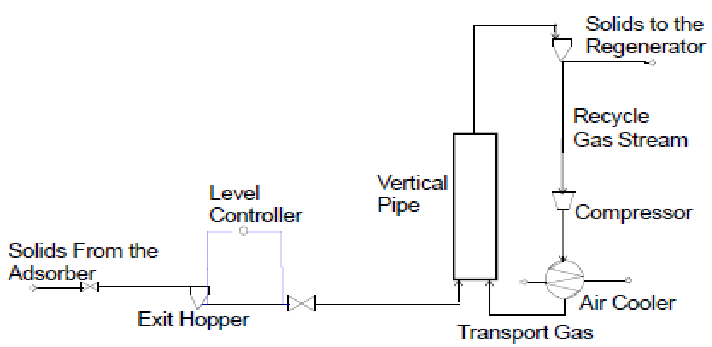
Heat-Recovery System

- Dynamic model of heat recovery system including pre and post-heat exchangers has been completed

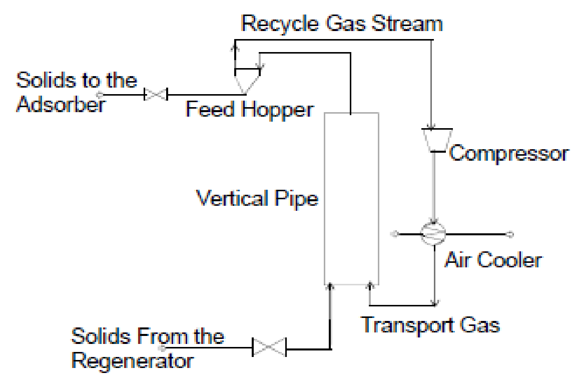
Solids Transport

- Model of pneumatic transport system has been completed by considering various options for transport gas with the design objective of minimizing auxiliary power consumption

Adsorber to Regenerator

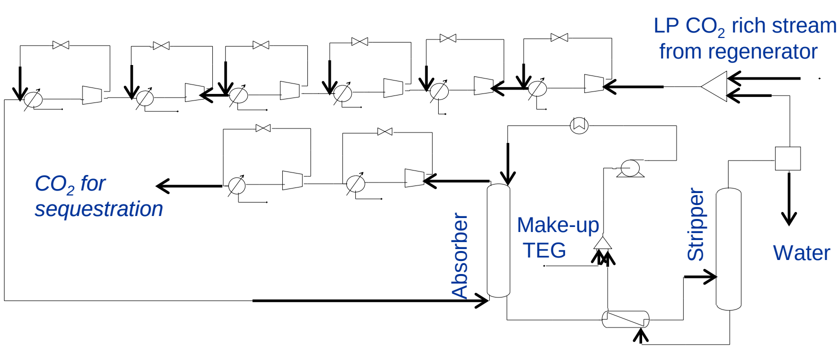


Regenerator to Adsorber



CO_2 Compression System

- Multi-stage integral gear compressor with inter-stage coolers, recycle valves
- Glycol absorption system modeled for moisture control in the sequestration-ready CO_2
- Typical performance curves obtained from a commercial vendor



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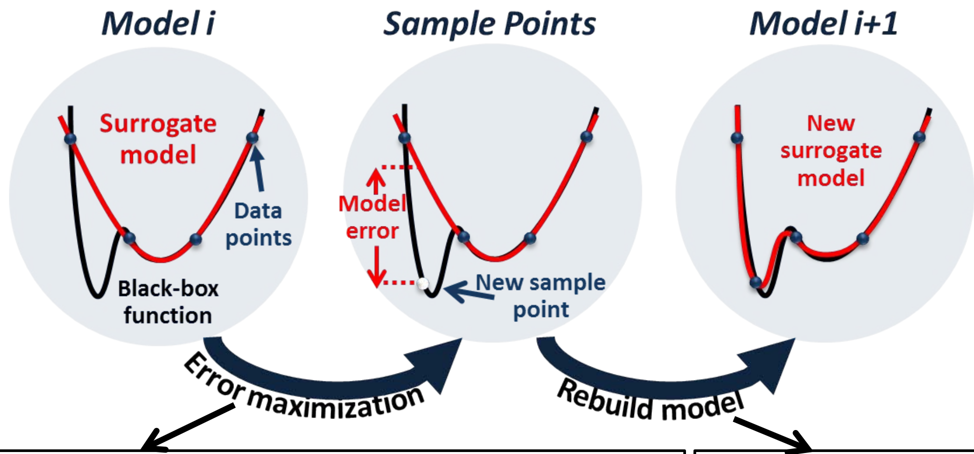
Automated Learning of Algebraic Models for Optimization



For building accurate, simple algebraic surrogate models of simulated processes

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

Surrogate model ($\hat{z}(x)$)

Simulation/black-box ($z(x)$)

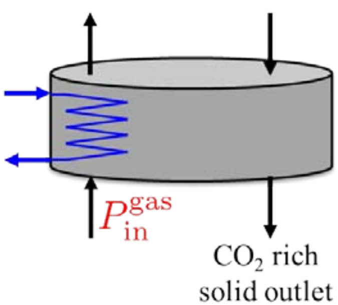
Step 1: Define a large set of potential basis functions

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

Step 2: Model reduction

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

Example Model: BFB Adsorber Inlet Gas Pressure



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

Pressure drop across length of bed

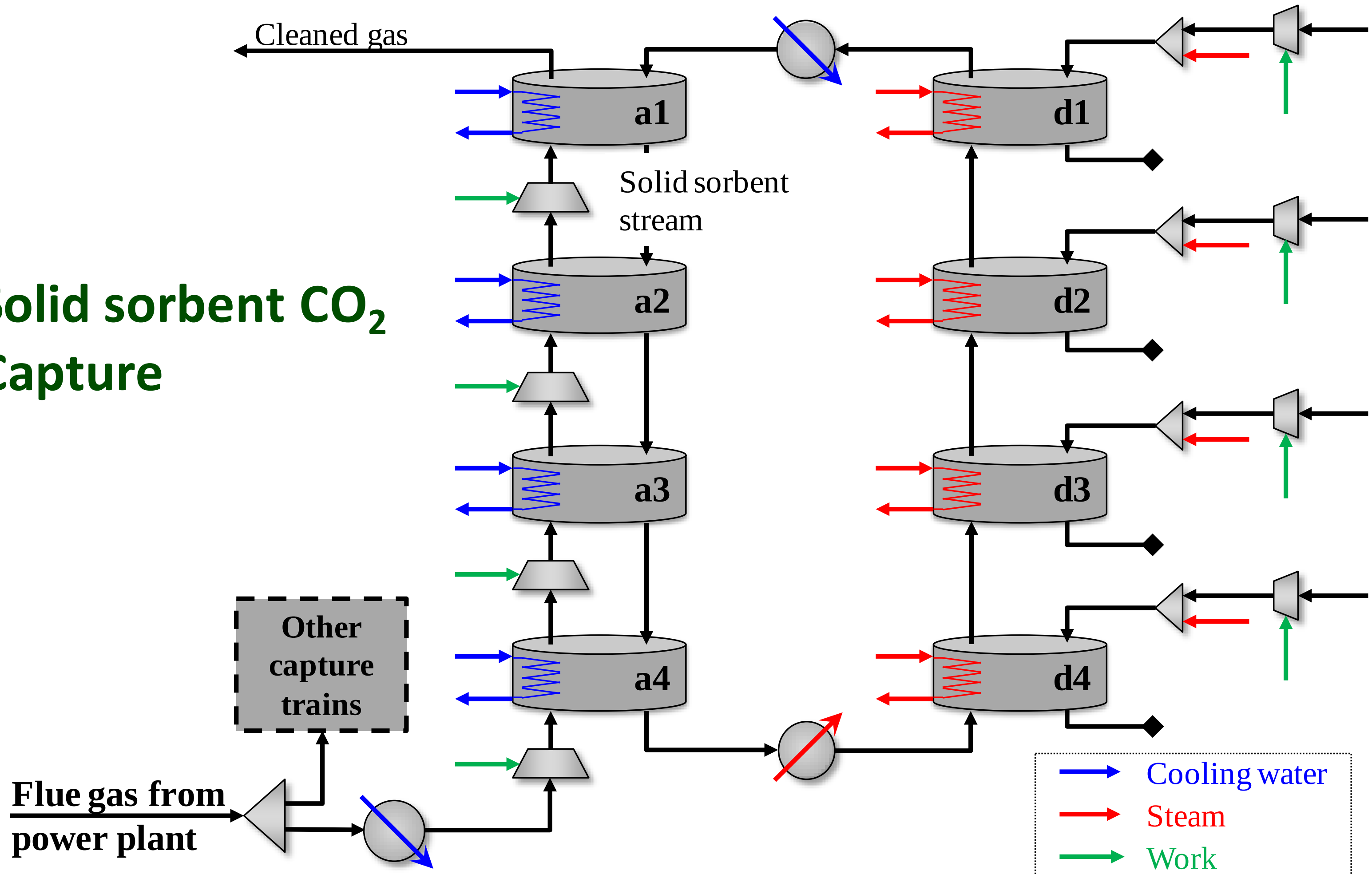
$$\hat{P}_{\text{in}}^{\text{gas}} = P_{\text{out}}^{\text{gas}} + 0.019\, L_b + 0.0055\, \sqrt{D_T}$$

Proportional to outlet pressure

Pressure drop due to bed diameter

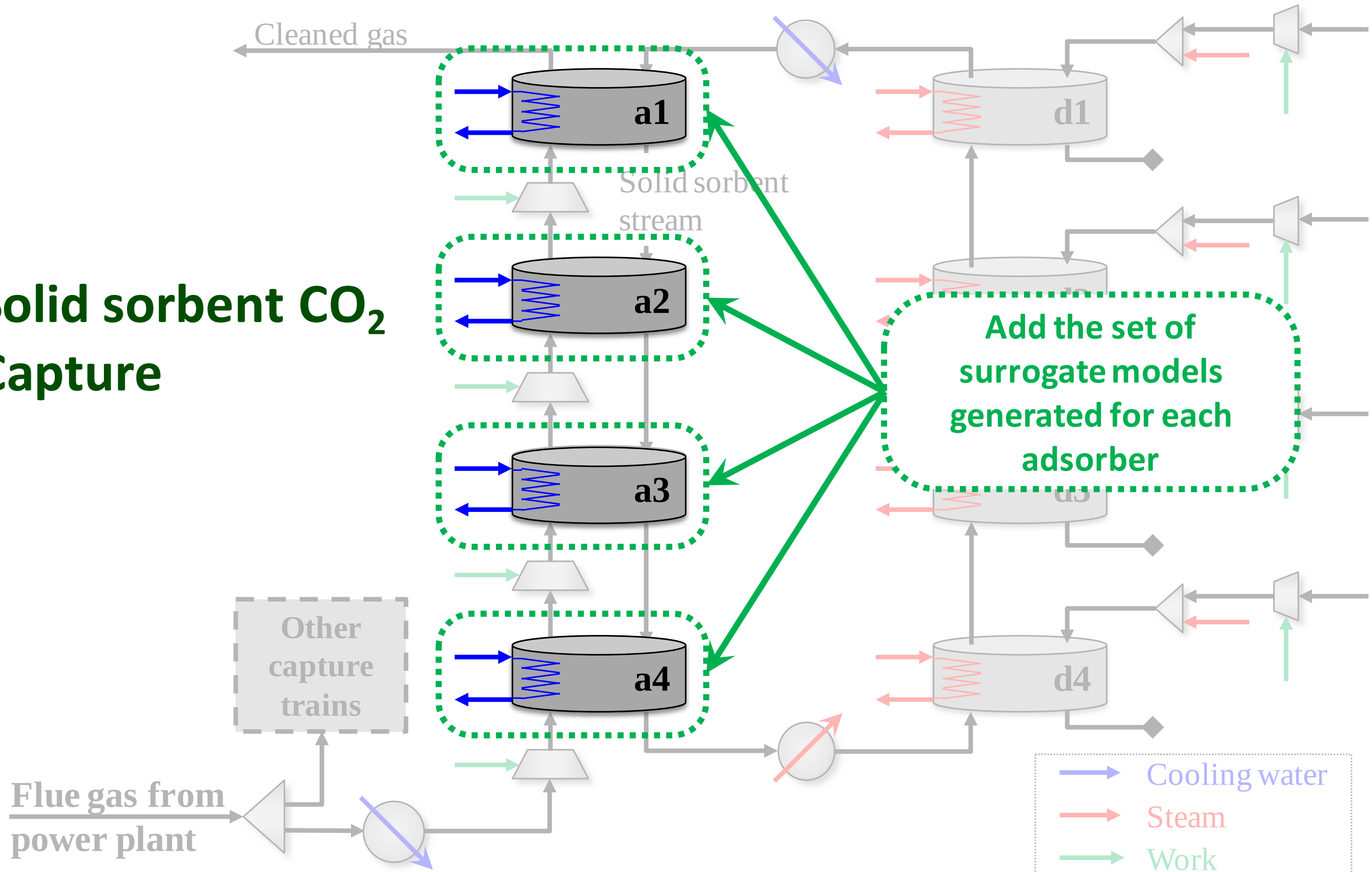
Superstructure Formulation & Optimization

Solid sorbent CO_2 Capture



Insert Algebraic Surrogates into Superstructure

Solid sorbent CO_2 Capture



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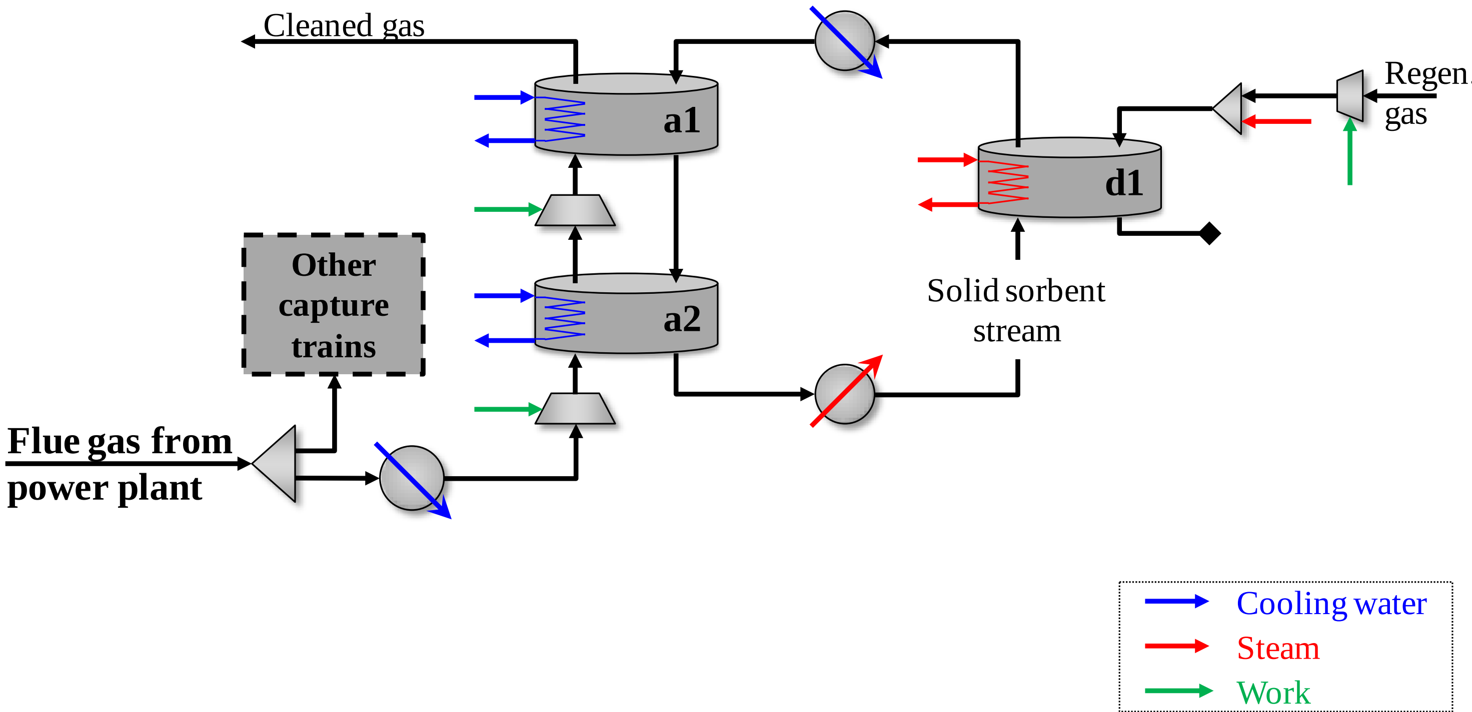
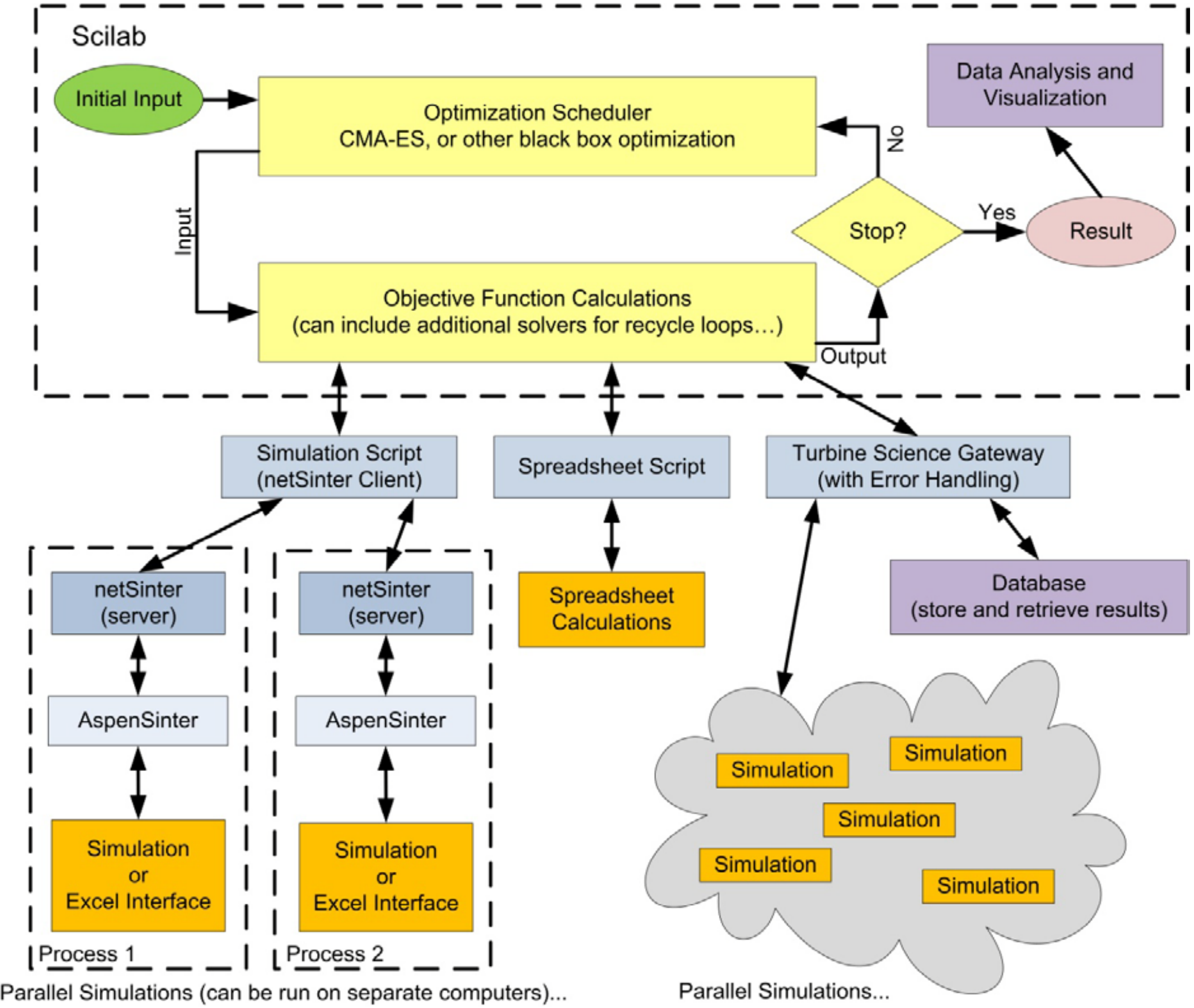
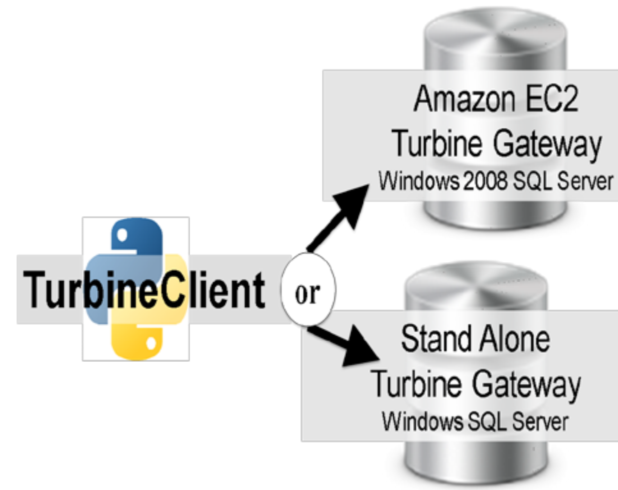
Initial Superstructure Solution

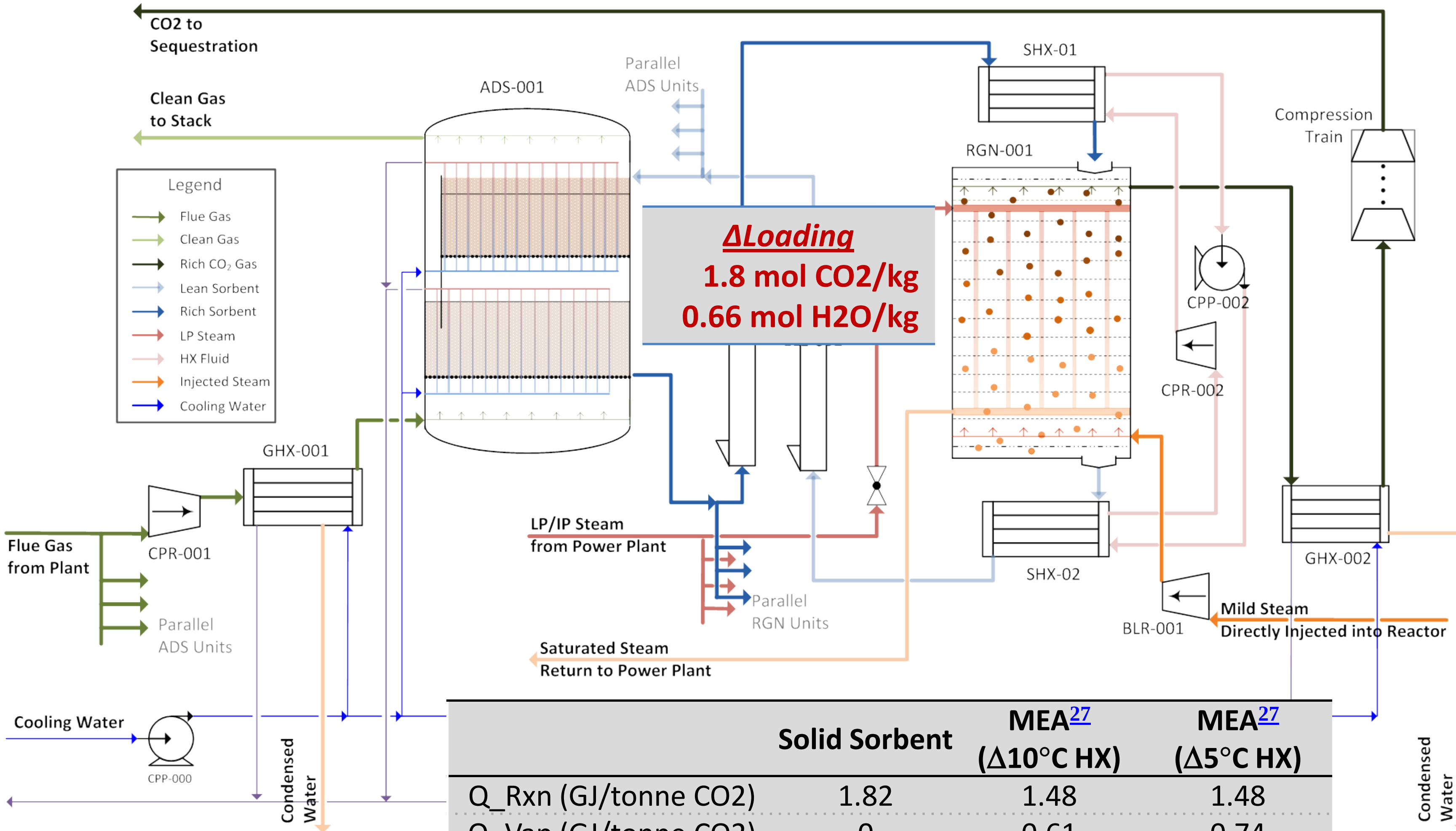


Simulation-Based Optimization: Verify Solution



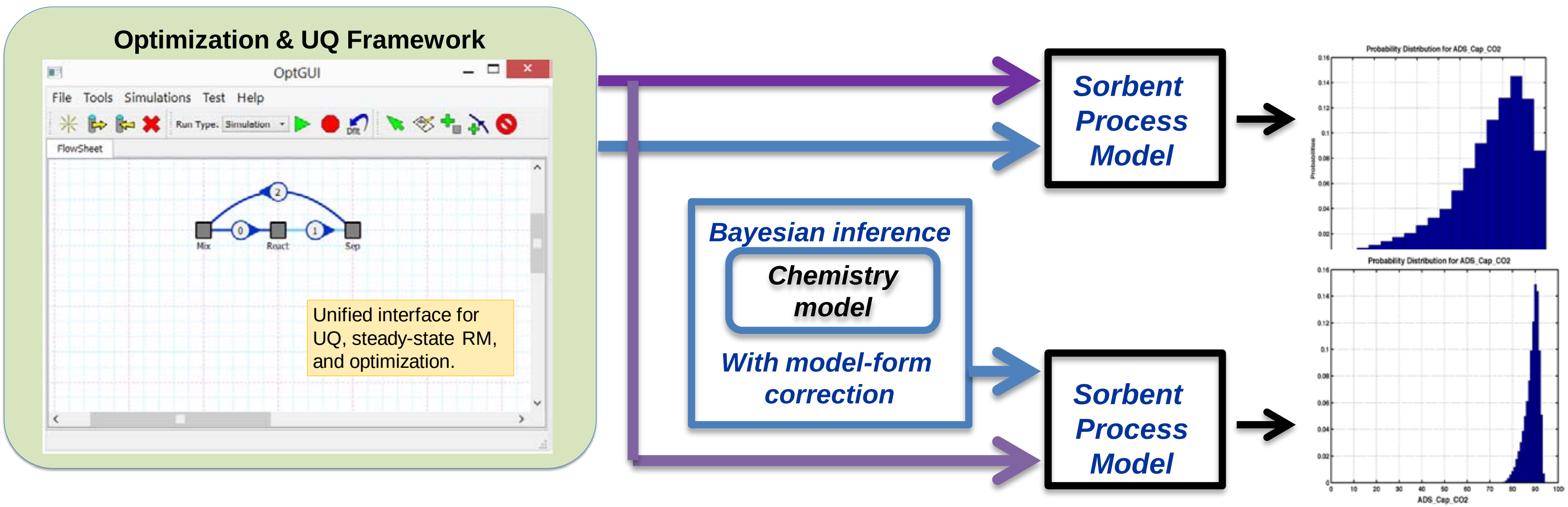


Optimized Process Developed using CCSI Toolset



	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

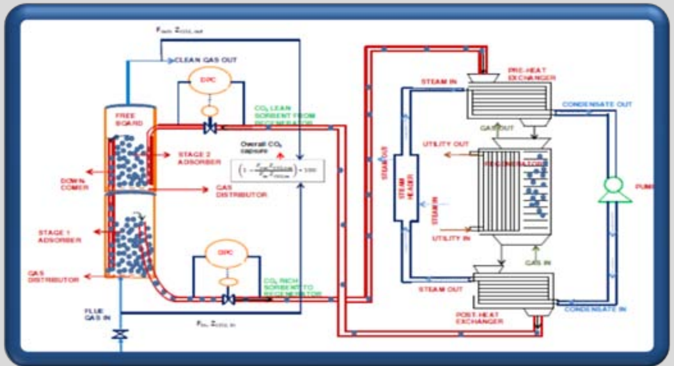
Multi-Scale Uncertainty Quantification Framework



- **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

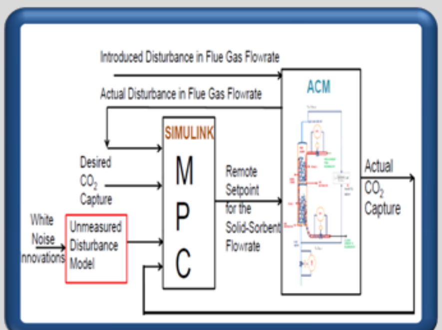
Dynamic Reduced Models & APC Framework

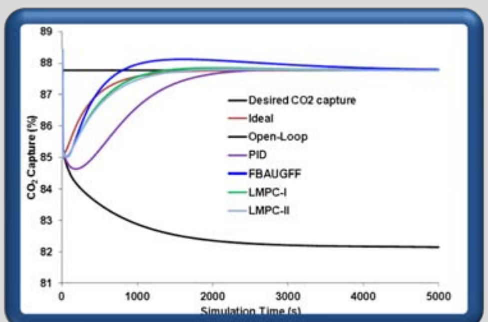
1-D Capture & Compression System Models

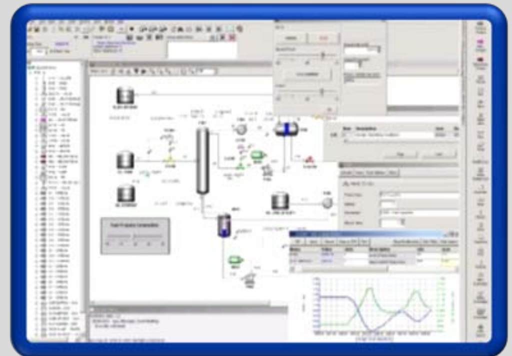


Dynamic Reduced Models

Advanced Process Control Framework







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Dynamic Reduced Models (D-RMs)

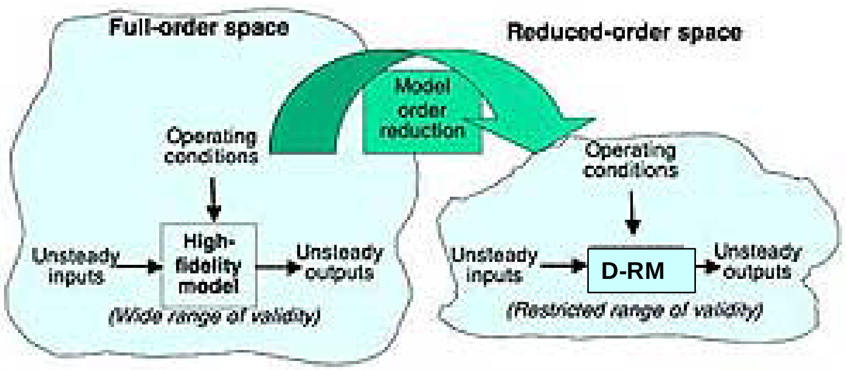
- **Motivation and Approaches**
  - First-principles dynamic models for CO_2 capture are computationally expensive. D-RMs are very useful for faster computation

On-Line Applications:

- Use in applications such as advanced process control (APC) and real-time optimization (RTO)
- Must be real-time
- Mainly input/output information is important
- *Data-driven* D-RMs based on pre-computed results from repeated simulations of a high-fidelity dynamic model over a range of input/output (I/O) variable values

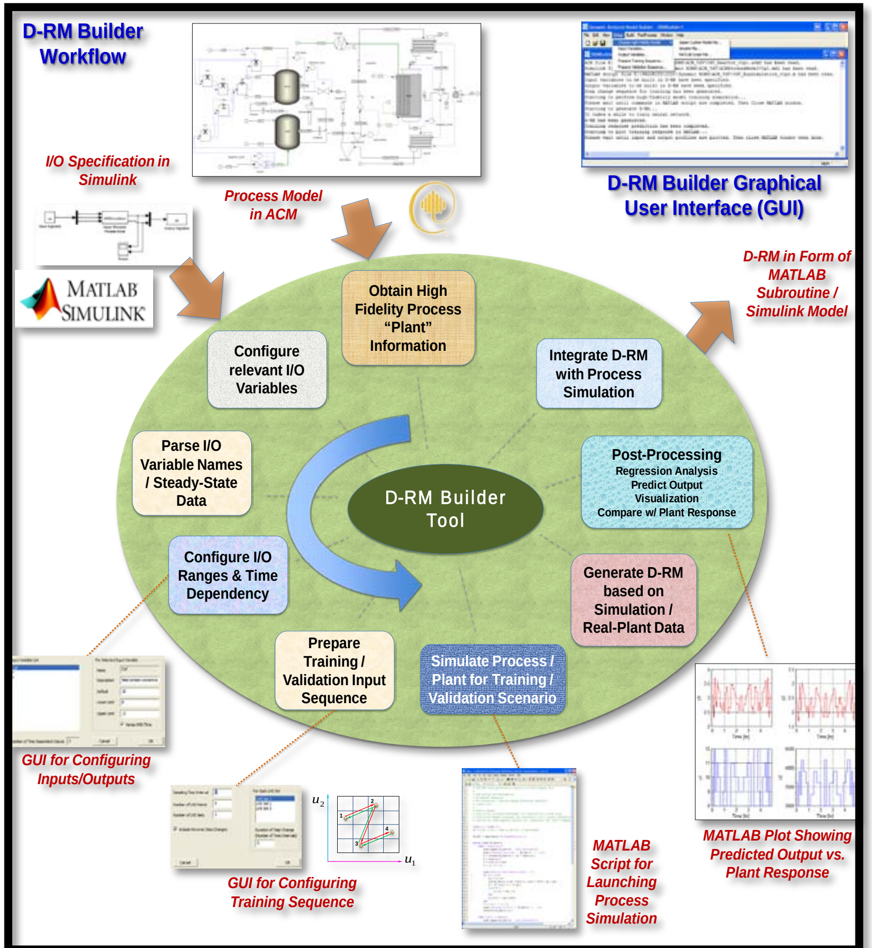
Off-Line Applications:

- Use as surrogate for process models
- Need not be real-time
- Provides state information
- *Reduced-order* D-RMs based on reduction of state space
  - o e.g., Proper Orthogonal Decomposition (POD)



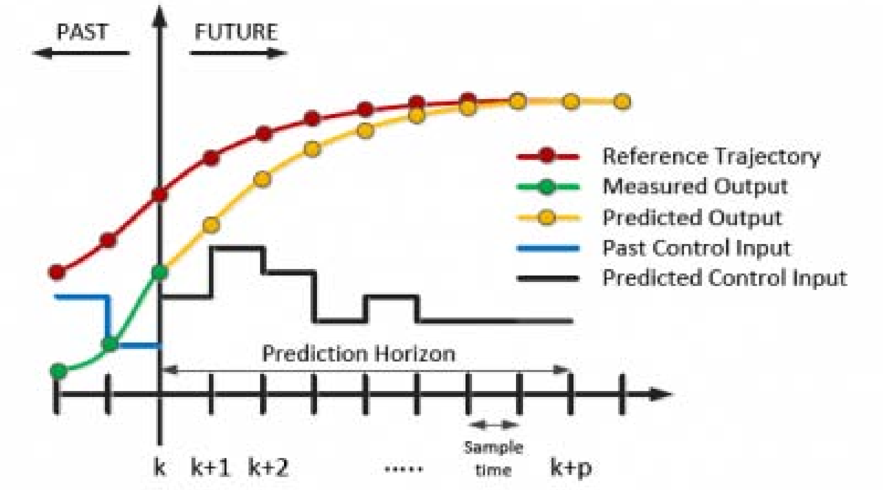
Dynamic Reduced Models (D-RMs)

- **Tool**
  - **D-RM Builder for On-Line Applications**
    - Use high-fidelity ACM/APD models embedded in Simulink to create D-RMs as MATLAB script files (.m files)
- **Accomplishments**
  - **Data-driven Black Box**
    - Implemented Nonlinear Autoregressive Moving Average (NARMA) based on Neural Networks
    - Implemented Decoupled A-B Net
      - Linear state-space (Laguerre)
      - Nonlinear mapping from state-space to output using Neural Network
  - **D-RM Builder**
    - Developed preliminary GUI
    - Tested on several benchmarks



Advanced Process Control Framework

- **Goal**
  - Develop estimator-based advanced process control (APC) framework using D-RM models
- **Approaches**
  - Model predictive control (MPC) with input/output constraints
  - Nonlinear state-estimation
    - o Recursive: Extended or Unscented Kalman Filter
    - o Optimization-based: Moving Horizon Estimation
  - Covariance estimation
    - o Autocovariance least-squares (ALS)
- **Tools**
  - APC Framework Tool
    - o Use data-driven D-RMs as prediction models embedded in Simulink for real-time APC
    - o Option of compiled MATLAB files for high execution speed

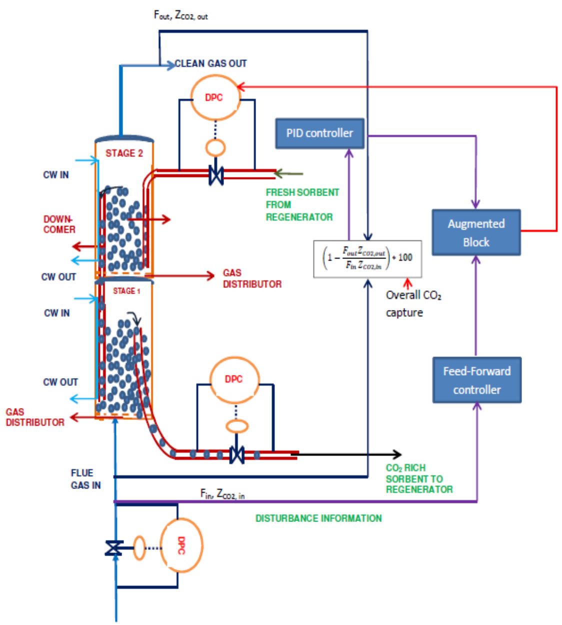


Model Predictive Control

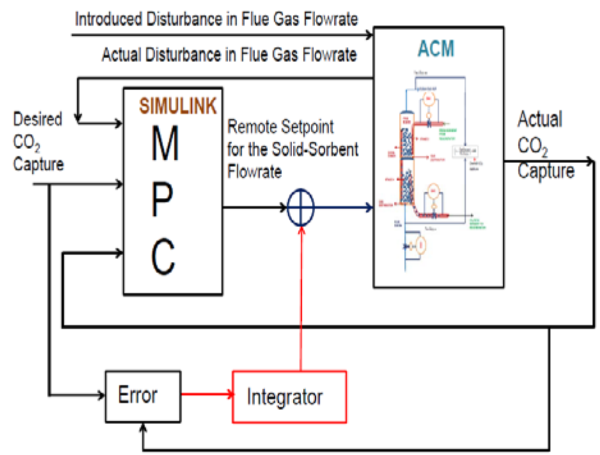
Controller Design for Maintaining CO_2 Capture

1. Traditional PID Control

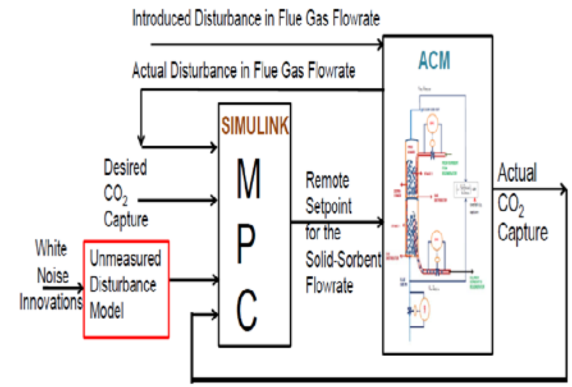
2. FEEDBACK-AUGMENTED FEEDFORWARD CONTROLLER



3. Offset-free LMPC Using an Integrator



4. Offset-free LMPC Using Unmeasured Disturbance



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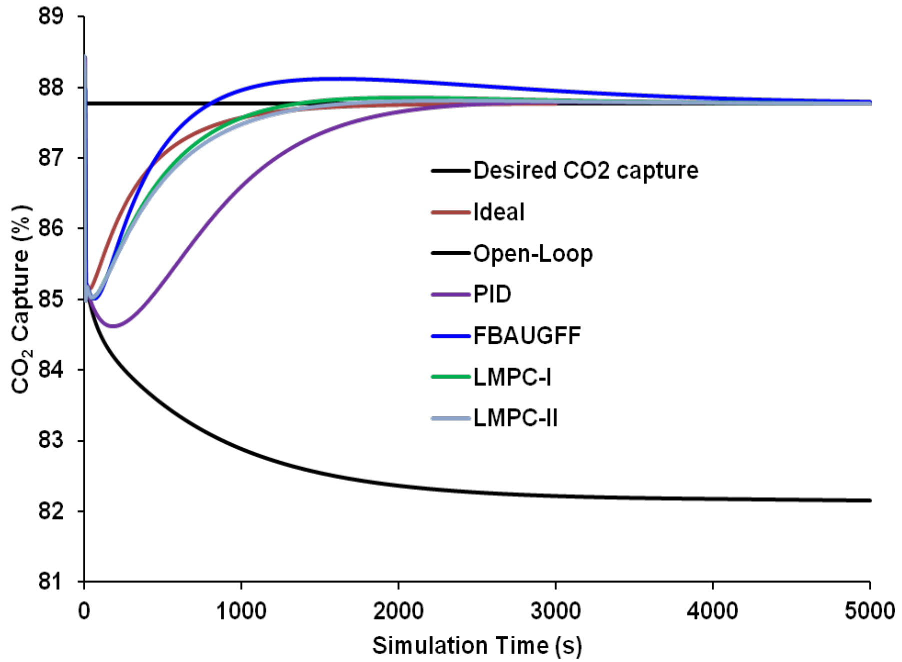
CONTROLLER PERFORMANCE COMPARISON

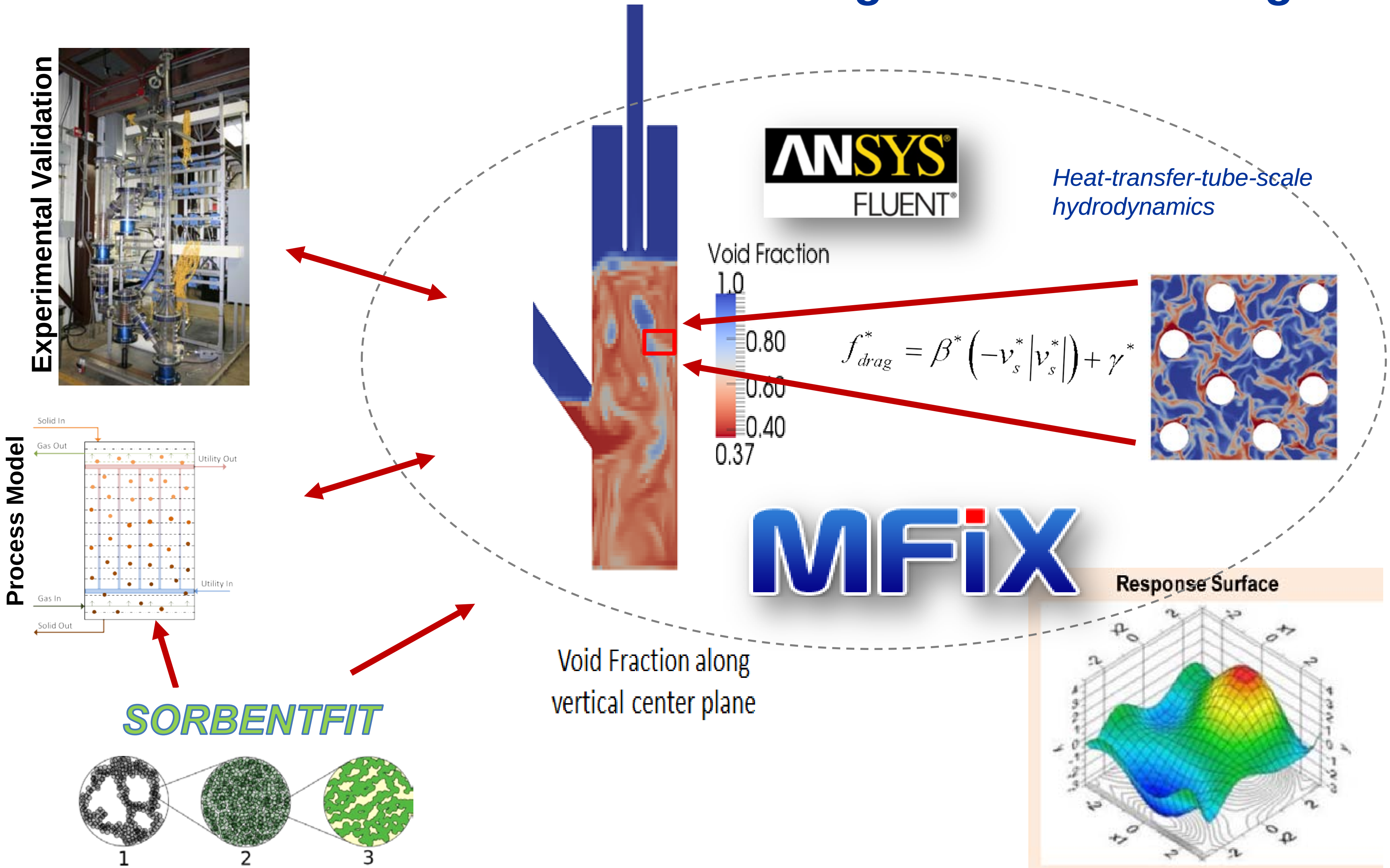


Control performances of LMPC-I and LMPC-II are superior to others

Control Performance Table

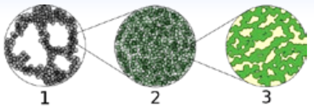
CONTROLLER	IAE	ISE	ITAE
	(hr)	(hr)	(hr^2)
(1) PID	0.8111	1.7551	1.12E-04
(2) FBAUGFF	0.4751	**0.5502**	6.60E-05
(3) LMPC-I	**0.3913**	0.6138	**5.57E-05**
(4) LMPC-II	0.4007	0.6386	6.30E-05

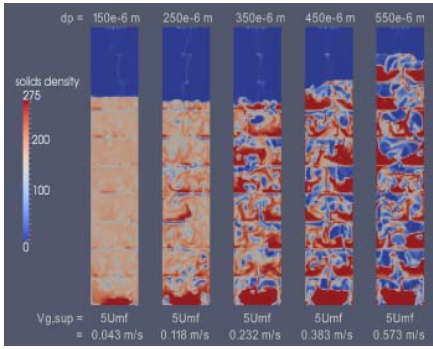
CFD models to reduce time for design/troubleshooting

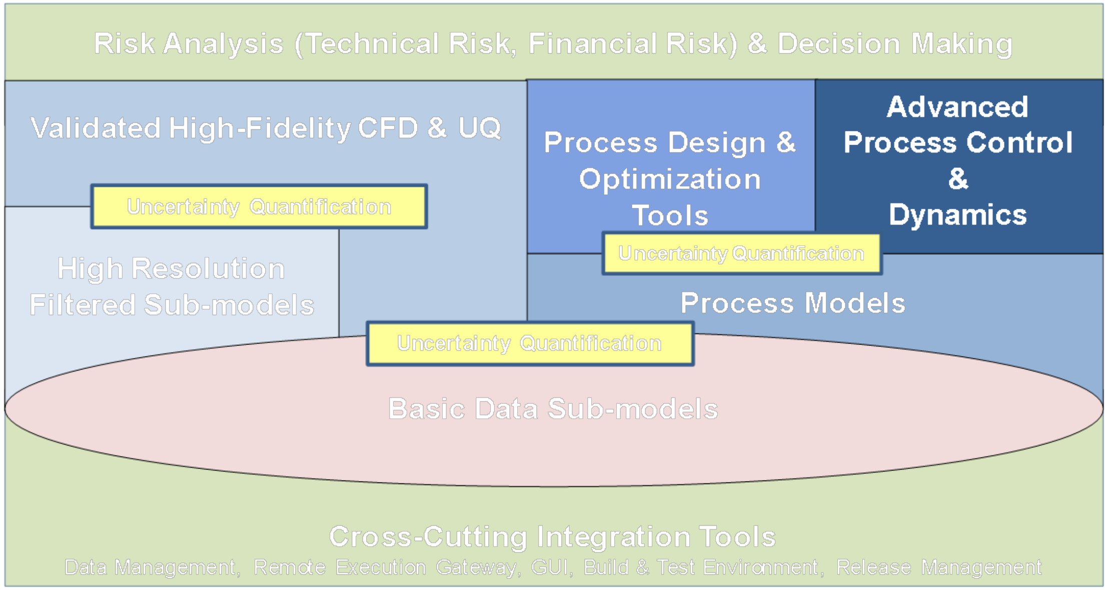


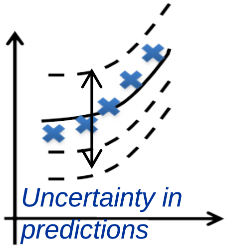
Deploys Initial Computational Toolset

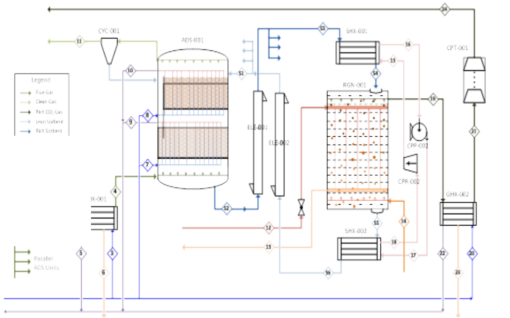
- Initial toolset released Oct. 2012, 1 year ahead of schedule due to industry request for early access
  - 3 companies already have already licensed
  - Other companies pursing license
- Additional releases planned for Fall 2013, 2014, 2015.
- Final release planned for Jan. 2016

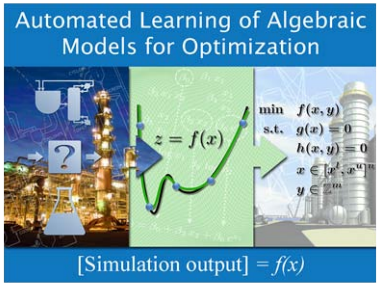


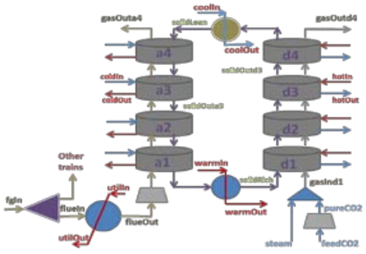












… and the people who made that happen!

57 Nat'nl Lab researchers
20 Industry representatives
13 Students/post-docs
9 Professors
5 National Labs
6 Universities

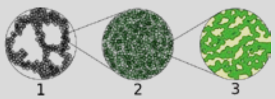
Thank you!

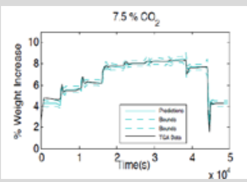
Disclaimer

Backup slides

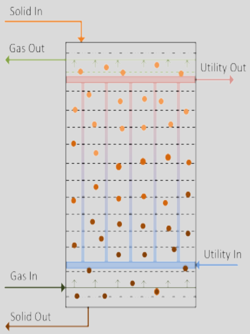
Advanced Process Systems Engineering Approaches

Basic Data Models

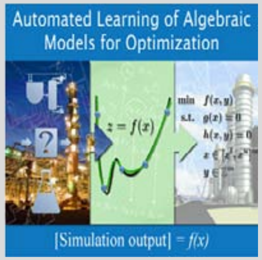




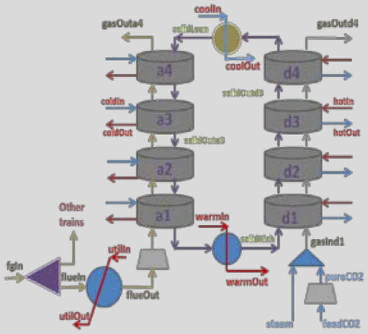
Process Models



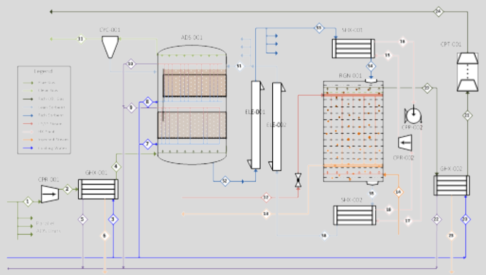
Algebraic Surrogate Models



Superstructure Optimization



Optimal Process



SORBENTFIT

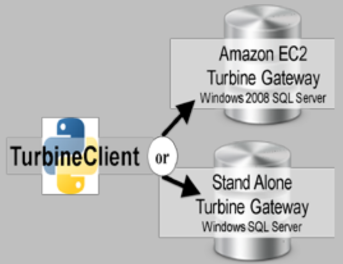
aspentech

gPROMS

GAMS

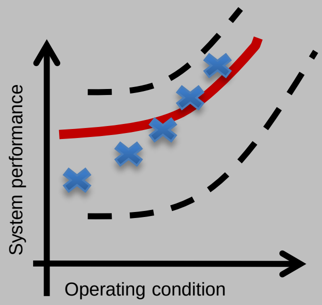
PSUADE

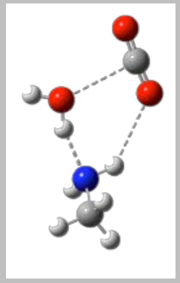
Simulation Gateway

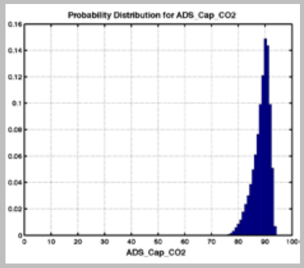


Simulation-Based DFO Framework

Uncertainty Quantification with Bayesian Calibration







CCSI™ Carbon Capture Simulation Initiative

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Berkeley Lab

Lawrence Livermore National Laboratory

Los Alamos National Laboratory EST.1943

Pacific Northwest National Laboratory

U.S. Department of Energy

CONSERVATION EQUATIONS

Bubble Region :

Gaseous Components

$$\frac{\partial(\delta V C_{b,i})}{\partial t} + \frac{V}{A}\frac{\partial(y_{b,i}G_{b,i})}{\partial x} + \delta V K_{bc,i}(C_{b,i} - C_{c,i}) + K_{g,bulk} = 0$$

$$\frac{\partial(C_{P,g}C_{bt}\delta V(T_{g,b} - T_{ref}))}{\partial t} + \frac{\partial(C_{P,g}G_b(T_{g,b} - T_{ref}))}{\partial x} + \delta A H_{bc}(T_{g,b} - T_{g,c}) - H_{g,bulk} = 0$$

Cloud-wake Region :

Gaseous Components

$$\frac{\partial(f_{cw}\delta\varepsilon_d V C_{c,i})}{\partial t} - V\delta K_{bc,i}(C_{b,i} - C_{c,i}) + V\delta K_{ce,i}(C_{c,i} - C_{e,i}) + V\delta(1-\varepsilon_d)f_{cw}r_{g,c} = 0$$

$$\frac{\partial(C_{P,g}C_{ct}V\delta f_{cw}e_d(T_{g,c} - T_{ref}))}{\partial t} - A\delta H_{bc}(T_{g,b} - T_{g,c}) + A\delta H_{ce}(T_{g,c} - T_{g,e}) + Af_{cw}\delta(1-\varepsilon_d)\rho_s a_p h_p(T_{g,c} - T_{s,c})$$
$$- f_{cw}\delta(1-\varepsilon_d)A\sum_j r_{g,c,i}C_{p,g,c,i}(T_{g,c} - T_{ref}) = 0$$

Adsorbed Species

$$\frac{\partial(Vf_{cw}\delta(1-\varepsilon_d)n_{c,j})}{\partial t} - \frac{V}{\rho_s}\frac{\partial(n_{c,j}J_c)}{\partial x} + K_{s,bulk,j} + V\delta K_{cebs}(n_{c,j} - n_{e,j}) - Vf_{cw}\delta(1-\varepsilon_d)r_{s,c} = 0$$

$$\frac{\partial\left(A\Delta x f_{cw}\delta\rho_s C_{P,s}(1-\varepsilon_d)(T_{s,c} - T_{ref})\right)}{\partial t} + A\frac{\partial(J_c C_{P,s}(T_{s,c} - T_{ref}) + h_{ads,c})}{\partial x} + H_{s,bulk}$$
$$+ A\delta\rho_s K_{cebs}(C_{P,s}(T_{s,c} - T_{ref}) + h_{ads,c} - C_{P,s}(T_{s,e} - T_{ref}) + h_{ads,e})$$
$$+ f_{cw}\delta(1-\varepsilon_d)A\sum_j r_{g,c,i}C_{p,g,c,i}(T_{g,c} - T_{ref}) - Af_{cw}\delta(1-\varepsilon_d)\rho_s a_p h_p(T_{g,c} - T_{s,c}) = 0$$

CONSERVATION EQUATIONS CONTD.

Emulsion Region :

Gaseous Components

$$\frac{\partial\left(V(1-f_{cw}\delta-\delta)\varepsilon_d C_{e,i}\right)}{\partial \mathrm{t}} - \delta A \mathrm{K}_{\mathrm{ce,i}}\left(\mathrm{C}_{\mathrm{c,i}}-\mathrm{C}_{\mathrm{e,i}}\right) - \mathrm{K}_{\mathrm{g,bulk}} + (1-f_{cw}\delta-\delta)A(1-\varepsilon_d)\mathrm{r}_{\mathrm{g,e}} = 0$$

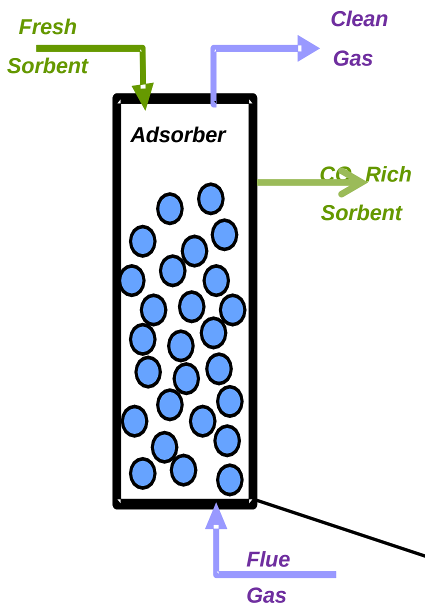
$$\frac{\partial\left(\mathrm{C}_{\mathrm{P,g}}\mathrm{C}_{\mathrm{et}}V(1-f_{cw}\delta-\delta)\varepsilon_d\left(T_{g,e}-T_{ref}\right)\right)}{\partial \mathrm{t}} - A\delta \mathrm{H}_{\mathrm{ce}}\left(\mathrm{T}_{\mathrm{g,c}}-\mathrm{T}_{\mathrm{g,e}}\right) + H_{g,bulk} + (1-f_{cw}\delta-\delta)(1-\varepsilon_d)A\rho_s a_p h_p\left(\mathrm{T}_{\mathrm{g,e}}-\mathrm{T}_{\mathrm{s,e}}\right)$$
$$-(1-f_{cw}\delta-\delta)(1-\varepsilon_d)A\sum\nolimits_j r_{g,e,i}C_{p,g,e,i}\left(T_{g,e}-T_{ref}\right) = 0$$

Adsorbed Species

$$\frac{\partial\left(V(1-f_{cw}\delta-\delta)(1-\varepsilon_d)n_{e,j}\right)}{\partial \mathrm{t}} + \frac{V}{\rho_s}\frac{\partial\left(n_{e,j}J_e\right)}{\partial x} - \mathrm{K}_{\mathrm{s,bulk,j}} - \mathrm{V}\delta\mathrm{K}_{\mathrm{cebs}}\left(n_{\mathrm{c,j}}-\mathrm{n}_{\mathrm{e,j}}\right) - V(1-f_{cw}\delta-\delta)(1-\varepsilon_d)r_{s,e} = 0$$

$$\frac{\partial\left(\mathrm{C}_{\mathrm{P,s}}\rho_s A(1-f_{cw}\delta-\delta)(1-\varepsilon_d)\left(T_{s,e}-T_{ref}\right)\right)}{\partial t} + A\frac{\partial\left(J_e \mathrm{C}_{\mathrm{P,s}}\left(T_{s,e}-T_{ref}\right)+h_{ads,e}\right)}{\partial x} - \mathrm{H}_{\mathrm{s,bulk}}$$
$$-\ A\delta\rho_s K_{cebs}\left(C_{P,s}\left(T_{s,c}-T_{ref}\right)+h_{ads,c}-C_{P,s}\left(T_{s,e}-T_{ref}\right)+h_{ads,e}\right)$$
$$+(1-f_{cw}\delta-\delta)(1-\varepsilon_d)A\sum\nolimits_j r_{g,e,i}C_{p,g,e,i}\left(T_{g,e}-T_{ref}\right) - (1-f_{cw}\delta-\delta)(1-\varepsilon_d)A\rho_s a_p h_p\left(\mathrm{T}_{\mathrm{g,e}}-\mathrm{T}_{\mathrm{s,e}}\right)$$
$$-\ \pi d_{HX}h_{t,x}\Delta T_{hx}N_{HX}C_r = 0$$

HYDRODYNAMIC MODEL



$$\left(\frac{\sqrt{d_{b,u,x}}-\sqrt{d_{b,e,x}}}{\sqrt{d_{b,0}}-\sqrt{d_{b,e,x}}}\right)^{\left(1-\frac{\gamma_1}{\gamma_{3,x}}\right)}\left(\frac{\sqrt{d_{b,u,x}}-\sqrt{\gamma_{2,x}}}{\sqrt{d_{b,0}}-\sqrt{\gamma_{2,x}}}\right)^{\left(1+\frac{\gamma_1}{\gamma_{3,x}}\right)}=e^{\left(-\frac{0.3x}{D_t}\right)}$$

where $\gamma_1=\frac{2.56\times10^{-2}}{v_{mf}}\sqrt{\frac{D_t}{g}}$ and $\gamma_{3,x}=\sqrt{\gamma_1^{\,2}+4\frac{d_{b,m,x}}{D_t}}$

$$d_{b,e,x}=\frac{D_t}{4}\left(-\gamma_1+\gamma_{3,x}\right)^2$$

$$d_{b,m,x}=2.59\,g^{-0.2}\left(A_x\left[v_{g,x}-v_{e,x}\right]\right)^{0.4}$$

$$d_{b,0}=1.38\,g^{-0.2}\left(a_o\left[v_{g,0}-v_{e,0}\right]\right)^{0.4}$$

Mori and Wen (1975)

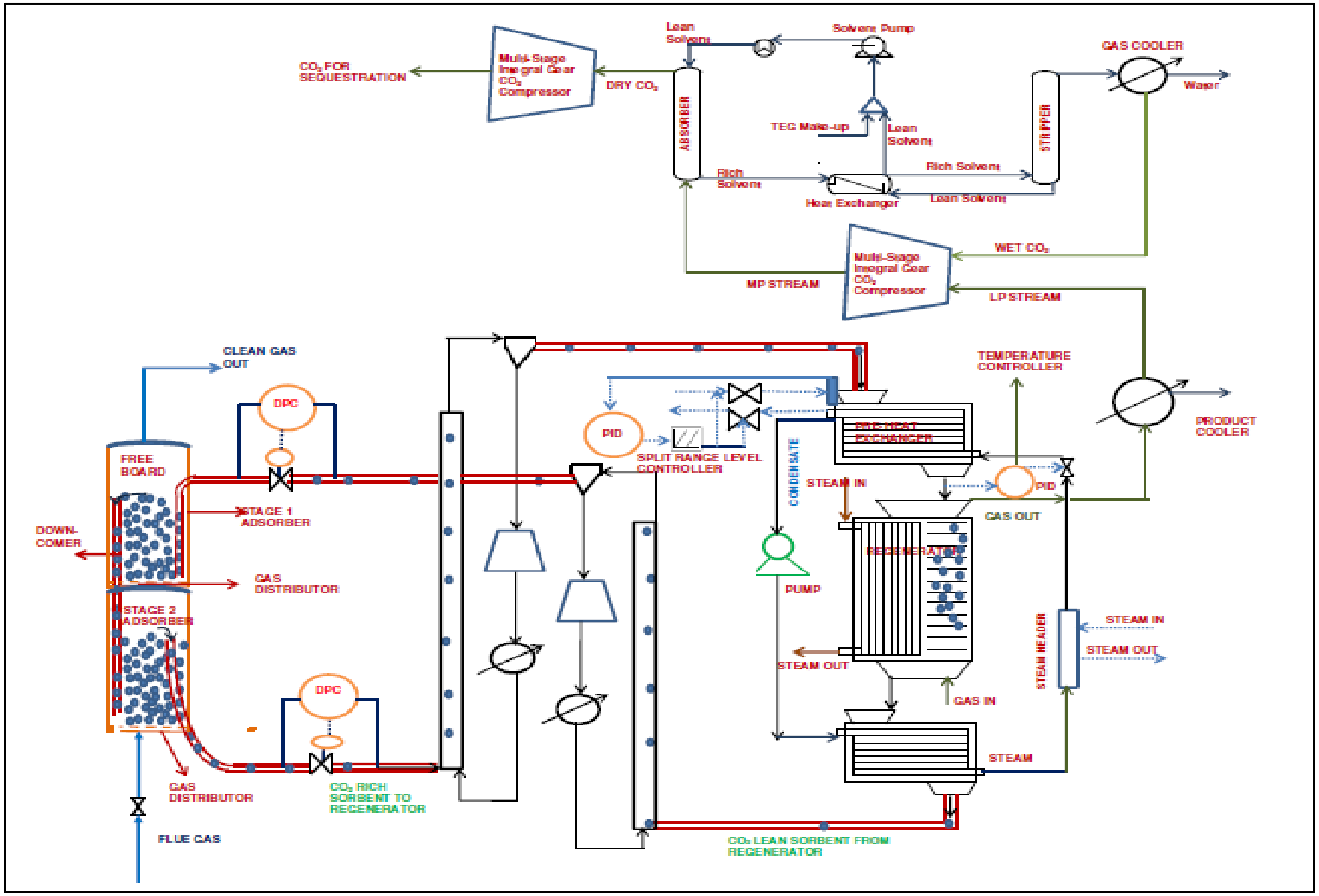
$$v_{b,x}=v_{g,x}-v_{mf}+0.35\sqrt{gD_{t,h}}$$

$$K_{bc,j,x}=1.32\times4.5\frac{v_{mf}}{d_{b,x}}+5.85\frac{D_{j,x}^{\;0.5}\,g^{0.25}}{d_{b,x}^{\;5/4}}$$

$$K_{ce,j,x}=6.78\sqrt{\frac{\varepsilon_{d,x}^{\;2}D_{j,x}v_{b,x}}{d_{b,x}^{\;3}}}$$

Sit and Grace (1981)

Process Model of the Integrated System



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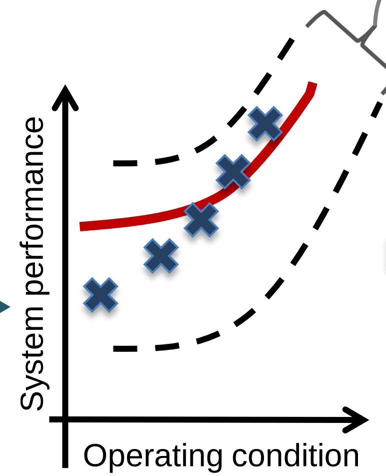
Uncertainty Quantification: How certain are we that our model can predict the system performance accurately?

- How to quantify these error bounds *a priori*?
- How to reduce these bounds?

CCSI simulation

Scaled-up design



Risk analysis

How does the uncertainty in the prediction affect the risk assessment outcome?