BIAS Sorbent NCCC Testing/CCSI Modeling

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National Energy Technology Laboratory

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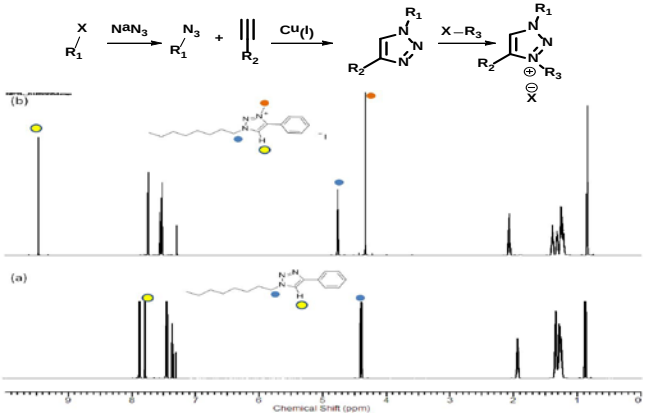
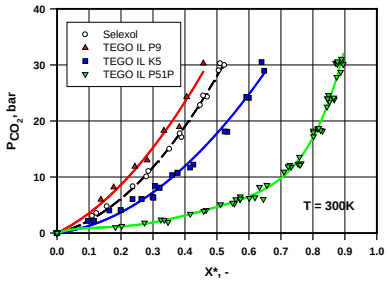
Integrated Materials Development

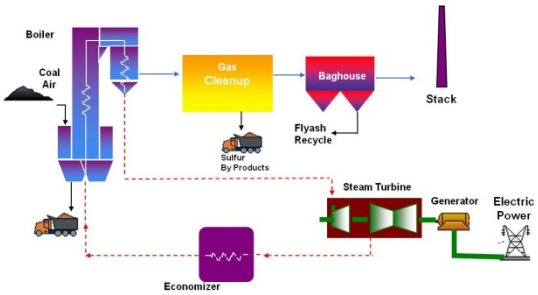
Characterization



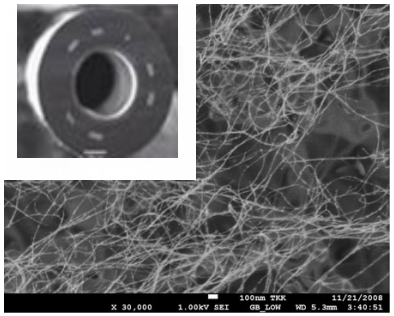
Performance Testing



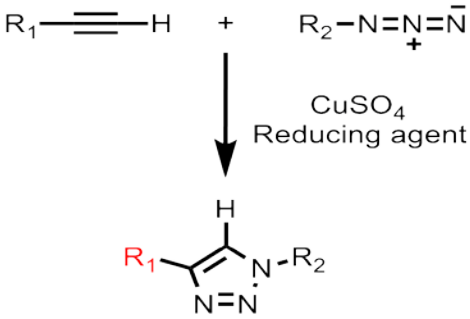
CCSI Simulation & Analysis



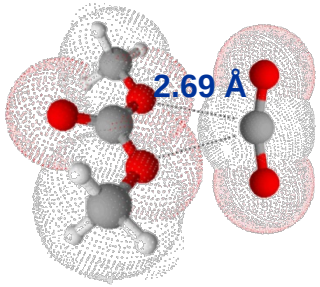
Fabrication



Synthesis

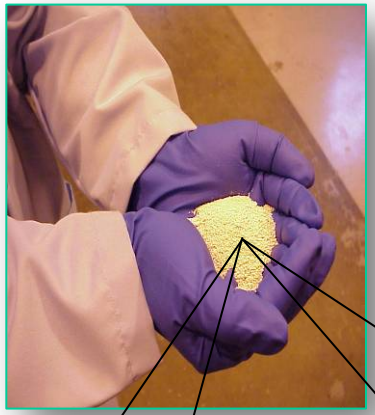


Molecular Modeling



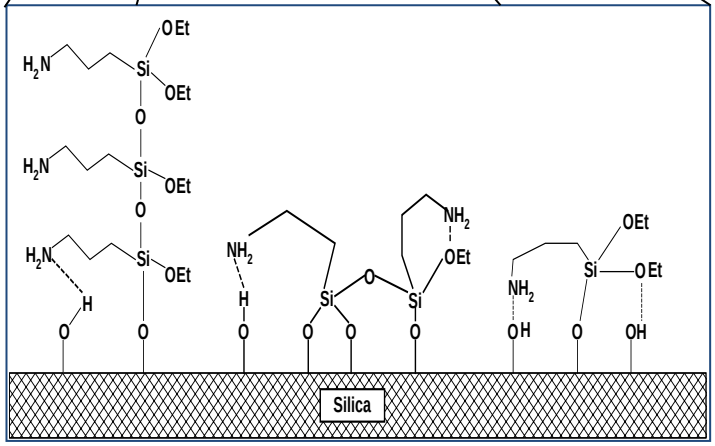
Carbon Capture

Supported Amine Sorbents

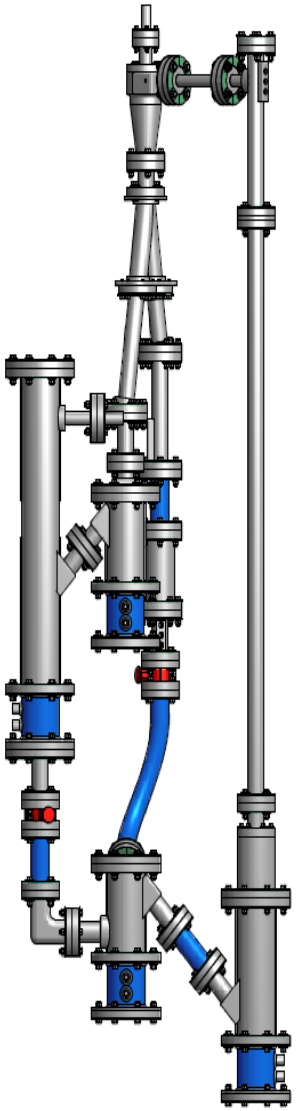


Objective: Deliver a test stand with a sorbent to NCCC facilities for slip stream testing AND deliver data for CCSI validation

Approach: Simultaneously develop a sorbent and full circulation test stand

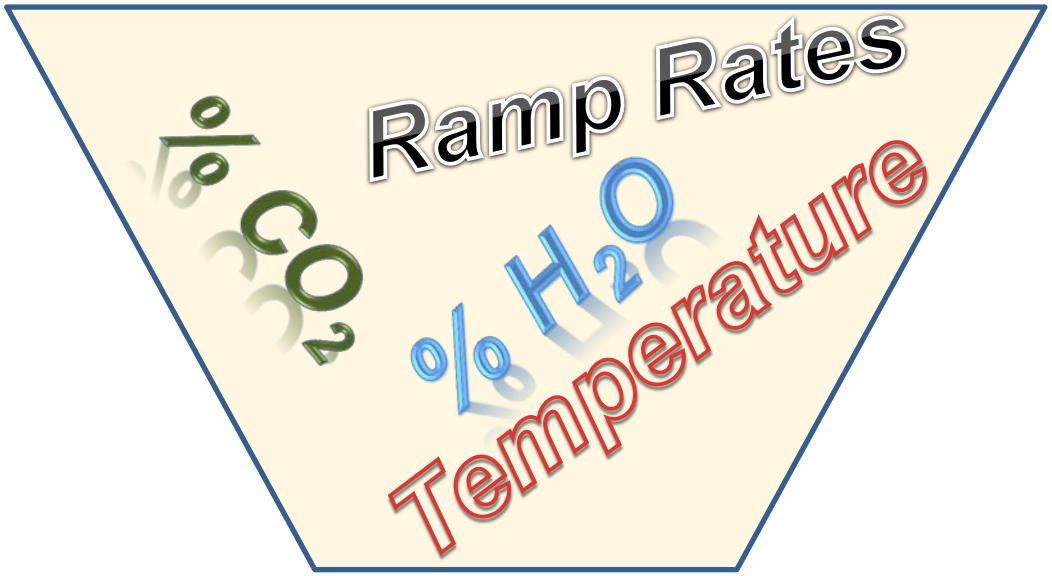


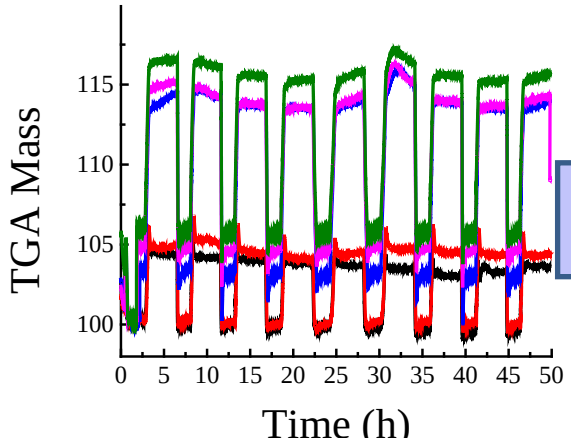
Scale-up



2012 R&D 100

TGA & Performance Data Collection





CCSI

Sorption Kinetics

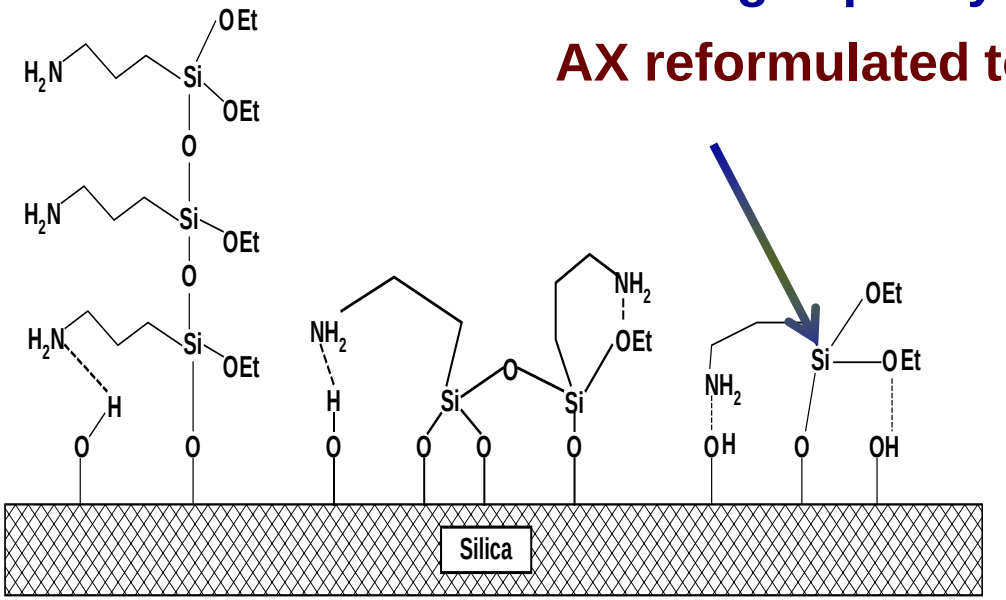
Sorbent Development: CCSI communication

Provided AX sorbent properties to CCSI

Feedback on working capacity and moisture requirements

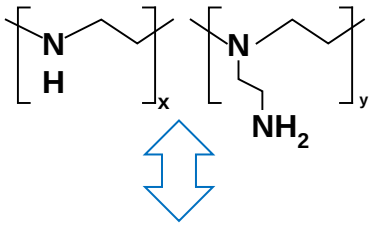
Reformulates sorbent based moisture and working capacity requirements

AX reformulated to 32D sorbent



Polyethyleneimine Silane Coupling

Polyethyleneimine Mn 423-2000



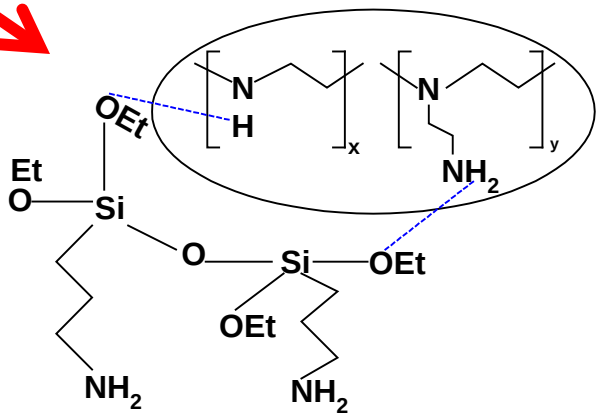
Aminosilanes

Methanol 80 C

Vacuum atm- 10 mm Hg

- Simple
- Scalable
- Acceptable Capacity
- Moisture Resistance
- Stability
- Saleable

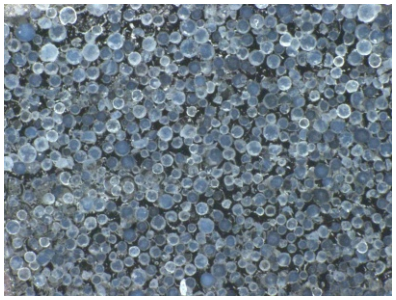
Pressure Chemical – Pan Dyer



Synthesis was scaled to 1,000 lb production

Summary for Basic Immobilized Amine Sorbent

- Silica substrate candidate of choice
- High capture capacity - 3-4 mol/kg
- Working capacities in the 2 mol/kg range
- Loading results confirmed by TVA and ADA-ES
- CO_2 regeneration improbable
- Stable at 110-115^oC
- Reduced moisture loading to minimize regeneration duty
- Kinetic study conducted
- Scaled to large production scale

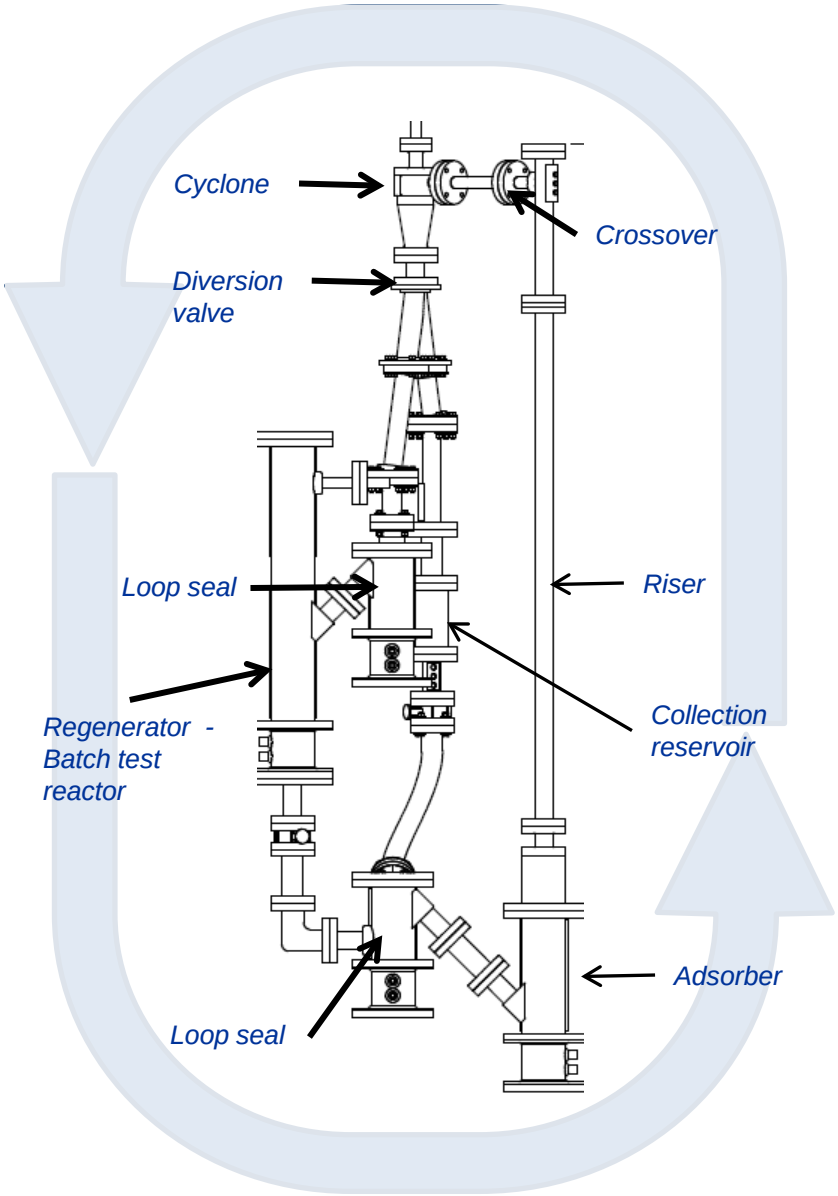


PEI on CARiACT Q10
(100 to 350 µm dia.)

Schematic and actual pilot unit

Circulating Reactor Development (C2U)

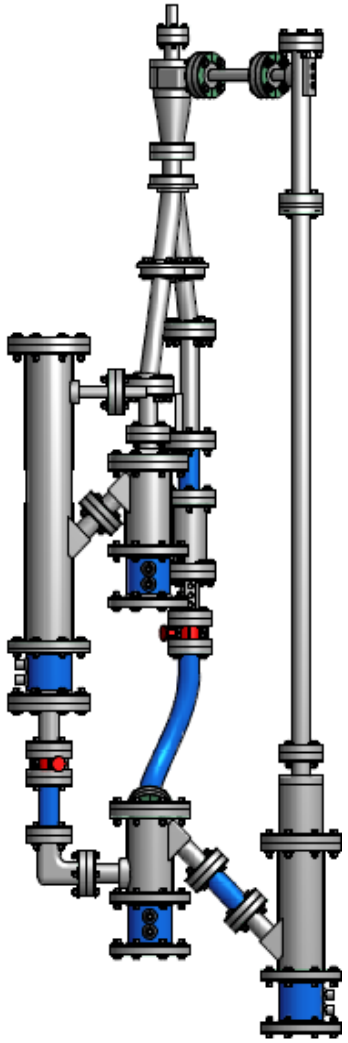
- **Integrated circulating fluid bed reactor**
- **Develop an understanding of engineering challenges**
- **System has not been optimized for 32D sorbent – currently achieve about 0.5 mol/kg with 32D**
- **Full post analysis of material available at NETL and partners**
  - Particle Size Distribution
  - Amine Loading
  - Capacity Testing



C2U Operation and Testing Modes

Full loop Circulation

1. Real experience in Dual CFB Reactor Design
2. Allows the Sorbent to be circulated
3. System is not optimized for 32D – low capacities observed
4. Circulation Rate is difficult to control
5. Sorbent was too light, pressure drops to small



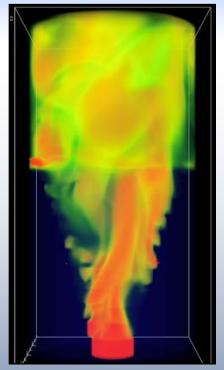
Batch Testing

1. Bubbling Fluid Bed
2. Easy to control fluidized bed
3. Bed holds ~ 2 kg
4. Multi-port gas extraction
5. Rapid testing procedure
6. Ease of modeling

CCSI For Accelerating Technology Development

Carbon Capture Simulation Initiative






Rapidly synthesize optimized processes to identify promising concepts → **Better understand internal behavior to reduce time for troubleshooting** → **Quantify sources and effects of uncertainty to guide testing & reach larger scales faster** → **Stabilize the cost during commercial deployment**

National Labs

Berkeley Lab
Pacific Northwest National Laboratory
NETL
Los Alamos National Laboratory
Lawrence Livermore National Laboratory

Academia

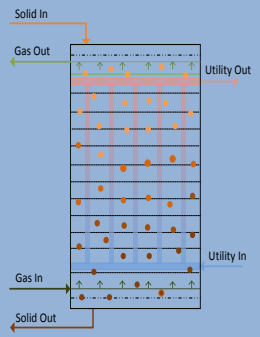
Carnegie Mellon
Princeton University
West Virginia University
Boston University
The University of Texas at Austin

Industry

ADA Environmental Solutions
Alstom
B&W
GE
EPRI Electric Power Research Institute
Fluor
Southern Company
Phillips 66
AEP American Electric Power
Southern California Edison
An Edison International Company
San Onofre Nuclear Generating Station
Chevron
URS
ExxonMobil
Air Products
Eastman
ANSYS
aspentech
invensys
PSE

Tools to develop an optimized process using rigorous models

Process Models



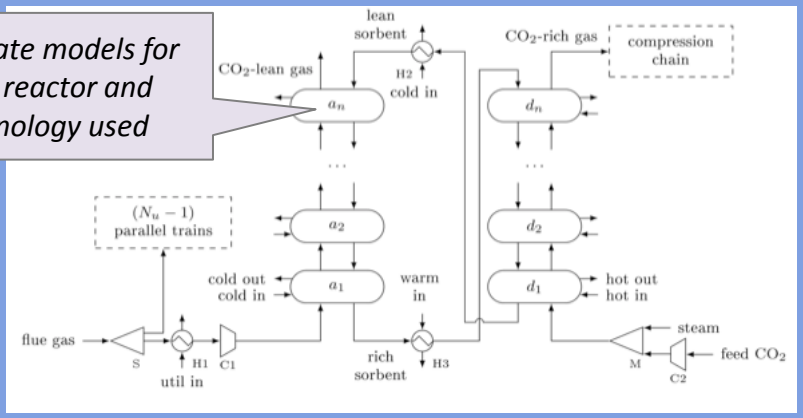
Basic Data Submodels

Algebraic Surrogate Models

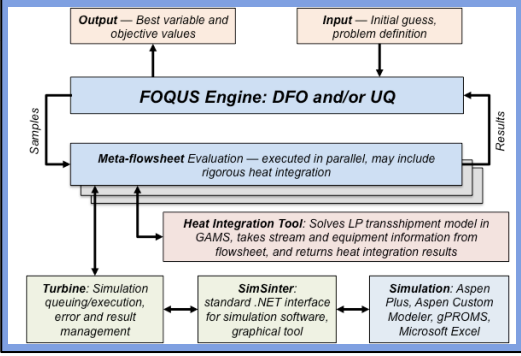
ALAMO

Surrogate models for each reactor and technology used

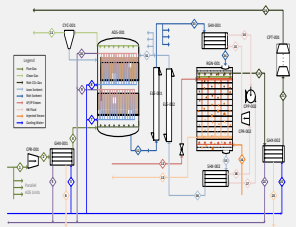
Superstructure Optimization



Simulation-Based Optimization



Optimized Process



Uncertainty Quantification

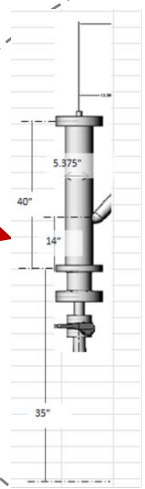
Process Dynamics and Control

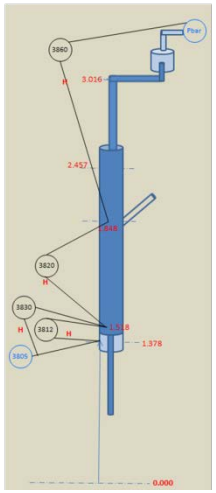
CFD Device Models

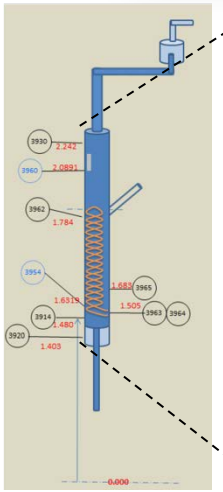
Simulation & Experiments to reduce time for design/troubleshooting

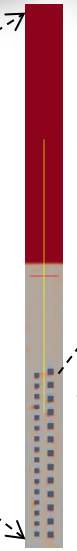
Experimental Validation

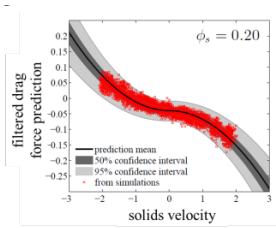
MFiX

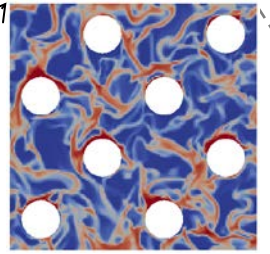




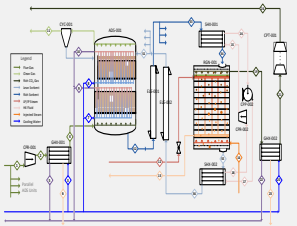




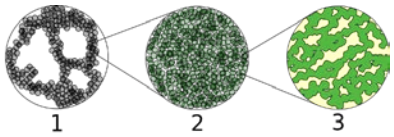


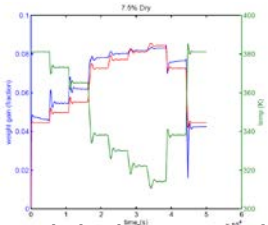


Process Models & Optimized Process



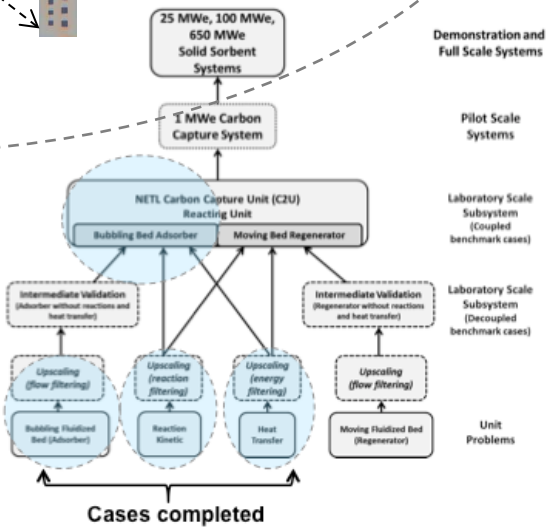
SORBENTFIT





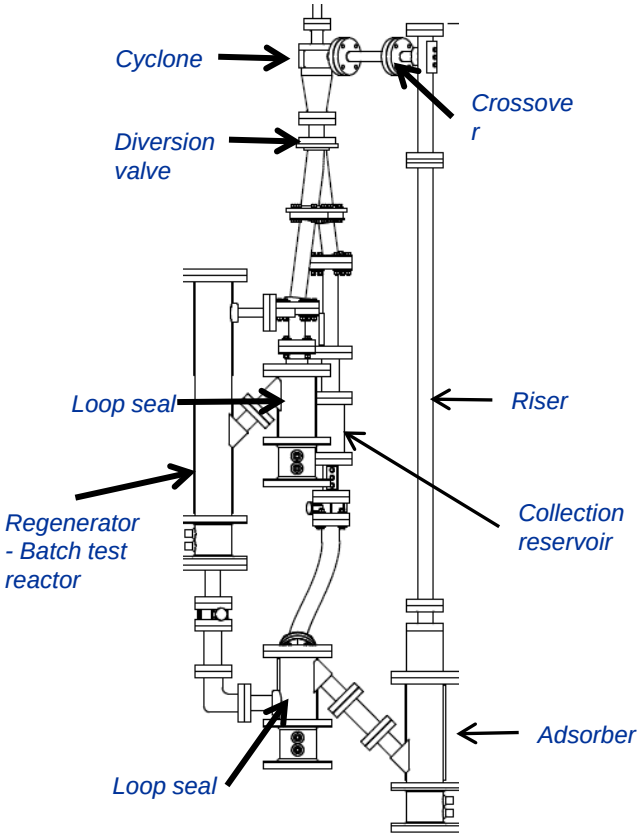
Experimental Kinetic/Mass Transfer Data

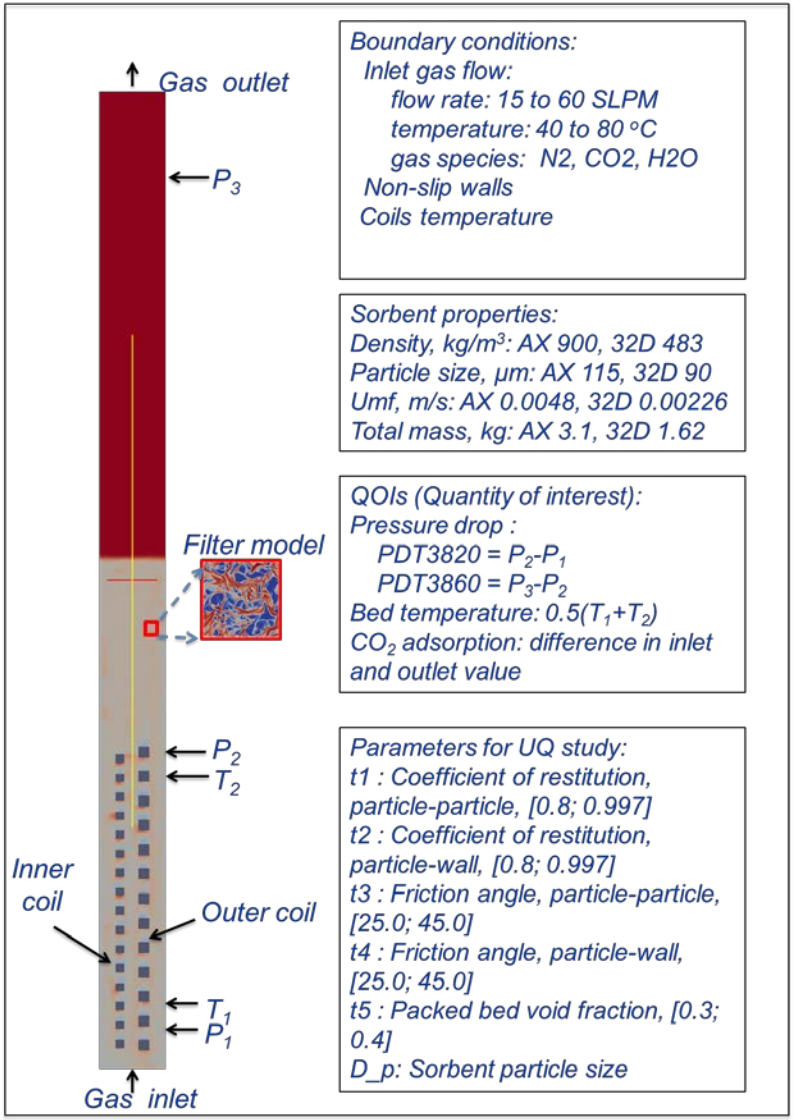
CCSI CFD Validation Hierarchy



C2U Experimental Design and CFD Model

Sketch of C2U batch unit experiments
71 experiments conducted





C2U and validation data

- **Statistical, space-filling experimental design**
  1. **Cold Flow testing – hydrodynamics**
  2. **Hot Flow testing – heat transfer, hydrodynamics**
  3. **Reaction testing – reaction kinetics, heat transfer, hydrodynamics**

- **Experiment parameters**
  - **Gas flow rate**
  - **CO_2 fraction in gas**
  - **Coil temperature**

- **Quantities of interest (QOI)**
  - **Bed pressure**
  - **Bed temperature**
  - **CO_2 total adsorption**
  - **CO_2 breakthrough curves**

Sorbent AX			Sorbent 32D					
Cold Flow	Hot Flow		Cold Flow	Hot Flow		Reacting Flow		
Flow (SLPM)	Flow (SLPM)	Temp(°C)	Flow (SLPM)	Flow (SLPM)	Temp(°C)	Flow (SLPM)	Temp(°C)	CO_2 Conc.
49.8	16.9	70.3	19.2	21.9	60.4	51.3	62.9	18.9
15	48.8	60.2	23.6	39.5	66.7	40	62.3	10.8
58.9	35.4	56.3	50.3	43.8	45.3	37	68.2	14.6
43.7	38.6	67.4	51.7	46.3	40.3	27.3	72.8	15.7
35.7	57.1	43.5	37	36.7	65	23.3	57.5	14.2
29.8	20.8	58.4	31.9	31.9	52.1	59	40.7	17.4
25.1	27.1	52.4	45.9	16.4	71.1	33.7	69.8	16.3
20.4	30	42.7	57.5	26.7	47.7	35.6	41.6	10.4
54.6	48.6	49	39.7	22.7	53.4	23.1	64.3	16.9
40.3	26	77.2	25.4	52.7	78.1	32.8	59	18.3
38.4	54.7	65.6	59.6	58.1	57.7	41.3	70.4	20
23.2	41.9	74.2	33.3	51	73.4	20.5	44.8	14.3
31.6	40.6	61.8	16.1	30.6	79.1	56.4	63.6	13.7
28	52	73	27.4	59	68.8	17.9	48	10.5
47.8	23	47.4	21.6	48.1	55.2	43	71.7	18.2
18	15.8	45.3	43.3	19.3	65.7	56.9	57.9	10.2
33.4	29.5	69.7	54.9	39.3	43.5	32	79.1	15.3
52.6	44.4	40.5	41.4	49.4	63	49.1	61.6	17.1
46	36	50	29.6	29.7	76	44.8	65.4	19.7
56.9	19.2	76.3	47.7	56.1	42.6	50.2	46.2	16.5
15	32.2	63.8	16.1	35.2	58.5	59.7	44.3	13
31.6	46.1	54.4	45.9	17.1	48.5	57.5	59.3	15.9
49.8	53.3	56.8	57.5	42.3	51.6	38.2	76.9	14.9
35.7	58.7	79.4	41.4	25.8	71.9	24.5	67.8	12
20.4	15.8	45.3	25.4	17.1	48.5	49.3	52.7	19.5
46	38.6	67.4	33.3	30.6	79.1	52.2	50.2	11.4
25.1	36	50	21.6	58.1	57.7	45.9	60.1	12.6
43.7	58.7	79.4	29.6	51	73.4	15.9	67	12.2
56.9	53.3	56.8	51.7	19.3	65.7	35.8	53.1	13.9
54.6	19.2	76.3	50.3	43.8	45.3	55	54	14.6
29.8			37			48.2	54.9	13.1
38.4			43.3			54.4	75.7	11.9
47.8			19.2			15.1	56.4	15.1
23.2			27.4			34.6	47	12.7
58.9			54.9			30.2	77.6	16.7
33.4			39.7			26.7	48.3	10.8
18			31.9			19.9	44	17.9
40.3			47.7			28.6	50.7	13.3
28			59.6			25.1	74.5	11.6
52.6			23.6			22.2	76.4	16.1
						46.8	40.9	19.2
						39.2	66.1	18.4
						30.8	42.7	13.4
						44.5	69.1	15.6
						42.3	56	11.1
						53.4	72.5	18.8
						19	79.3	17.7
						27.9	73.7	19.3
						17.6	51.8	17.5
						40.5	49.4	11.6
						19	79.3	17.7
						32.8	59	18.3
						54.4	75.7	11.9
						46.8	40.9	19.2
						38.2	76.9	14.9
						24.5	67.8	12
						20.5	44.8	14.3
						57.5	59.3	15.9
						56.9	57.9	10.2
						35.6	41.6	10.4

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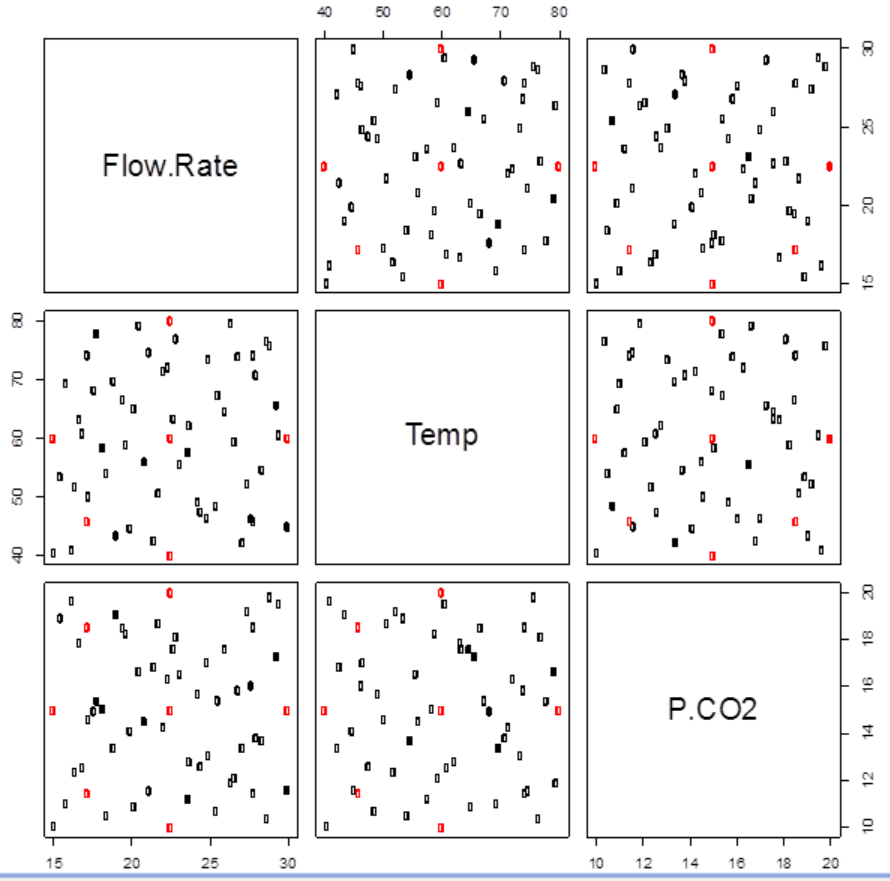
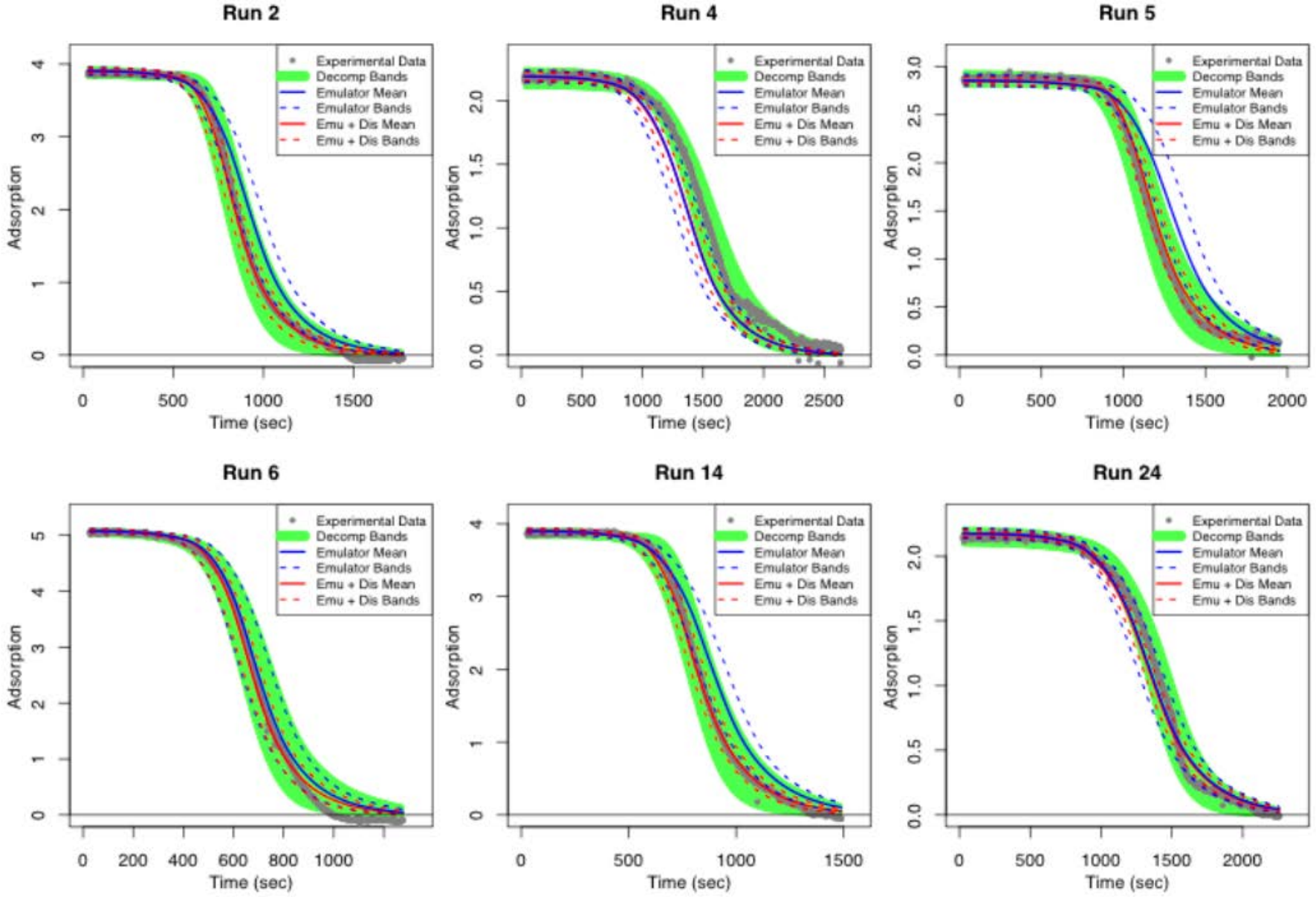
- **Quantities of interest (QOI)**
  - **Bed pressure**
  - **Bed temperature**
  - **CO_2 total adsorption**
  - **CO_2 breakthrough curves**



Calibrated Model Results & Experimental Data



Deliverables and Next Steps

- **C2U Validation Milestone Report**
  - **Model setup, input data files, parameter determinations and comparison data sets for easy implementation with a different software or for a different application**
  - **Statistical tools and methods used in the calibration/validation process with best-practices documentation**

- **Next steps:**
  - **Simulation with quantified confidence for 1MW BFB adsorber**
  - **Prediction/Validation for 1 MW pilot system**

C2U Moves to NCCC For Additional Testing

- **Dismantled, shipped, and reassembled the C2U in Wilsonville, Alabama**
- **Conducted 50 hours of circulating flow without sorbent performance degradation**
- **Currently conducting 1,000 hour exposure in batch test mode for contamination**

U.S. Department of Energy
National Carbon Capture Center
at the Power Systems Development Facility
PARTICIPANTS:
Managed by Southern Company Services, Inc.

Acknowledgements

Sorbents/C2U

- Dave Luebke
- Mac Gray
- Jim Hoffman
- Larry Shadle
- Jim Spenik
- Rupen Panday
- NCCC Support Team

CCSI

- Xin Sun
- Curt Storlie
- Kevin Lai
- Wenxiao Pan
- Zhijie Xu
- Tingwen Li
- Jeff Dietiker
- The other 80+ researchers on the CCSI Technical Team

CCSI Toolset: Info Session This Evening @ 5:45 in Ellwood

Basic Data Submodels	High viscosity solvent model
	SorbentFit – Kinetic/diffusion basic data fitting tool with UQ
High Resolution Filtered Submodels	Attrition Model
	Cylinder Filtered Models with quantified uncertainty bounds
Validated high-fidelity CFD models & UQ tools	1 MW Adsorber and Regenerator CFD Models (validated)
	Large scale adsorber and regenerator CFD Models
	Statistical Model Validation Tool for Quantifying Predictions
	REVEAL: Reduced Order Modeling Tools for CFD and ROM Integration Tools
Process Models	Bubbling Fluidized Bed Reactor Model
	Moving Bed Reactor Model
	Multi-stage Centrifugal Compressor Model
	Membrane CO_2 Separation Model
	Reference Power Plant Model
Optimization and UQ Tools	FOQUS – Optimization & Quantification of Uncertainty
	ALAMO – Surrogate models for optimization
	Process Synthesis Superstructure
	Oxy-Combustion Process Optimization Model
Dynamics & Control	D-RM Builder
Risk Analysis Tools	Technical Risk Model
	Financial Risk Model
Crosscutting Integration Tools	SimSinter – Links simulation files to FOQUS/Turbine
	Turbine Science Gateway – Runs hundreds of thousands of simulations