BIAS Sorbent NCCC Testing/CCSI Modeling

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Integrated Materials Development

Characterization

Fabrication

Synthesis

Performance Testing

CCSI Simulation & Analysis

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
TGA & Performance Data Collection

Ramp Rates

% CO₂

% H₂O

Temperature

Sorption Kinetics

CCSI

0 5 10 15 20 25 30 35 40 45 50

Time (h)

TGA Mass

100

105

110

115
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

Sorbent Development: CCSI communication
Polyethyleneimine Silane Coupling

Polyethyleneimine Mn 423-2000

Aminosilanes

Simple
Scalable
Acceptable Capacity
Moisture Resistance
Stability
Saleable

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
- CO₂ regeneration improbable
- Stable at 110-115°C
- 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
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

Academia

Carnegie Mellon

PRINCETON UNIVERSITY

West Virginia University

BOSTON UNIVERSITY

The University of Texas at Austin

Industry

ADA

ALSTOM

B&W

GE

EPRi

FLUOR

PHILLIPS

APT

AMERICAN ELECTRIC POWER

FLUOR

SOUTHERN COMPANY

66

ExxonMobil

ANSYS

URS

aspentech

invensys

PSE
Tools to develop an optimized process using rigorous models

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**Process Models**

- Solid In
- Solid Out
- Gas In
- Gas Out
- Utility In
- Utility Out

**Algebraic Surrogate Models**

**Basic Data Submodels**

**Simulation-Based Optimization**

- Output: Best variable and objective values
- Input: Initial guess, problem definition

**FOQUIS Engine: DFO and/or UQ**

**Meta-sheet Evaluation** — executed in parallel, may include rigorous heat integration

**Heat Integration Tool** — Solves LP transshipment model in GAMS, takes stream and equipment information from Design, and returns heat integration results

**Simulation** ( Aspen Plus, Aspen Custom Modeler, gPROMS, Microsoft Excel)

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**Superstructure Optimization**

Surrogate models for each reactor and technology used

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**Optimized Process**

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**Uncertainty Quantification**

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**Process Dynamics and Control**

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**CFD Device Models**
Simulation & Experiments to reduce time for design/troubleshooting

Experimental Validation

Process Models & Optimized Process

SORBENTFIT

Experimental Kinetic/Mass Transfer Data

Cases completed
C2U Experimental Design and CFD Model

Sketch of C2U batch unit experiments
71 experiments conducted

Boundary conditions:
- Inlet gas flow: flow rate: 15 to 60 SLPM
  temperature: 40 to 80 °C
- gas species: N2, CO2, H2O
- Non-slip walls
- Coils temperature

Sorbent properties:
- Density, kg/m³: AX 900, 32D 483
- Particle size, μm: AX 115, 32D 90
- Umf, m/s: AX 0.0048, 32D 0.00226
- Total mass, kg: AX 3.1, 32D 1.62

QOIs (Quantity of interest):
- Pressure drop:
  PDT3820 = P2-P1
  PDT3860 = P3-P2
- Bed temperature: 0.5(T1+T2)
- CO₂ adsorption: difference in inlet and outlet value

Parameters for UQ study:
- t1: Coefficient of restitution, particle-particle, [0.6; 0.997]
- t2: Coefficient of restitution, particle-wall, [0.6; 0.997]
- t3: Friction angle, particle-particle, [25.0; 45.0]
- t4: Friction angle, particle-wall, [25.0; 45.0]
- t5: Packed bed void fraction, [0.3; 0.4]
- D_p: Sorbent particle size
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
C2U and validation data

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• Experiment parameters
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  – CO₂ total adsorption
  – CO₂ 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
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## CCSI Toolset: Info Session This Evening @ 5:45 in Ellwood

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