NATIONAL ENERGY TECHNOLOGY LABORATORY

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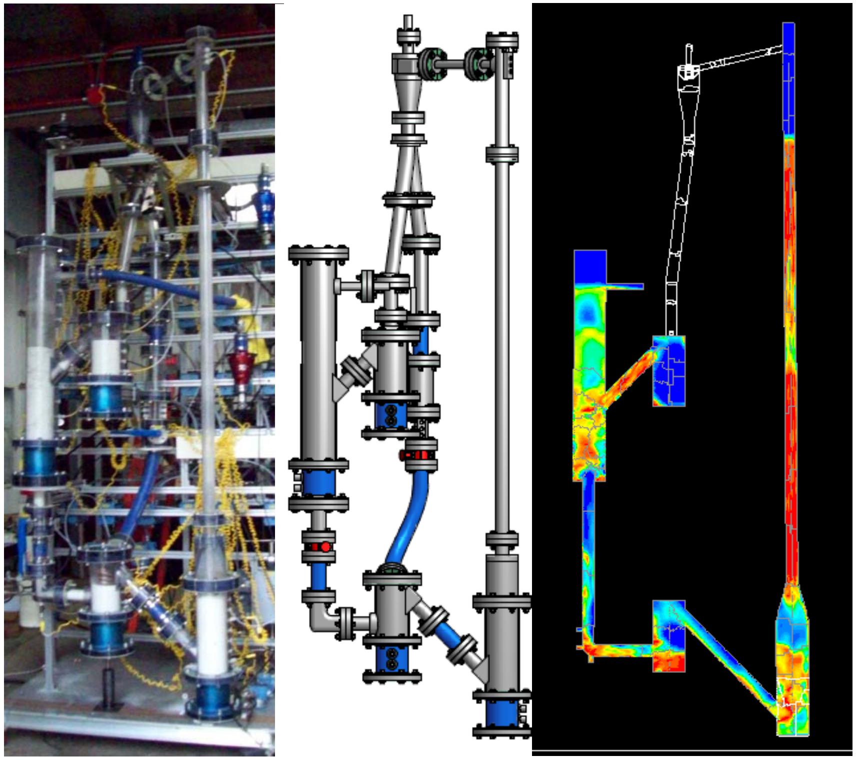


Model Validation Experimental Activities

Larry Shadle

2012 Multi Phase Flow Conference

at WVU NRCCE

May 23, 2012

Outline

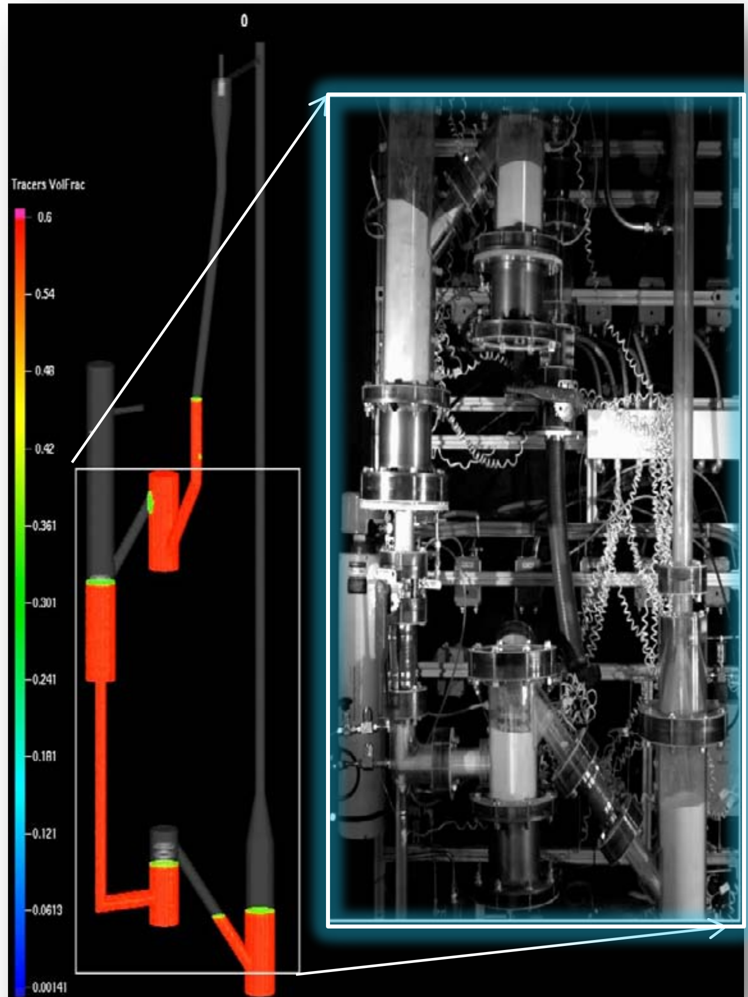
- **Carbon Capture Experiments**
  - C2U video compared to CPFD simulations
  - Sorbent kinetics
  - Batch tests
  - Elutriation

- **Side Inlet jet in 12-inch Riser**
  - Installation and plans
  - ECVT measurements issues and solutions
- **Small Scale Challenge Problem**
  - Proposed test matrix
  - Schedule

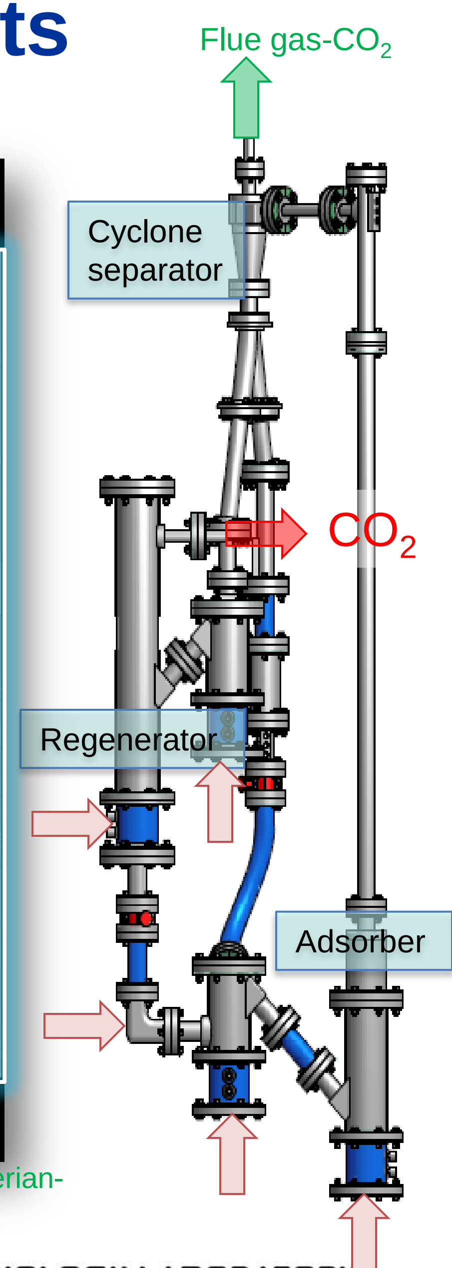
Carbon Capture with Sorbents

Model Validation Experiments

- Carbon Capture Unit -- C2U
- An integrated CO_2 adsorber and sorbent regeneration unit
- Temperature swing adsorption/regeneration
- CPFD simulation and video of initial system startup
  - glass beads
  - solids flow from aeration
  - fluidization character
  - shifting of bed inventory
  - leading to slugging in adsorber



Clark, et al. (2012) CO2 Absorption Loop Experiment with Eulerian-Lagrangian Simulation, , Powder Tech. Sp issue.
[3]Video courtesy Balaji GoPalan

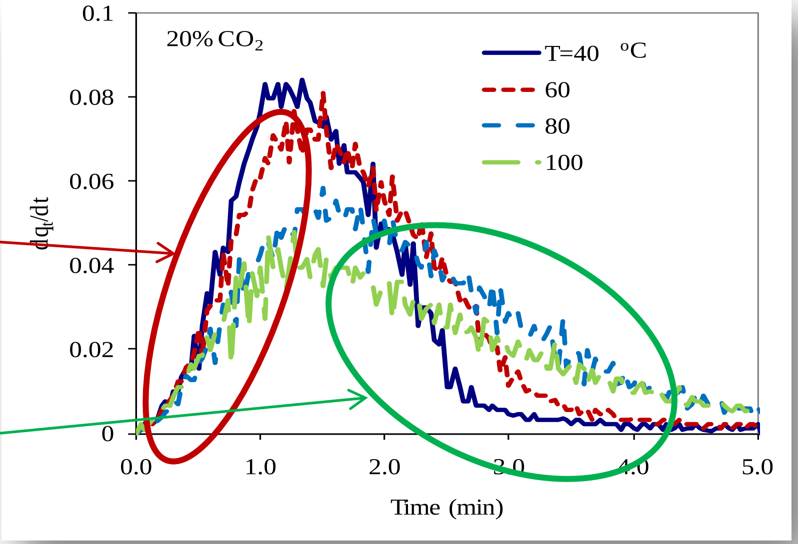


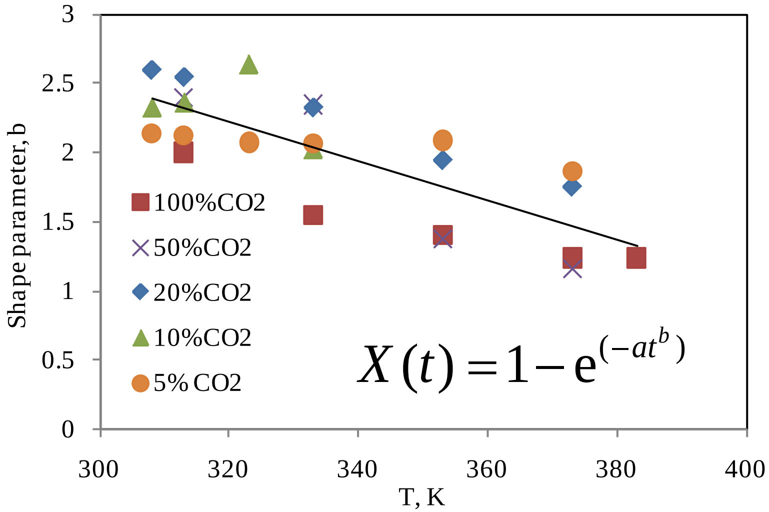
CO_2 Capture on PEI Si Sorbent

Follows Diffusion Controlled Nucleation and Growth Kinetics

- **Product Nuclei formation was reduced at higher T**
  - Increased reverse reaction rates
  - Heterogeneous sites tend towards homogeneous
- **Nuclei growth increased with increased T**
- **Diffusion controlled growth theory:**
  - b = 1.5 for zero nucleation rate
  - b = 1.5 to 2.5 for decreasing nucleation rate
  - b > 2.5 for increasing nucleation rate
- **Overall Nucleation and Growth Rate:**

$$\frac{dX}{dt} = 0.42e^{\frac{662}{T}} y_{CO_2}^{0.693} (1-X)\sqrt{-\ln(1-X)}$$





Monazam, et al. (2012)…Absorption Kinetics…by Solid Supported Amine Sorbent, AIChE Journal.

Theile Modulus Analysis

PEI impregnated sorbent (196C)

General Theile Modulus is the ratio of the kinetic rate to the diffusion rate

$$\emptyset = \frac{d_p}{6}\left[\frac{(n+1)k^n RT}{2D_A^{eff}} P_{A,i}^{n-1}\right]^{1/2}$$

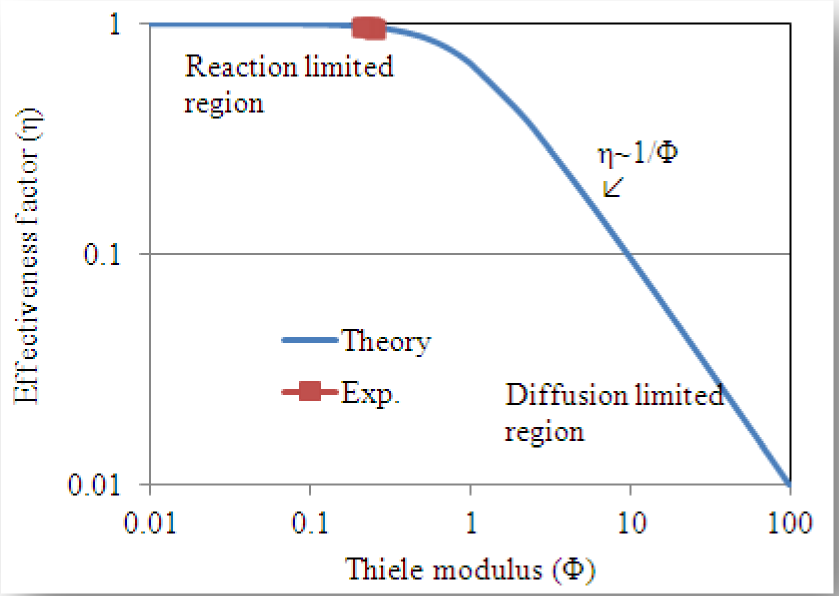
Kinetic rate, k^n, from diffusion controlled nucleation growth model.

$$\frac{dX}{dt} = 2a^{1/2}(1-X)\sqrt{-\ln(1-X)} \quad where \quad k = 2a^{1/2}$$

When the effectiveness factor, η, is near 1 the reaction is kinetically controlled

$$\eta = \frac{1}{3\emptyset^2}\left(\frac{3\emptyset}{\tanh(3\emptyset)} - 1\right)$$

When the effectiveness factor approaches 0 then diffusion is the rate controlling process



Experimental data taken between 40 and 110°C and 5-100% CO_2

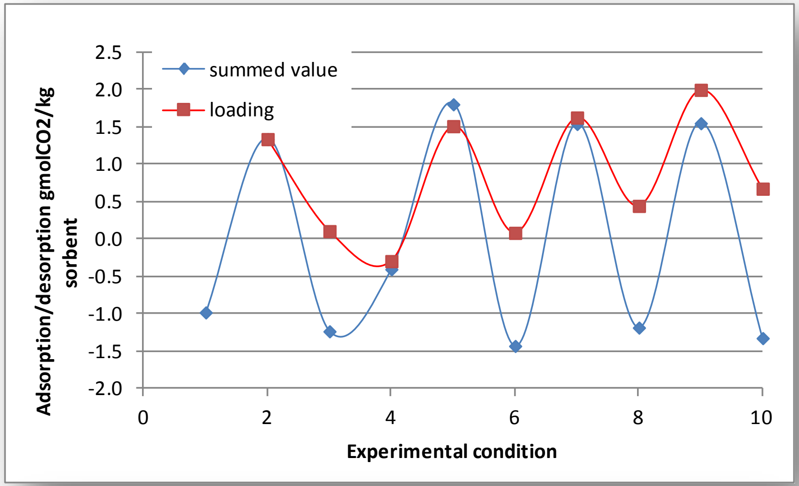
Monazam, et al. (2012). Absorption Kinetics…by Solid Supported Amine Sorbent, AIChE Journal.

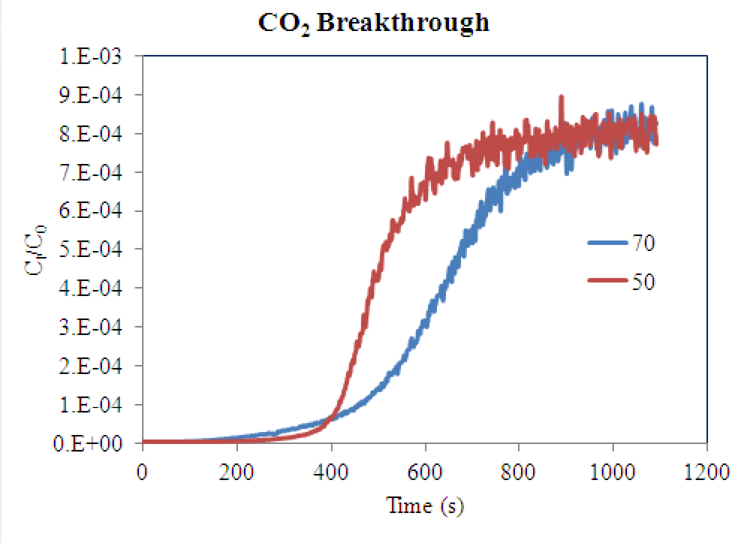
Preliminary C2U Batch Test Results

Sorbent AX

	liters CO_2
70 deg rep 1 =	90.28
70 deg rep 2 =	121.80
40 deg rep 1 =	104.20
40 deg rep 2 =	105.70

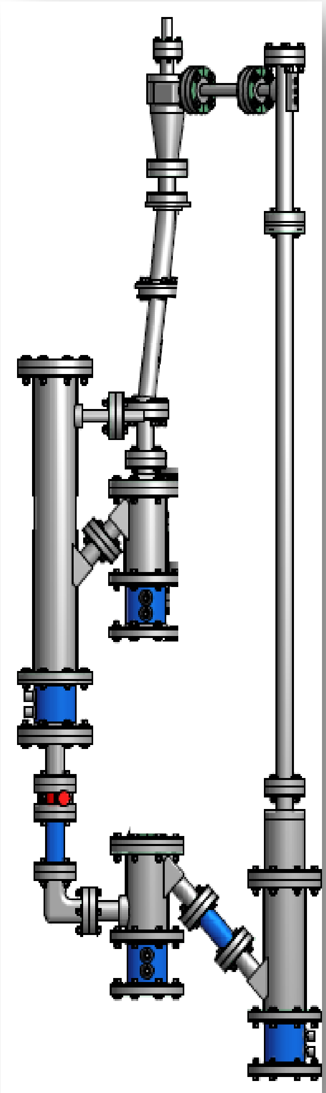
- Batch tests conducted on sorbent capacity, heats of reaction, and heat transfer coefficient.
- Improved adsorption repeatability
- Regeneration incomplete
  – Loading crept up for later cycles
- Same negative T dependence observed in TGA with 196C
  – Rate increased at lower T

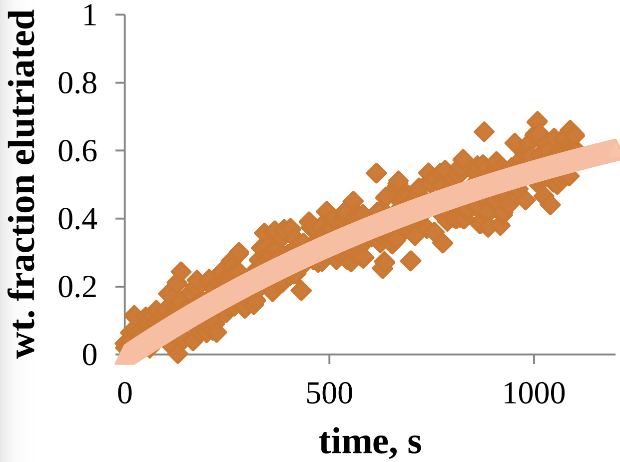


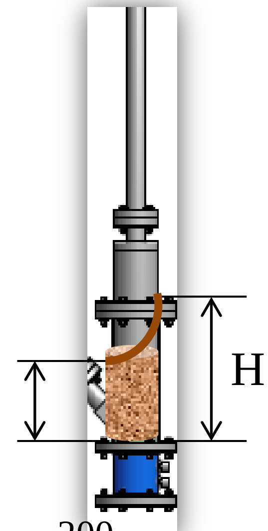


Role of Elutriation in C2U Operations

circulation rate and approach to steady state







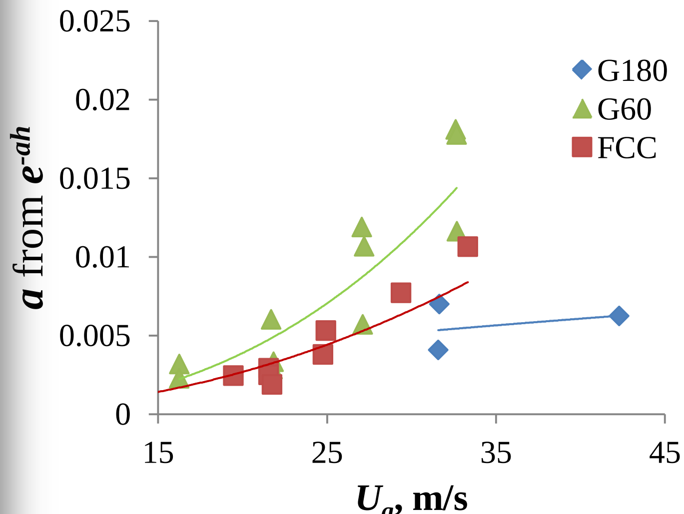
Entrainment*

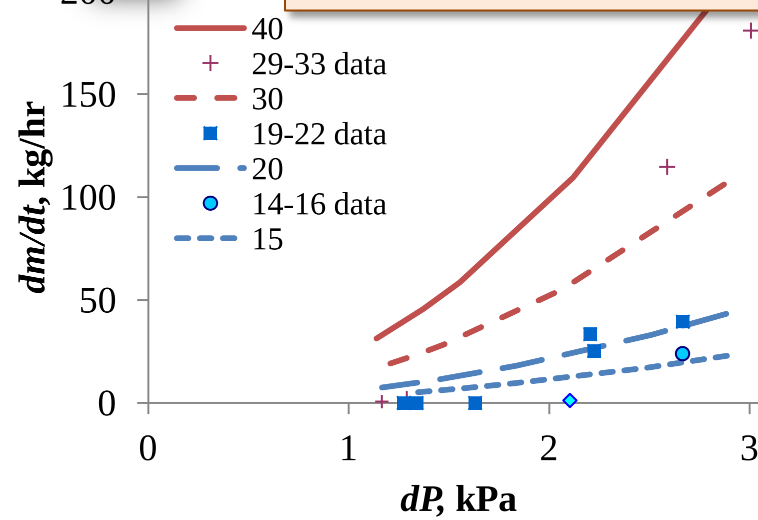
$$\varepsilon = \varepsilon_0 \cdot e^{-ah}$$

where a is f(U_g, d_p, ρ_s, ρ_g)

Want dm/dt as f(P):

$$\frac{dm}{dt} = m_0 \cdot e^{-at}$$

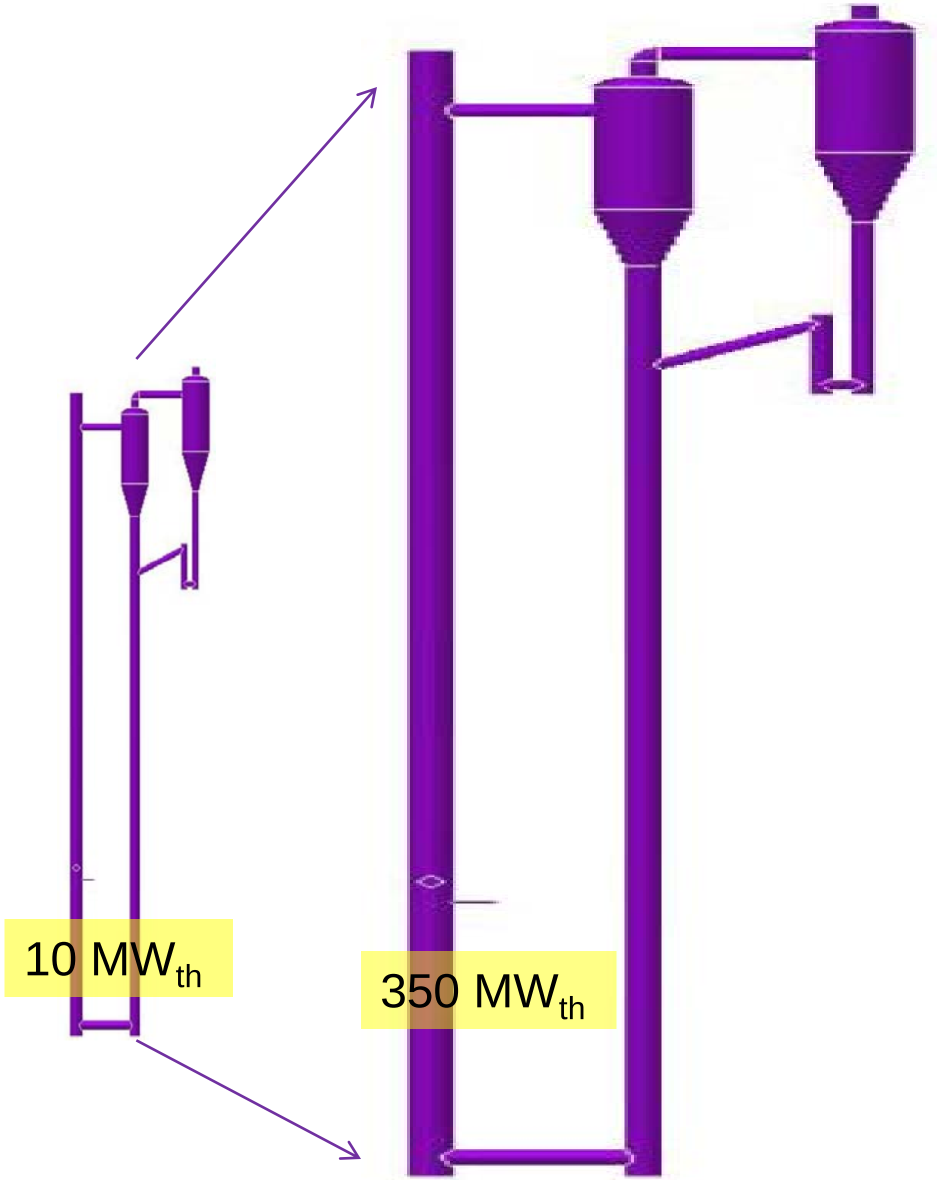




*Kunii and Levenspiel (1995). Fluidization. Engineering, Butterworth & Heineman. p. 165-176.

Motivation for Side Jet Validation

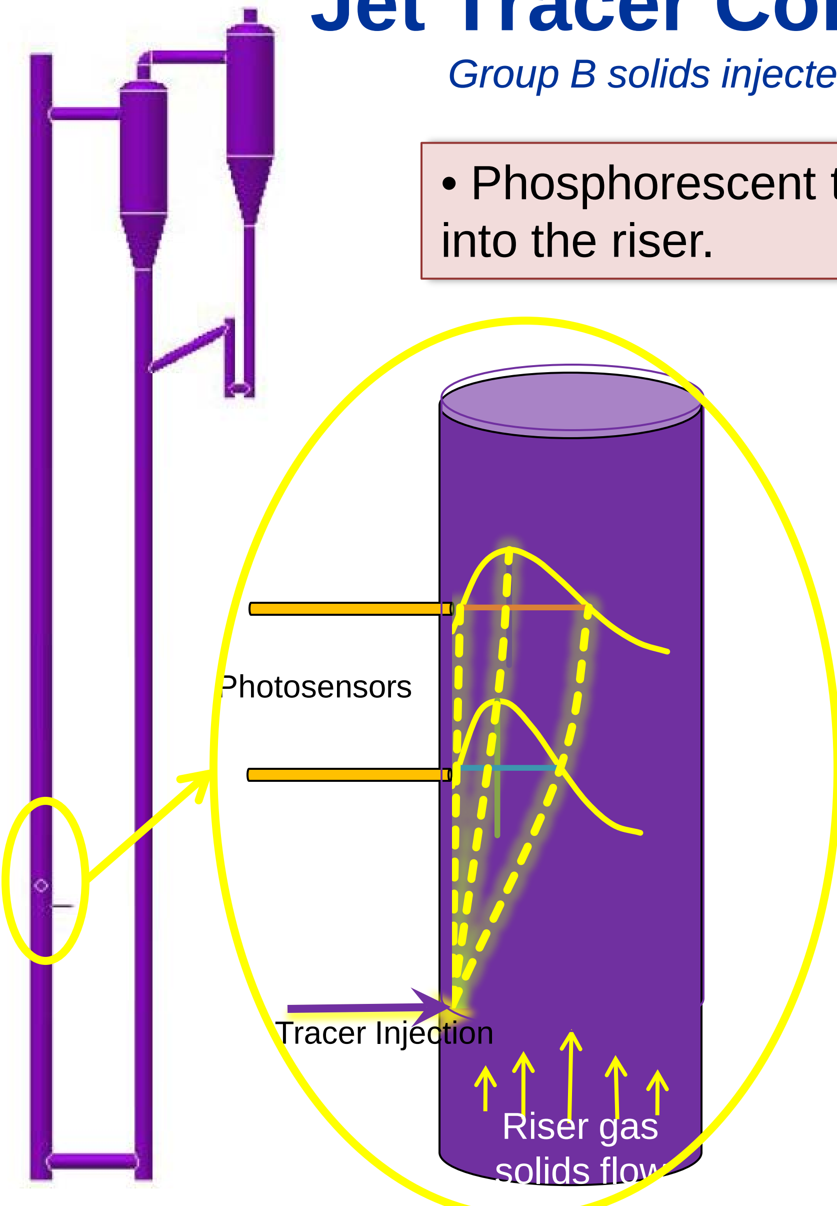
- **Pilot scale such as TRIG use side coal feed and gas supply ports**
- **Commercial scale transport gasifier is a larger diameter.**
- **Goal: to avoid channeling and achieve mixing, efficient conversion, and process stability.**
- **Approach: to measure jet penetration, validate CFD simulations, and use CFD to assist designs and optimize performance**



Jet Tracer Concentrations

Group B solids injected with v_s=3.75 m/s

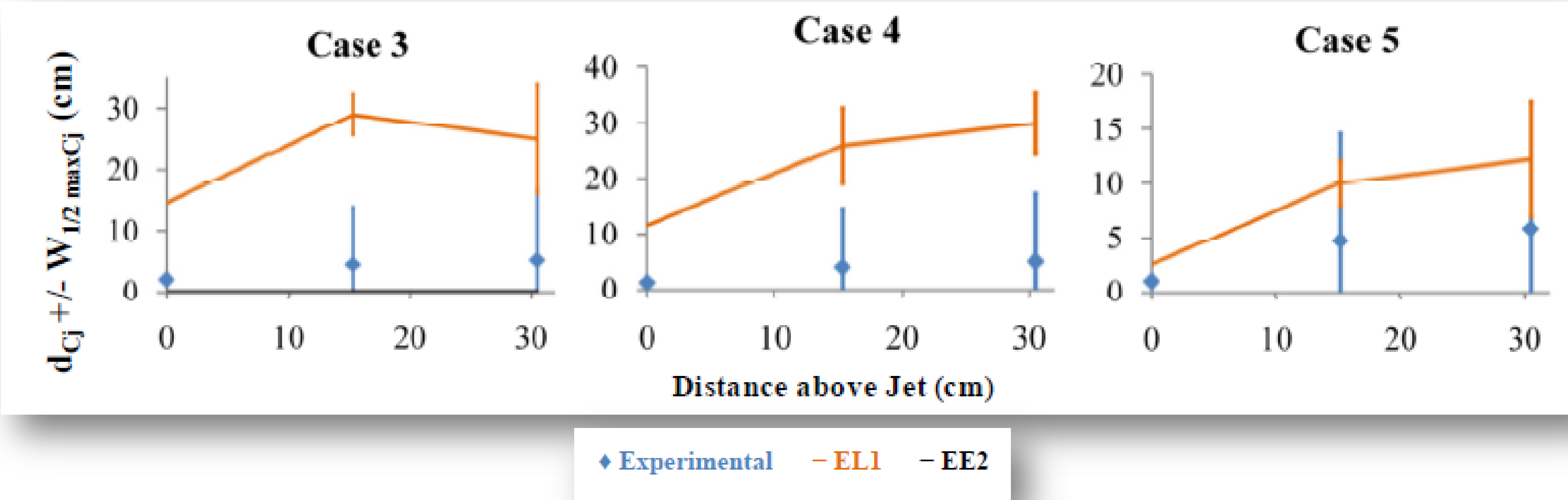
• Phosphorescent tracers enabled tracking solids injected into the riser.



- **Phosphorescent particles are activated and immediately injected at known mass flux and gas velocity.**
- **Photosensors are used to traverse the cross section above and below the solids injection.**
- **Relative concentration of tracer particles provide:**
  - **Distance to peak conc. d_{Cj}**
  - **Spread of jet, $W_{1/2maxCj}$**

Jet Penetration

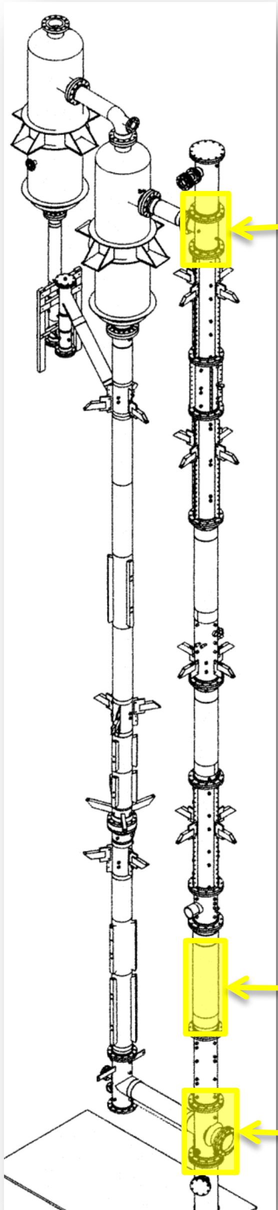
Challenge Problem III

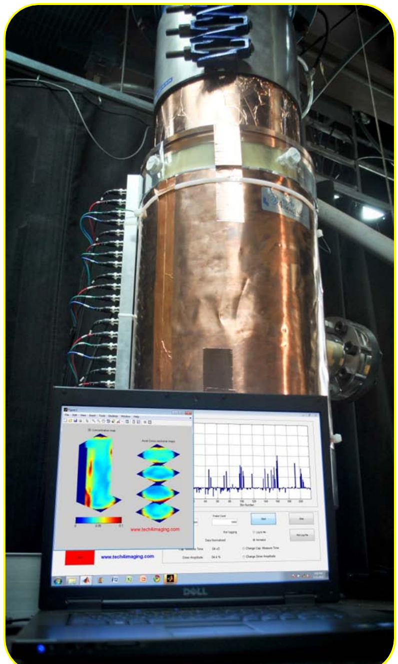


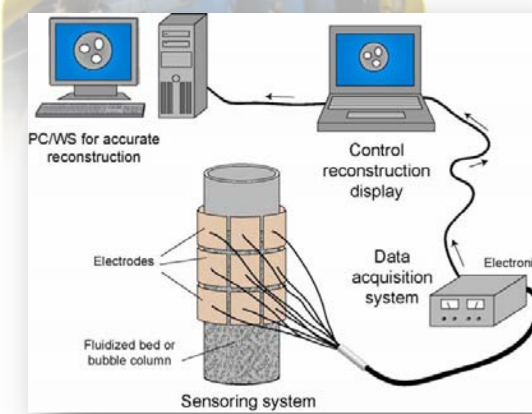
Jet penetration across radius of CFB riser from point of injection

- **Penetration simulated accurately in DSU case 5 (EL1)**
- **Penetration was over predicted (EL1) both:**
  - o at lowest gas velocity Fast Fluid Bed Case 3 and
  - o In core annular Case 4
- **No Penetration was predicted (EE2)**

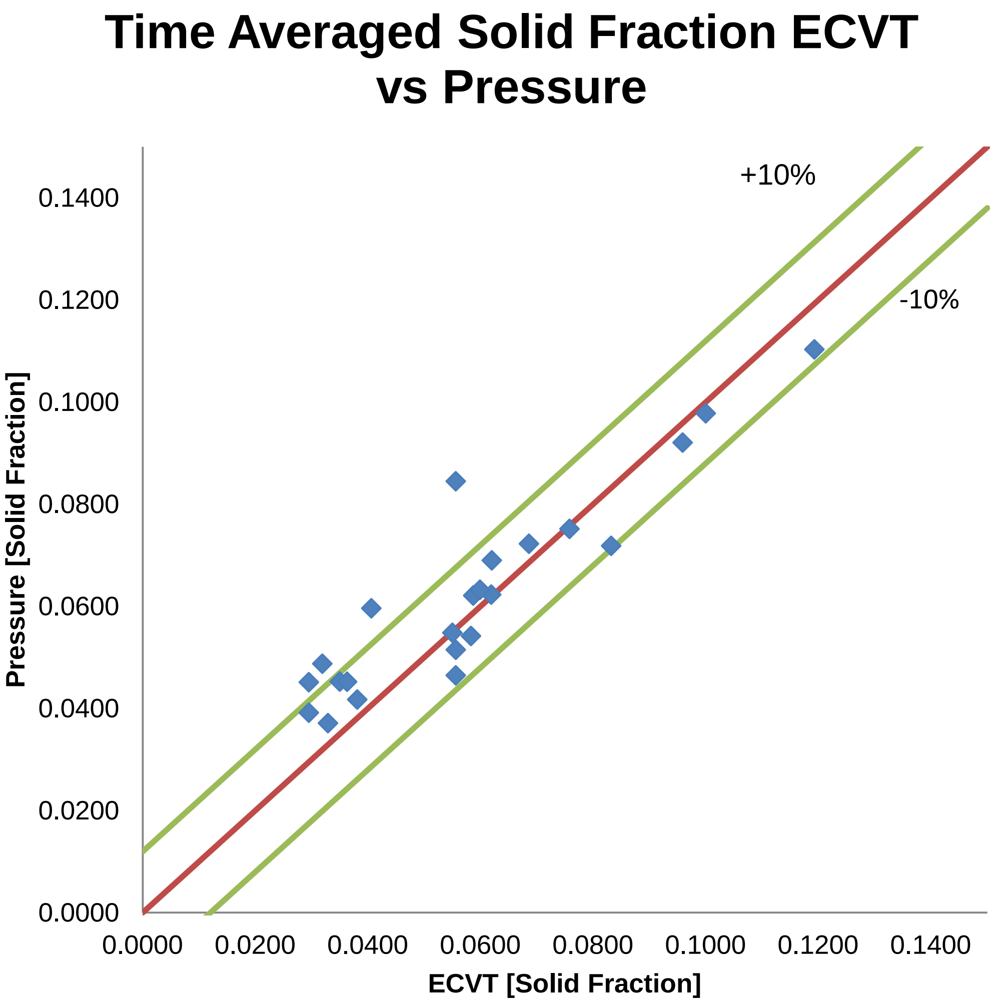
ECVT Sensors on 12-inch ID CFB Riser

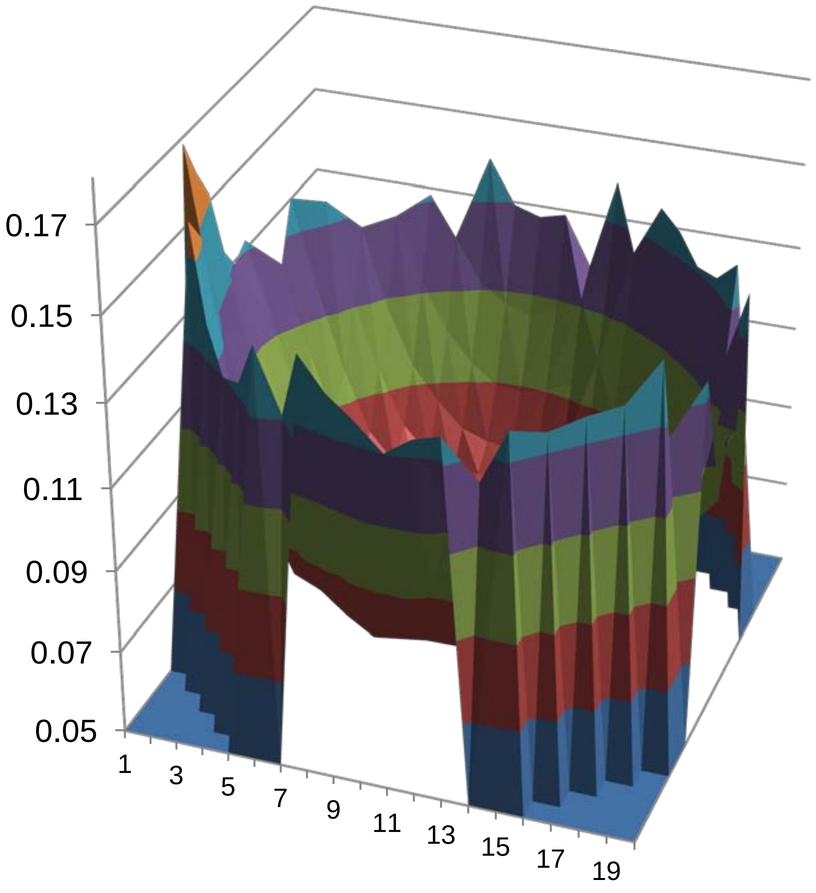






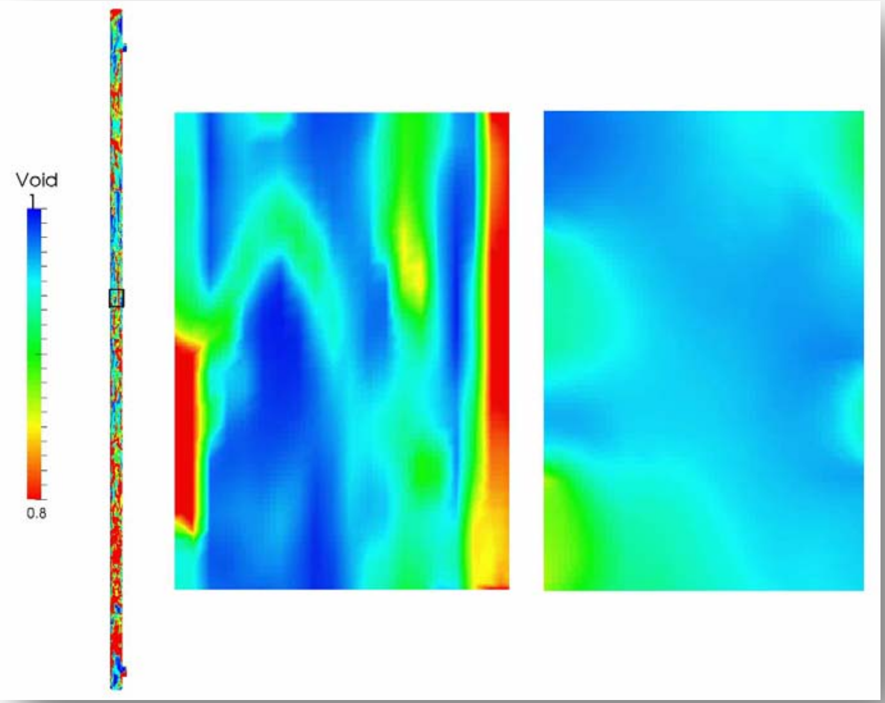
Pressure estimation compared to ECVT

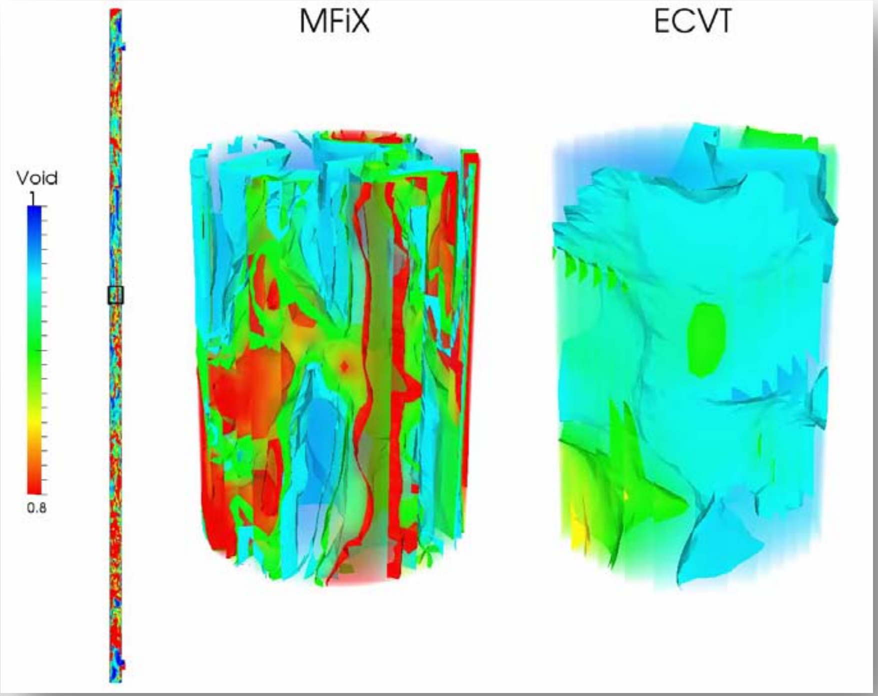




Modeled and Measured Voidage Across 30 cm ID Riser

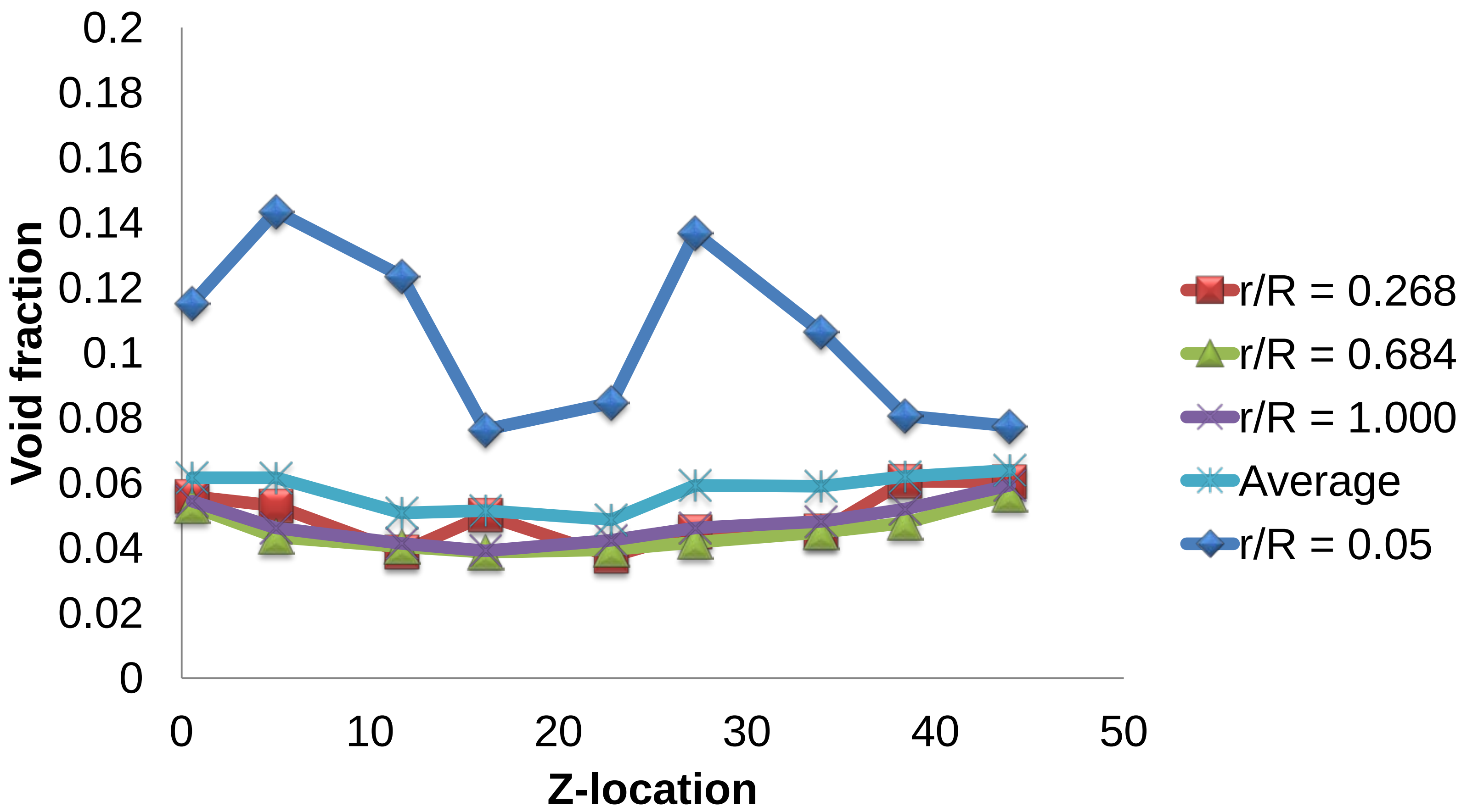
2D slice across a plane





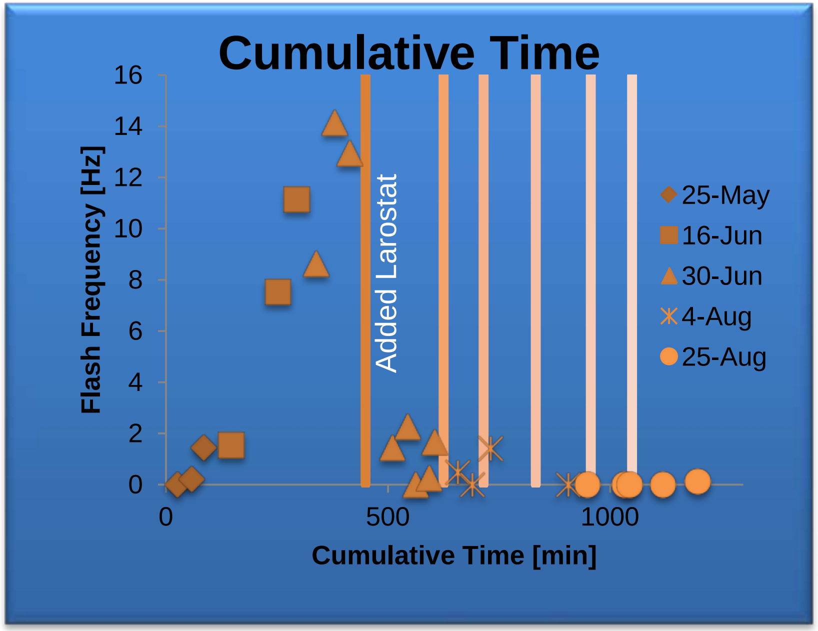
3D Rendering with Isosurface at 10% Void Fraction

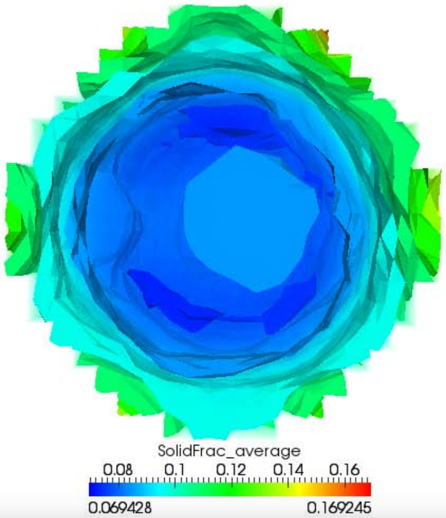
Radial Solid Fraction Profile in CFB Riser

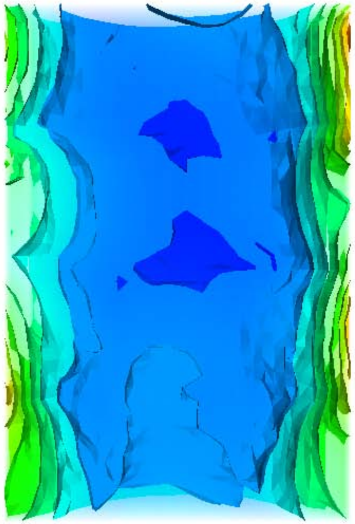


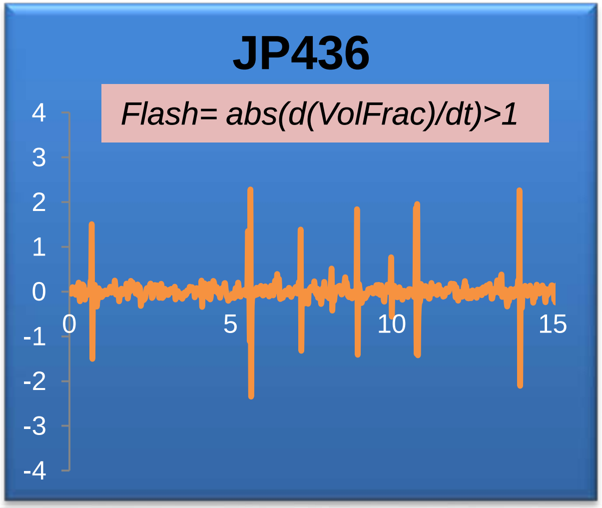
Resolving Artifacts in Preliminary ECVT Measurements

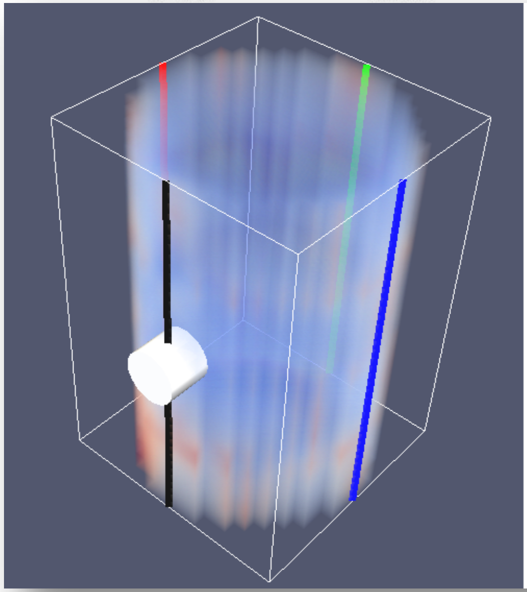
Electrostatic and Deconvolution Issues

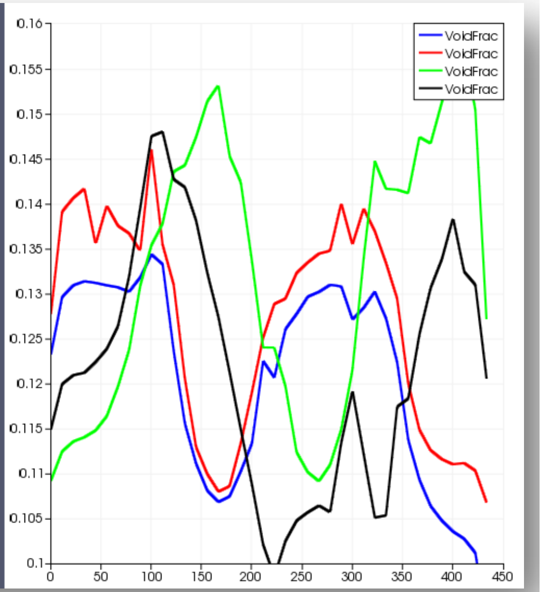








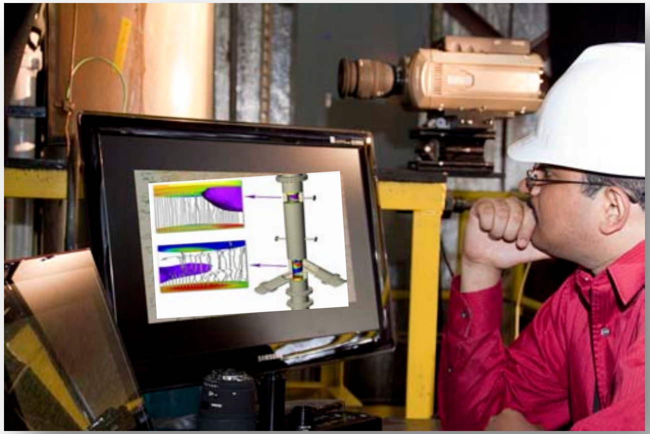




Motivation for Small Scale CPs (SSCP)

CP Goal was benchmarking computational models on industrial scale.

Shadle et al. (2011) CP Workshop, CFB X ed T. Knowlton, Sun River Oregon; and 2010 AIChE Annual Meeting Conference Proceedings, Salt Lake City, UT, 297i, pp.10.



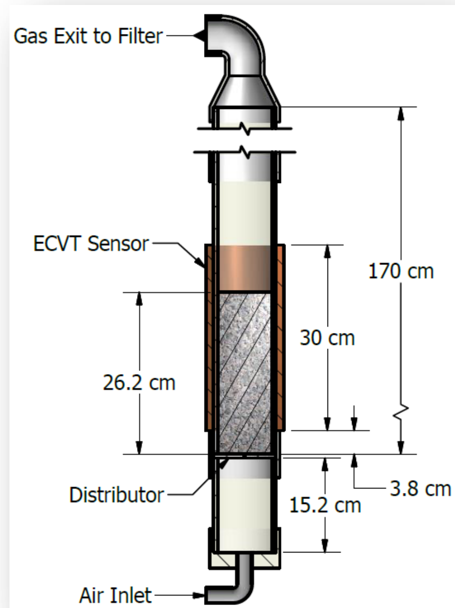
SSCP Goal is to assist in the improvement and development of multiphase CFD models.

- Desirable features include:
  - Expand testing to include other models: DEM…
  - Encourage model sensitivity studies
  - Reduce scale and complexity of test cases; needed human and computational resources
  - Conduct CP's at regular, more frequent intervals
  - Increase participation; Seek funding sources similar to IFPRE
- A series of highly controlled, well-defined small-scale CP's will be undertaken.

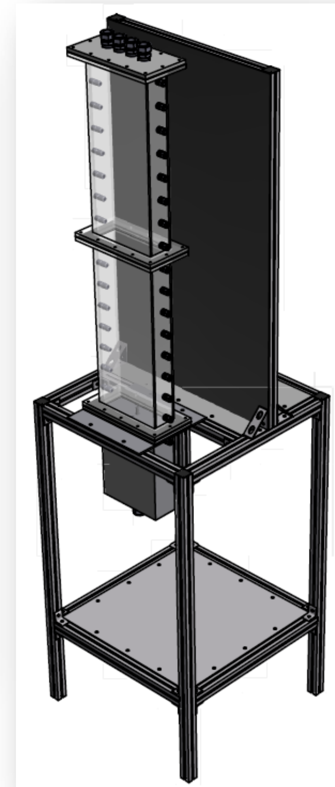
https://mfix.netl.doe.gov

SSCP: 10-cm ID and 2D FBs with Group D granular materials

- **Granular Materials**
  - 3000&6000 *μm* plastic (PSD)
- **Independent Parameters**
  - $U/U_{mf\ largest}$=1.5 and 3
- **Controlled/tracked Parameters**
  - Initial H_{bed} H/D=1.5
  - T, Barometric P, dP across the distributor
- **Dependent Parameter**
  - dP/dL across the bed
  - 3D voidage profile
  - HS-PIV particle velocity statistics



BFB
10-cm diam.



Rectangular FB
7.5x23x122 cm

Small-Scale Challenge Problem – SSCP1

- Baseline Models Against U_{mf}, U_{mb} and Bed Density Data
- → Model Challenge Problems
- → Compare Against Results
- → Refine Models

SSCP1: FB with Group D granular materials

2012												
10-cm BFB	Mon 1	Mon 2	Mon 3	Mon 4	Mon 5	Mon 6	Mon 7	Mon 8	Mon 9	Mon 10	Mon 11	Mon 12

Schedule

- Proof of concept – demonstrate all aspects of testing, ability to achieve stated test conditions and record stated measurements in 3 months
- Post Announcement of SSCP1 by Jun 30, 2012 (month 0 = start time)
- Tune drag model on minimum fluidization data by month 3
- Finalize experimental testing by month 4
- Analyze uncertainty of test data by month 5
- Release test results by month 6
- Compare tests against model simulations by month 9
- Recommend modifications to models and revise simulations by month 12

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