NATIONAL ENERGY TECHNOLOGY LABORATORY

Challenge Problem – Next Steps

PSRI

Particulate Solid Research, Inc.

Larry Shadle, Mehrdad Shahnam, Chris Guenther, & Ray Cocco

NETL 2011 Workshop on Multiphase Flow Science

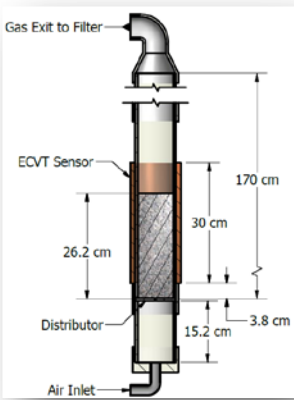
Airport Marriott Station Square, Pittsburgh, PA

August 16-18, 2011

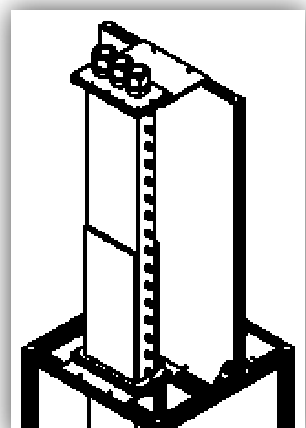
U.S. DEPARTMENT OF ENERGY

Outline

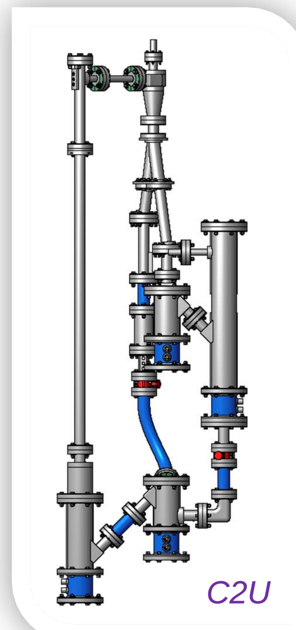
- **Motivation and Objectives**
  - Highlights of past industrial scale "Challenge Problems"
- **Upcoming Small-Scale Challenge Problems (SSCP)**
- **SSCP Release Schedule**



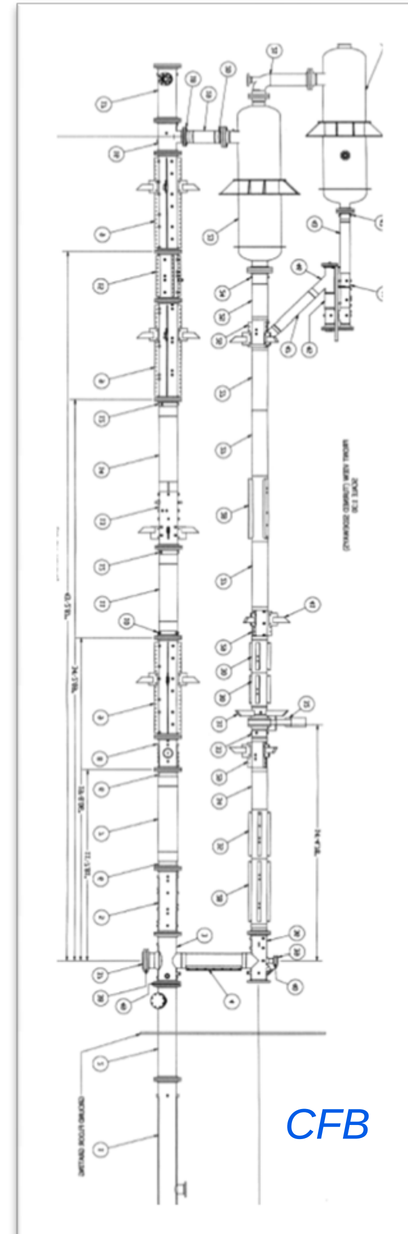
10cm BFB



Rectangular FB



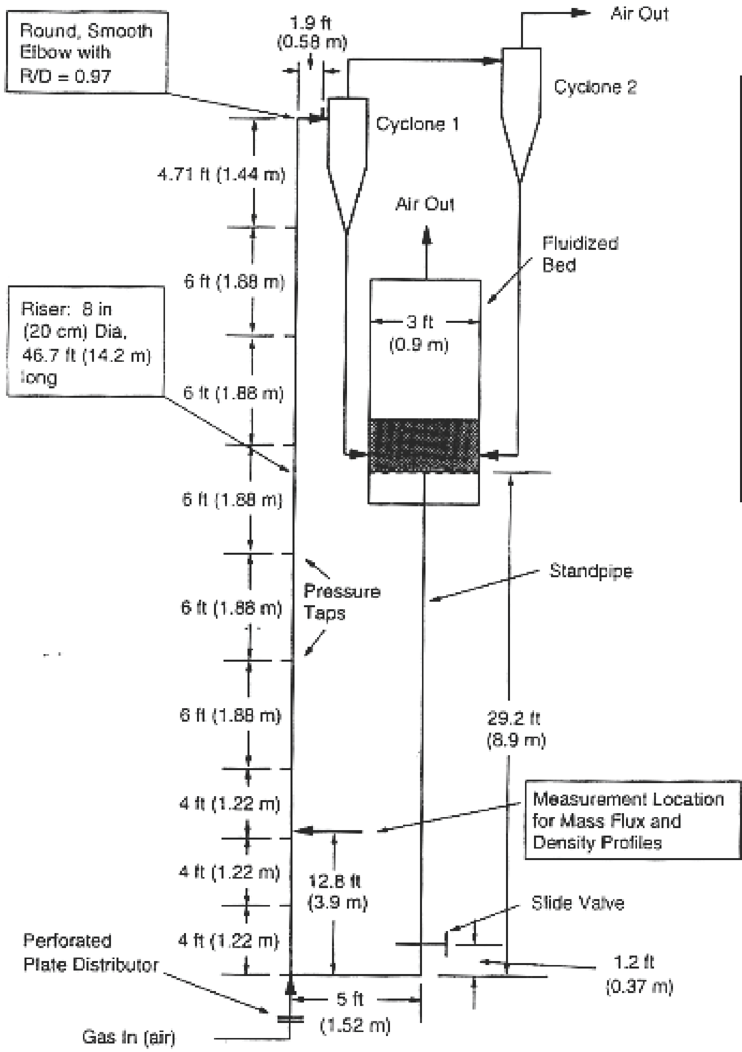
C2U



CFB

1995 PSRI Challenge Problem

Proprietary & Confidential



SCHEMATIC DRAWING OF 20-CM-DIA CFB TEST UNIT

I-12

FCC Catalyst (d_{p50} = 76 microns, ρp=107 lb/ft^3(1715 kg/m^3))

Superficial Velocity	Solid Mass Flux (Circulation Rate)			
	10 lb/ft^2-s (49 kg/m^2-s)	40 lb/ft^2-s (196 kg/m^2-s)	100 lb/ft^2-s (489 kg/m^2-s)	160 lb/ft^2-s (782 kg/m^2-s)
17 ft/s (5.2 m/s)			X	
25 ft/s (7.6 m/s)			X	
36 ft/s (11 m/s)	X	X	X	X

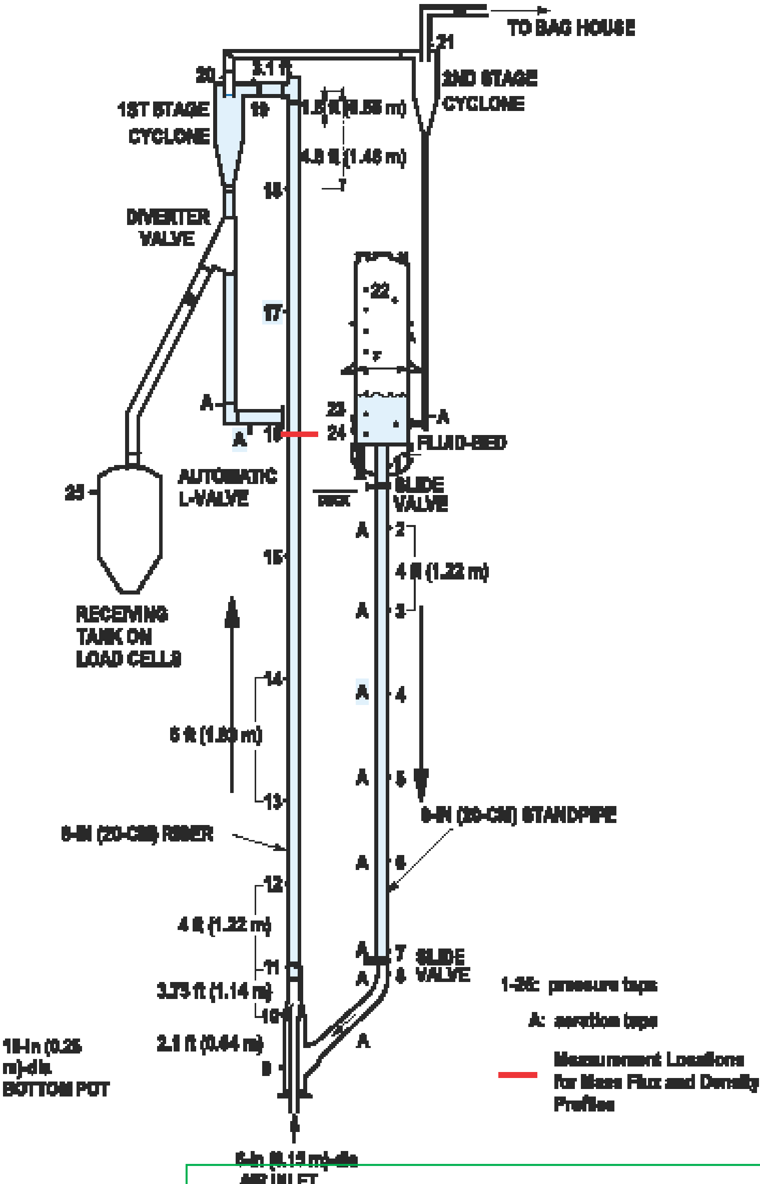
Sand (d_{p50} = 175 microns, ρp=165 lb/ft^3(2644 kg/m^3))

Superficial Velocity	Solid Mass Flux (Circulation Rate)		
	3 lb/ft^2-s (15 kg/m^2-s)	6 lb/ft^2-s (29 kg/m^2-s)	10.5 lb/ft^2-s (51 kg/m^2-s)
8 ft/s (2.4 m/s)		X	
13 ft/s (4 m/s)	X	X	X
19 ft/s (5.8 m/s)		X	

Ref: Laguerie & Large, Fluidization VIII Workshop, 1995.

10 Respondents

2001 PSRI Challenge Problem



FCC Catalyst (d_{p50} = 67 microns, ρp=75 lb/ft^3(1200 kg/m^3))

Superficial Velocity	Solid Mass Flux (Circulation Rate)	
	10 lb/ft^2-s (50 kg/m^2-s)	80 lb/ft^2-s (400 kg/m^2-s)
12 ft/s (3.7 m/s)	x	x
39 ft/s (12 m/s)	x	

Same DOE

Sand (d_{p50} = 178 microns, ρp=165 lb/ft^3(2644 kg/m^3))

Superficial Velocity	Solid Mass Flux (Circulation Rate)	
	10 lb/ft^2-s (50 kg/m^2-s)	80 lb/ft^2-s (400 kg/m^2-s)
12 ft/s (3.7 m/s)	x	x
39 ft/s (12 m/s)	x	

13 Respondents

Ref: Kwauk and Yang, Fluidization X Workshop, 2001.

Challenge Problem I & II

Challenge Problem I

1995

PSRI

Industrial Scale

20-cm-Diameter & 40-cm-Diameter Riser

FCC & Sand

Responses from 10 Groups

Three groups were successful

"Models were not sophisticated enough to be used to predict all of the hydrodynamics in a CFB".

Challenge Problem II

2001

PSRI

Industrial Scale

20-cm-Diameter riser with a blind tee and an elbow at the riser exit

FCC & Sand

Responses from 13 Groups

Range of total percent errors: 77 to 334%. The highest individual percent error was 838 %

"Models still needed substantial development to be able to predict CFB hydrodynamics".

2011 PSRI & NETL Challenge Problems

- **Two Systems this time, both with a twist**
  – "Bubbling" fluidized bed => with gas bypassing
  – CFB Riser => side mounted solids fed jet

- **Objectives**
  – Meet 2006 Multi-Phase Flow Roadmap goal:
    Benchmark model capabilities at industrial scale
  – Provide vetted data set

2011 Challenge Problem III

16-m-Long & 30.5-cm-Diameter CFB Riser

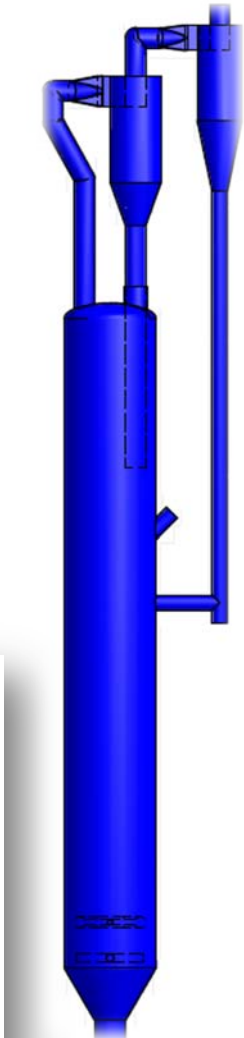
Responses from 5 Groups

4-64 hr to simulate 1s

6-m-Long & 92-cm-Diameter Bubbling FB

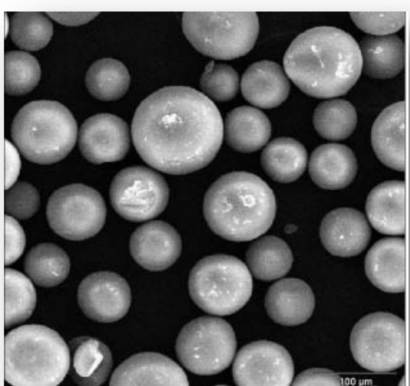
Responses from 3 Groups

15-24 hr to simulate 1s

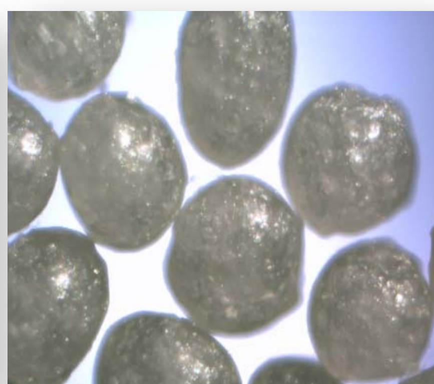


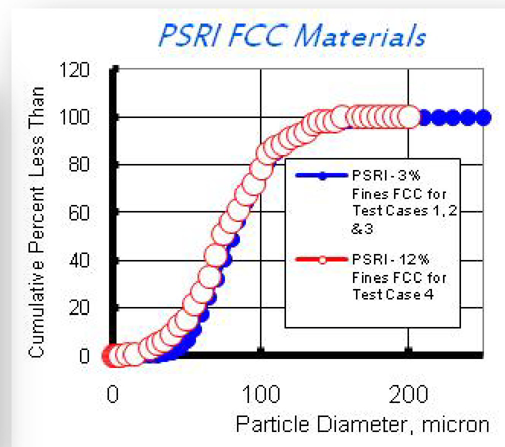
Ref: Shadle et al, Workshop at CFB X, 2011.

Geldart Group A



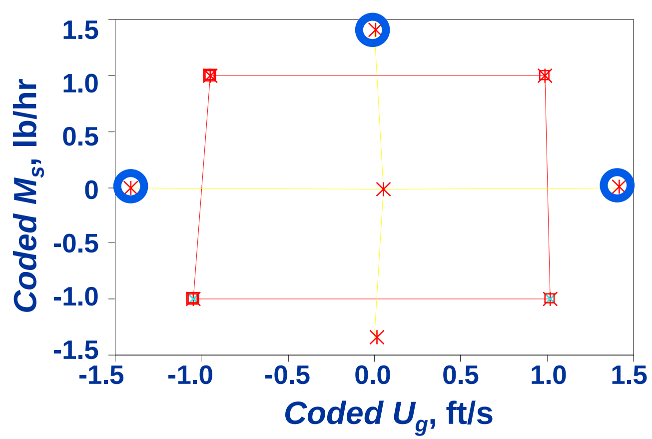
Geldart Group B

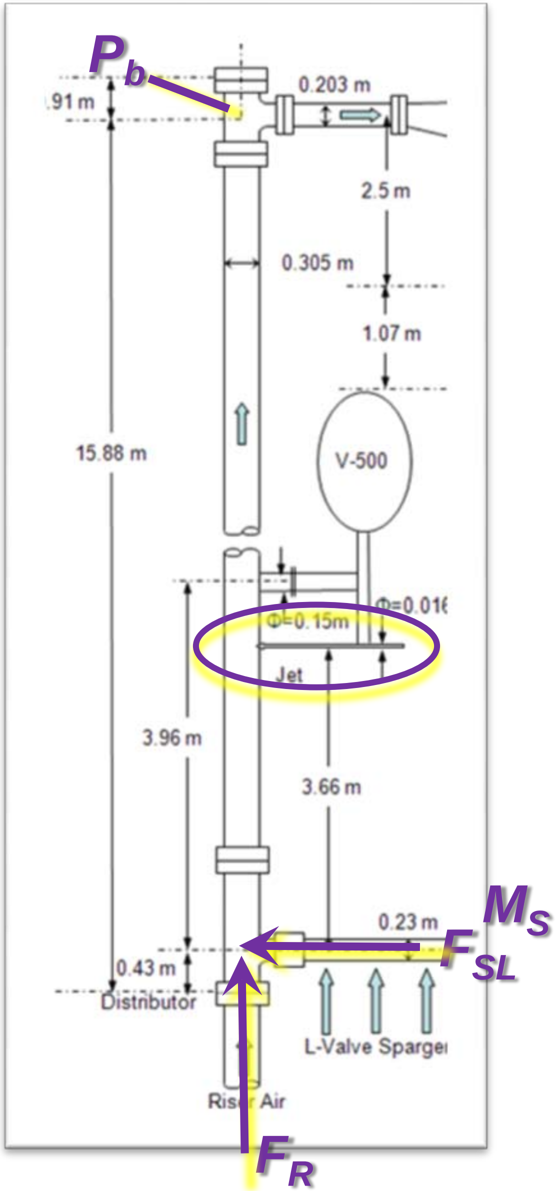




CFB Test Conditions

Material	Case	U_{gi} (m/sec)	M_s (kg/sec)	F_R (SCMs)	F_{SL} (SCMs)	RH (%)	T (°C)	P_b (kPa)
Group A	1	5.14	1.44	0.683	0.001	0.14	20.5	182
	2	5.14	9.26	0.682	0.002	0.14	20.5	167
Group B	3	5.71	5.54	0.476	0.025	48	23	100
	4	7.58	7.03	0.599	0.025	49	23	102
	5	7.58	14.00	0.640	0.029	46	23	105





PSRI
Particulate Solid Research, Inc.

BFB Challenge Problem

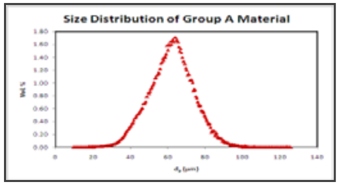
Test Case No.	Static Bed Height, ft (m)	FCC Fines Content % < 44 mm	*Ug* ft/s (m/s)	Fluidization Behavior
1	12 (3.66)	3	1 (0.3)	Gas bypassing
2	4 (1.22)	3	1 (0.3)	Uniform
3	8 (2.44)	3	2 (0.6)	Gas bypassing
4	8 (2.44)	12	2 (0.6)	Uniform

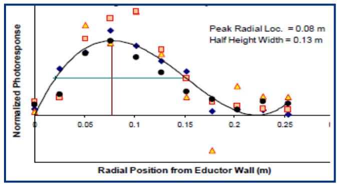
Gas bypassing more likely for tall beds, low fines content and low gas velocity

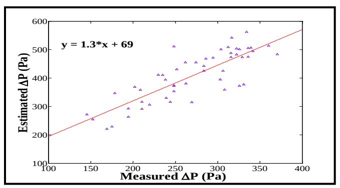
Modeling Benchmark

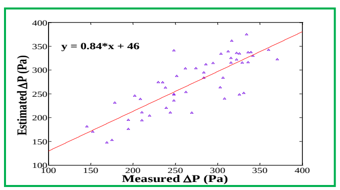
PSRI
Particulate Solid Research, Inc.

Measuring Our Success, Targeting Our Challenges
@
https://mfix.netl.doe.gov/challenge/index.php







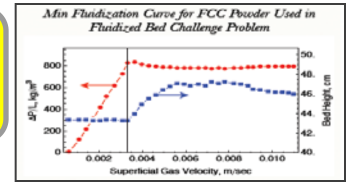


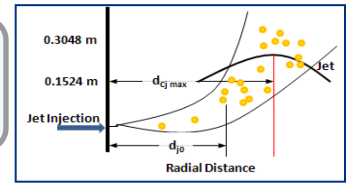
Validate Against U_{mf}, U_{mb} and Bed Density Data

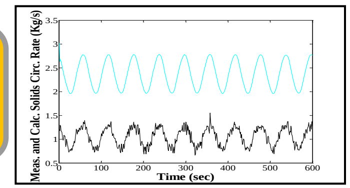
Model Challenge Problems

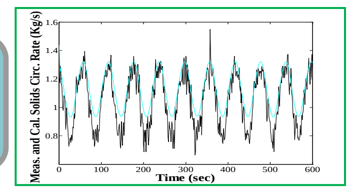
Compare Against Results

Refine Models









Important Timeline

May 2010 | Jun 2010 | Jul 2010 | Aug 2010 | Sep 2010 | Oct 2010 | Nov 2010 | Dec 2010 | Jan 2011 | Feb 2011 | Mar 2011 | Apr 2011 | May 2011 | Jun 2011 | Jul 2011

May 9, 2010: Problem Descriptions Available at https://mfix.netl.doe.gov

Oct 30, 2010: First Simulation Results Due

Nov 1, 2010: Experimental Data Released

Jan 31, 2011: Second Simulation Results Due

May 2, 2011: Workshop on Results at CFB 10

Jul 30, 2011: Publication of Results

Lessons Learned from CP-III

- **Data sets have been vetted and will remain available to continue to serve as model validation test cases.** *https:\\mfix.netl.doe.gov*
- **Industrial scale, non-reacting, multi-phase flow problems required:**
  - *10's of hours on multi-processor computers to simulate for 1 s, and*
  - *At least 30 to 60 s time to establish quasi steady state.*
- **Availability of computational and human resources limited participation and reduced modeler's ability to refine the solutions.**
- **The number of modeling responses was insufficient to assess progress in multiphase flow modeling and/or sensitivity to EE or EL model parameters.**

Motivation for Small Scale CPs (SSCP)

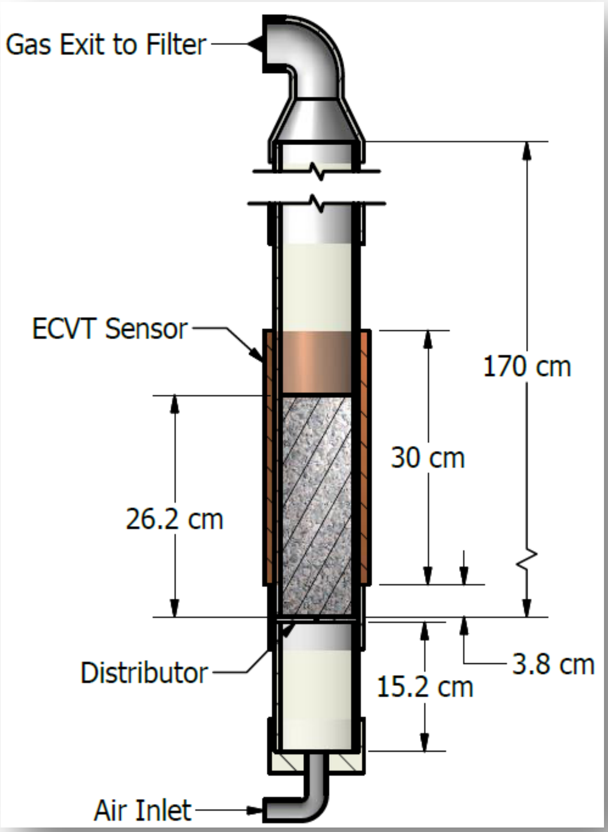
CP Goal was benchmarking computational models on industrial scale.

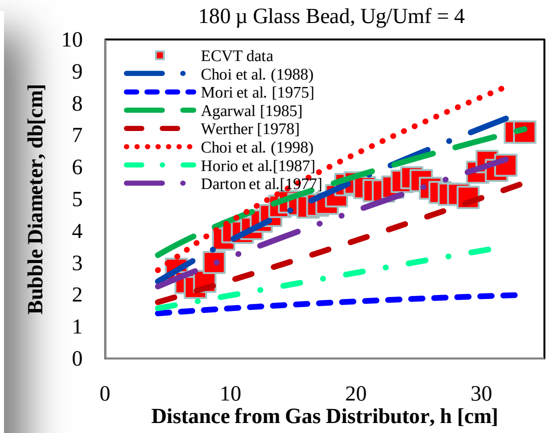
SSCP Goal is to assist in the improvement and development of multiphase CFD models.

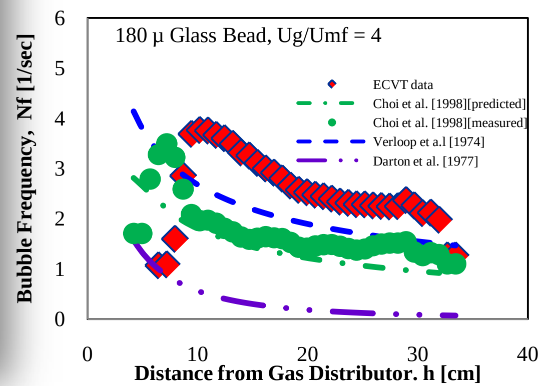
- **Desirable features include:**
  - **Expand testing to include other models: DEM…**
  - **Encourage model sensitivity studies**
  - **Reduce scale and complexity of test cases; needed human and computational resources**
  - **Conduct CP's at regular, more frequent intervals**
  - **Increase participation; Is funding necessary?**

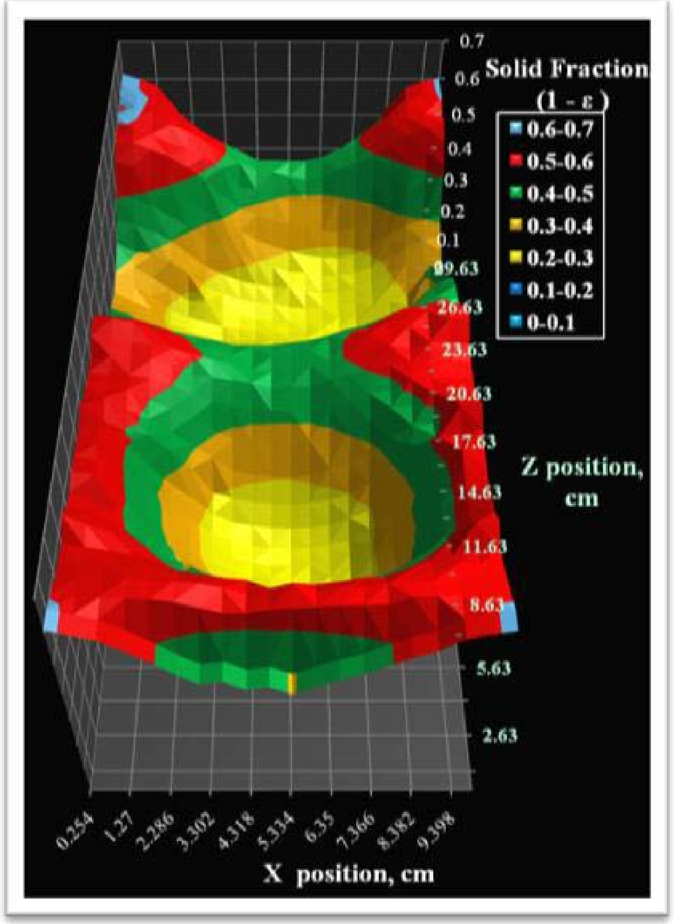
- **A series of highly controlled, well-defined small-scale CP's will be undertaken.**

10-cm Bubbling Fluidized Bed SSCP



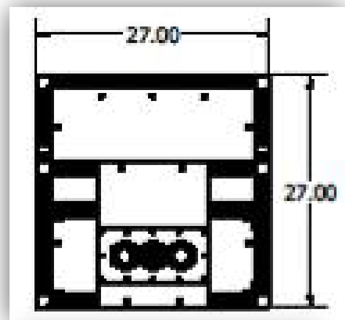


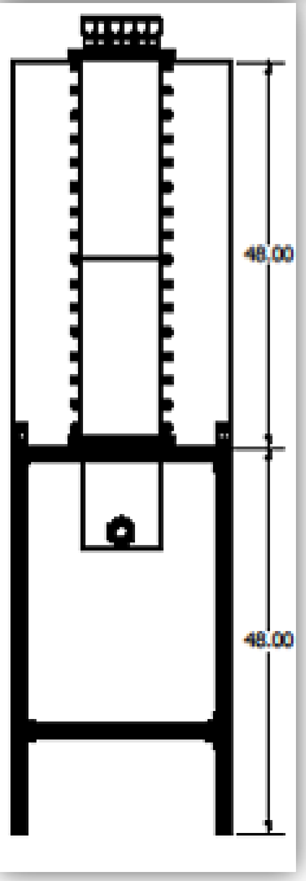




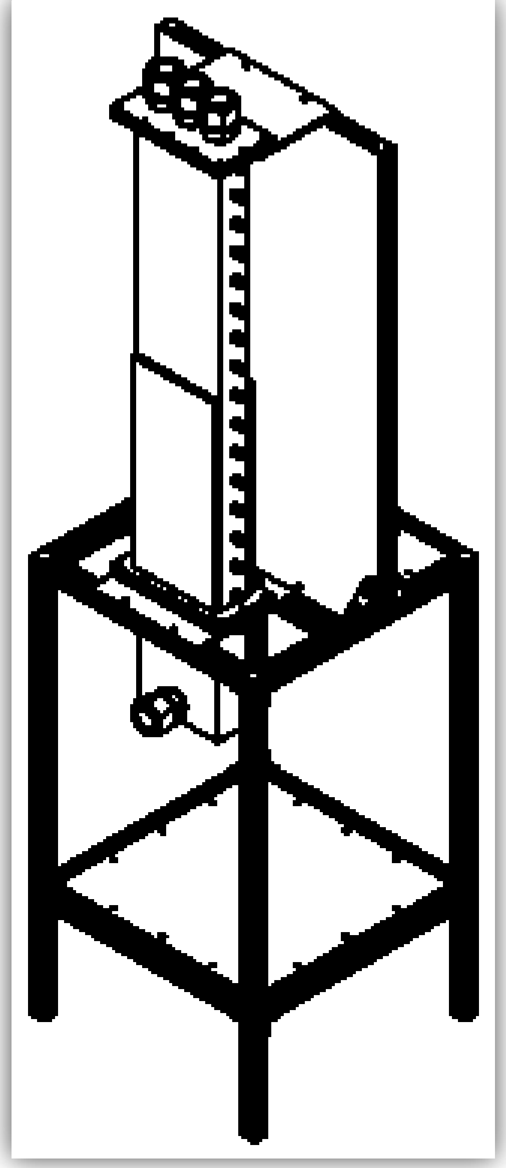
- Poly-disperse materials including at least one case with a particle count
- 4 to 6 test cases
- Non-intrusive measurements ECVT

Rectangular Fluidized Bed

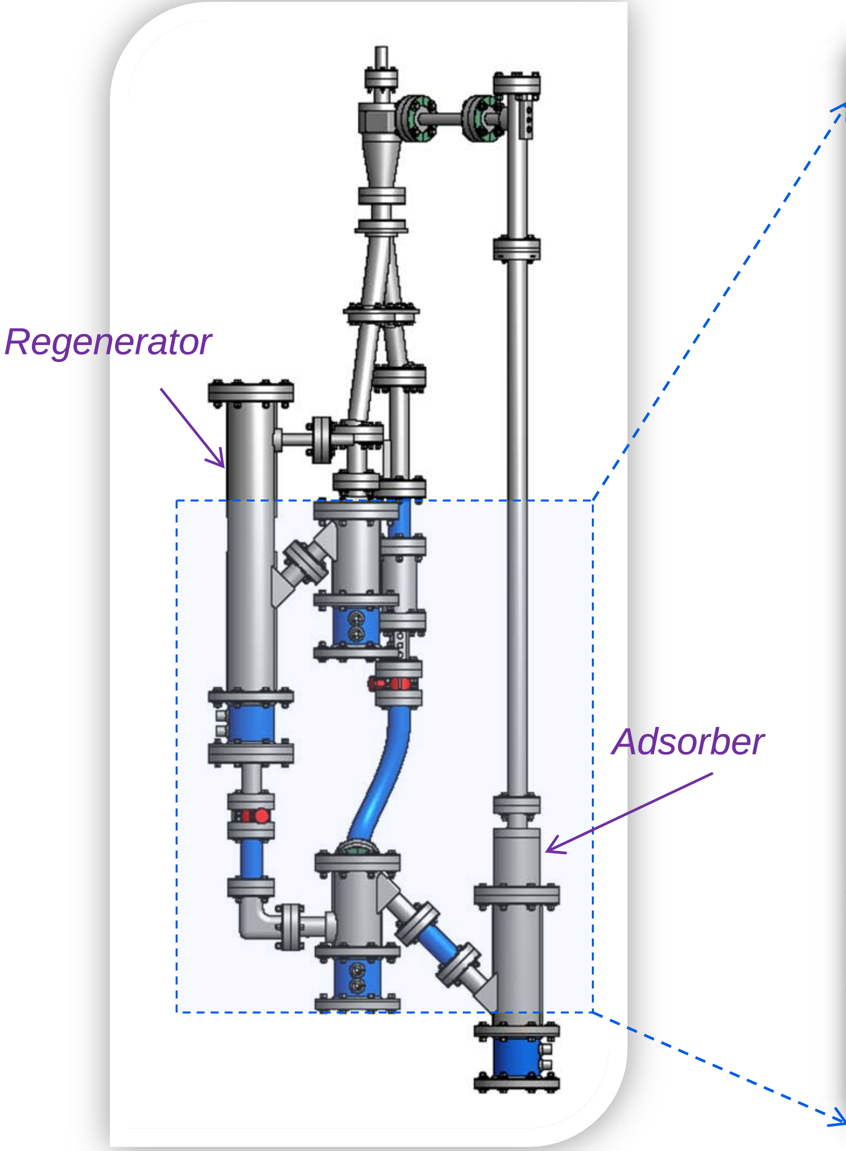




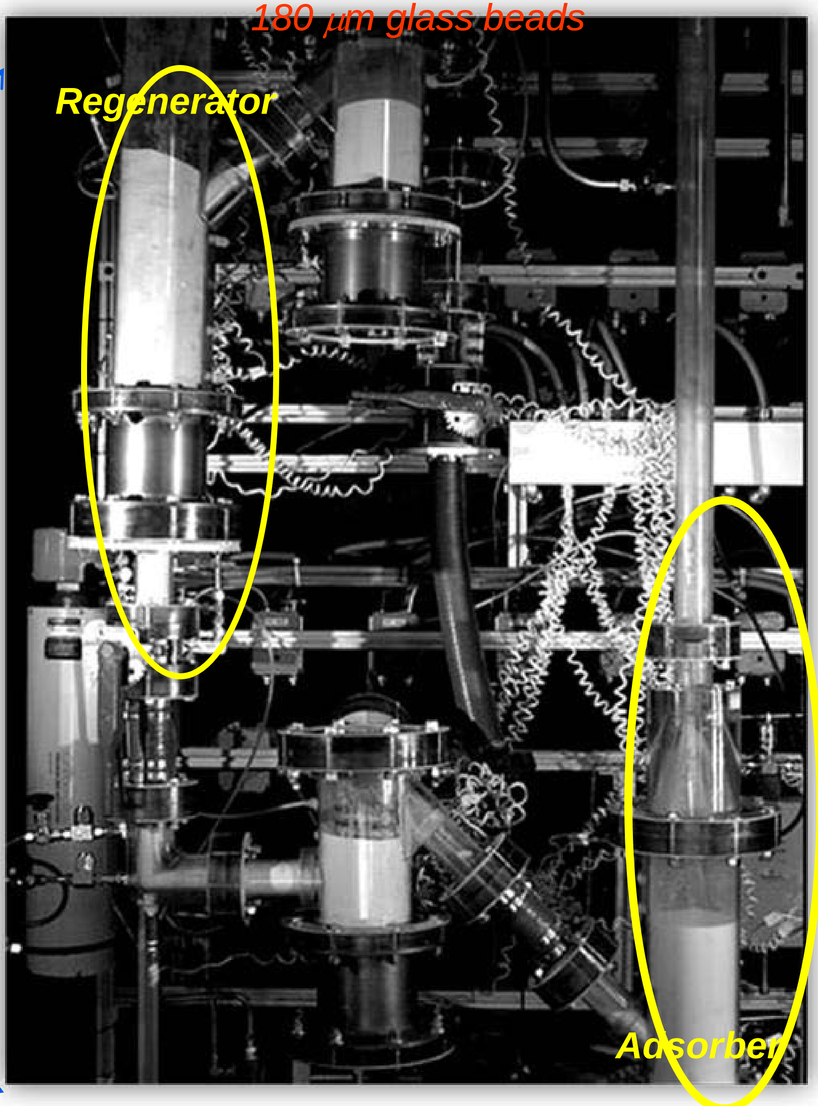
- 3"x9"x48" Rectangular bed
- Non-intrusive video imaging
- Instrumented with ECVT
- Capable of fluidizing 6 mm steel beads



Carbon Capture Unit (C2U)



video of design conditions with 180 μm glass beads



Upcoming Small-Scale Challenge Problems (SSCP)

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

2012

10-cm BFB

SSCP1: Poly-disperse mixtures with data on entrainment, voidage, pressures, and bubbles

Jan 2012	Feb 2012	Mar 2012	Apr 2012	May 2012	Jun 2012	Jul 2012	Aug 2012	Sep 2012	Oct 2012	Nov 2012	Dec 2012

2013

Rectangular BFB

SSCP2: Group D particles (6 mm) with data on gas and particle velocities, voidage, pressures, and bubbles

Jan 2013	Feb 2013	Mar 2013	Apr 2013	May 2013	Jun 2013	Jul 2013	Aug 2013	Sep 2013	Oct 2013	Nov 2013	Dec 2013

2014

CP-IV 30-cm CFB

CP-IV: industrial scale model validation of full CFB loop

Jan 2014	Feb 2014	Mar 2014	Apr 2014	May 2014	Jun 2014	Jul 2014	Aug 2014	Sep 2014	Oct 2014	Nov 2014	Dec 2014

2015

Carbon Capture Unit (C2U)

SSCP3: Gas adsorbing particles with data on adsorption, regeneration, temperatures, voidage, pressures, and bubbles

Jan 2015	Feb 2015	Mar 2015	Apr 2015	May 2015	Jun 2015	Jul 2015	Aug 2015	Sep 2015	Oct 2015	Nov 2015	Dec 2015

Challenge Problem schedules and updates will be posted on https:\\mfix.netl.doe.gov

Responses/Comments on “Challenge Problem: Next Steps”

The following comments were not taken verbatim but are rather recollections of thoughts and concepts discussed during the Workshop.

- **Dimitri Gidaspow:** In 1985 Syamlal and Gidaspow (AIChE Journal 31, 127-135.January 1985) have shown that wall heat transfer coefficients in bubbling beds can be computed using the IIT CFD code. This technique was verified by Professor Hans Kuipers. This year we have compared such calculations using our code for a commercial silicon production reactor and compared the results to the commercial BARRACUDA code. Both theories and codes give reasonable results. But the BARRACUDA theory gives a heat transfer coefficient that is half of that from the theory of Syamlal and Gidaspow. This is due to the lack of the thermal conductivity of silicon in the BARRACUDA code. Hence I suggest that the next challenge problem include a computation of the wall heat transfer coefficient.
- **Reply, Larry Shadle**: A heat balance is being conducted in the carbon capture unit and heat transfer coefficients will be estimated in both non-reacting and reacting flows for the challenge problem proposed for 2015.
- **Phil Smith:** The concept of posing a challenge problem in which the experiment is conducted by one group and simulated blindly by another is less productive than the learning that takes place when the two are done together.
- **Reply, Shadle:** Agreed, however very few research organizations have the facility and capability to do both well, especially at the industrial scale.
- **Reply, Ray Cocco:** The use of smaller scale units provides better opportunities for research to duplicate the experiments as well as participate in the computational model development because of the lower cost and simple nature of replicating the facility.
- **Smith:** Both the experimental and the modeling results need to be represented with their uncertainties including those of the independent /controlled parameters, as well as the variability of the dependent parameters.
- **Reply, Shadle:** A large part of my effort in preparing the challenge problem III data was in estimating the uncertainties. These experimental uncertainties are reported in both the problem statement on the independent parameters taking from the replicates and in the results as presented in the data release at the Fall 2010 AIChE meeting and on the MFIX website. For those experimental measurements where there were no replicates, confidence intervals were determined by lumping the measurement at different locations and assuming continuity either across the radius or along the height of the equipment. The model uncertainties were more difficult to estimate from the results provided at the operational setpoints. The approach was to compare all the simulations together to the experimental confidence intervals to get a general sense of simulation variability from model to model.

Responses/Comments on "Challenge Problem: Next Steps"

(Continued)

- **Ron Breault:** The use of smaller scale experiments does not necessarily reduce the size of the computational problem. Process internals require fine resolution often increasing the number of cells that must be simulated.
- **Reply, Shadle:** In the small scale challenge problems it is our intention to keep the experimental systems simple to avoid these problems.
- **Reply, Craig Myler:** An estimate of the resources required to simulate these problems using a well defined modeling approach should be provided to enable perspective research organizations to estimate the effort required to respond.
- **Arastoopour:** The ability for university researchers to respond requires more than simply scheduling the challenge problems on a regular and frequent interval. Research contracts and grants have stated goals and deliverables and the student's time and effort cannot be diverted to do other activities for the sake of validation even when validation is required, because the nature of the validation required under a given contract will likely be specific to the application being funded.
- **Reply, Madhava Syamlal:** I always encourage researchers to include a validation effort into every model development activity. Researchers should consider these challenge problem cases as available data resources to assist in that validation. We will look into our future solicitations and, where possible, add language to include this type of validation into the scope of work. Since the Workshop I talked to Ashok Sangani, who is the Program Manager for Particulate and Multiphase Processes at NSF, about potential support for US students to participate in the challenge problem. He is amenable to providing support, and someone from academia ought to follow up with him on setting that up.
- **Craig Myler:** A challenge problem to us in industry does not need to be blind in the sense presented here but rather should include experimental data for one or two small scale fluid bed units and then scale up to a third larger scale unit. It is that third larger scale unit which should be the blind unit and whose performance should be compared with simulated predictions.
- **Reply, Syamlal:** This would be precisely in-line with our 2006 Roadmap for Multi-phase flow development.
- **Reddy Karri:** The concept for the first three challenge problems has been PSRI/NETL selected the type of experiment. Instead, this time around we should let the modelers pick an experiment and we should perform that experiment and provide the test results. The next challenge problem should include both small scale (4 in at NETL) and a large scale (3 ft at PSRI) and both should run at the same test conditions such as, same material, same gas velocities and same gas and implement the same measurement techniques.

Responses/Comments on "Challenge Problem: Next Steps"

(Continued)

- **LS Fan:** The challenge problem can also be used to test the experimental techniques. The best approach would be for the experimentalists to bring their techniques to NETL and/or PSRI to test over instead of testing the techniques on the units built by the experimentalists on their own sites. The lack of high bay area in the academic setting these days and the difficulty to reproduce fully identical units are the reasons. This idea was discussed before but has not been implemented.
- **Alberto Passalacqua:** I am sending you a couple of links to CFD websites where news about CFD initiatives are usually posted. CFD review: http://www.cfdreview.com/ On this website you can post announcements, and users subscribed to it receive a weekly email with it inside. CFD-Online: http://www.cfd-online.com/ This is more a forum-oriented website, where people exchanges information about CFD and codes, however it is widely used by the CFD community, and their "CFD News and Announcements" section should be a good target.