NATIONAL ENERGY TECHNOLOGY LABORATORY

Overview of Multiphase Flow Science Needs at DOE-NETL

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National Energy Technology Laboratory

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J. Spenik, REM
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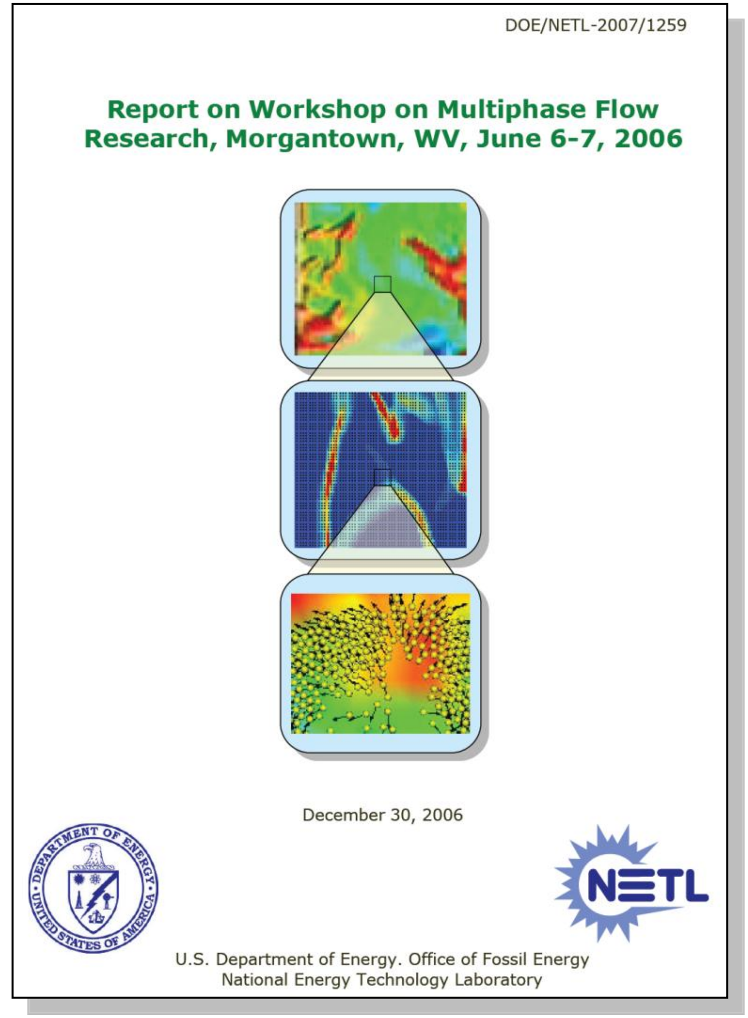
NETL 2011 Workshop on Multiphase Flow Science, Airport Marriott, Pittsburgh, PA, August 16-18, 2011

The goal is to use multiphase simulations to accelerate technology development

Vision

Ensure that by 2015 multiphase science based computer simulations play a significant role in the design, operation, and troubleshooting of multiphase flow devices in fossil fuel processing plants.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Report on Workshop on Multiphase Flow Research, Morgantown, WV, June 6-7, 2006

December 30, 2006

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National Energy Technology Laboratory

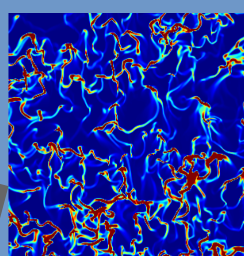
Workshop report at http://tinyurl.com/c9r7ux

Component of the toolset developed by Carbon Capture Simulation Initiative

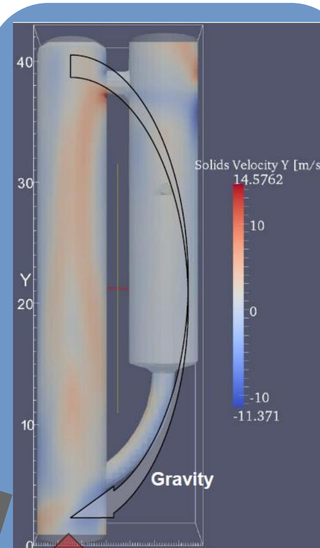
Single particle reaction kinetics

Particle

Effective lumped reaction kinetics



Cloud of particles



CO_2 capture device

CCSI
Carbon Capture Simulation Initiative

Data Management System

Particle/ Device Scale ⇔ *Process Synthesis & Design* ⇔ *Plant Operations & Control*

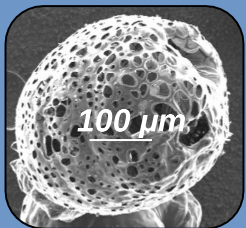
Uncertainty Quantification

Risk Analysis & Decision Support

- *Screen and optimize designs*
- *Evaluate technical risk of scale up*

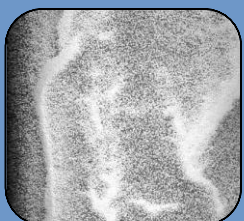
NETL · Berkeley Lab · Pacific Northwest National Laboratory · Los Alamos National Laboratory · Lawrence Livermore National Laboratory

Simulations support gasifier scale up



Coal gasification reactions

C_3M

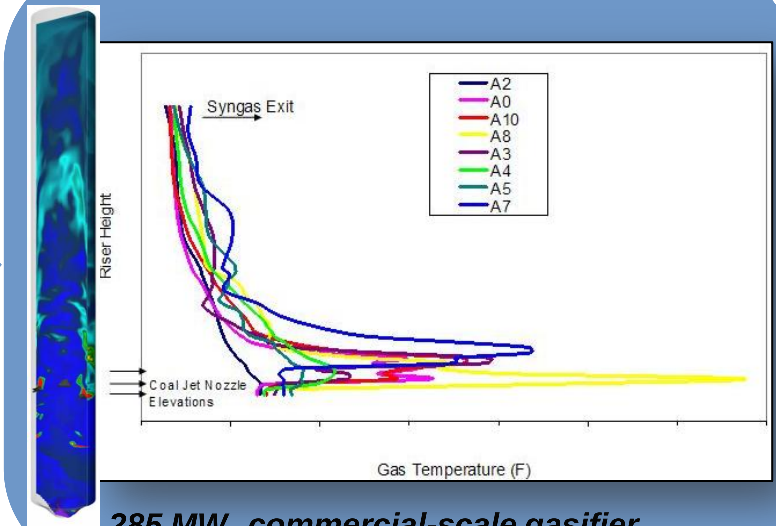


Gas-solids hydrodynamics

MFIX

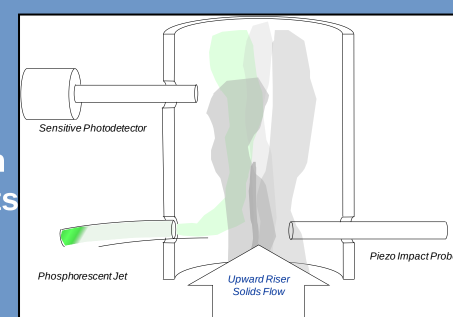
13 MW_{th} PSDF pilot-scale gasifier

Validated gasifier model



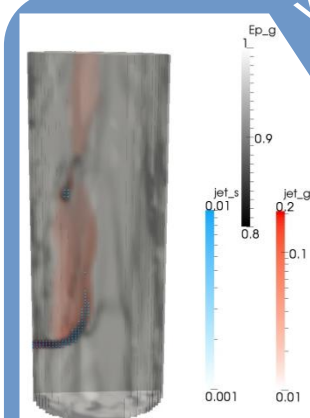
285 MW_e commercial-scale gasifier

Need to study jets in cross flow



Jet penetration experiments

Validation data on jets

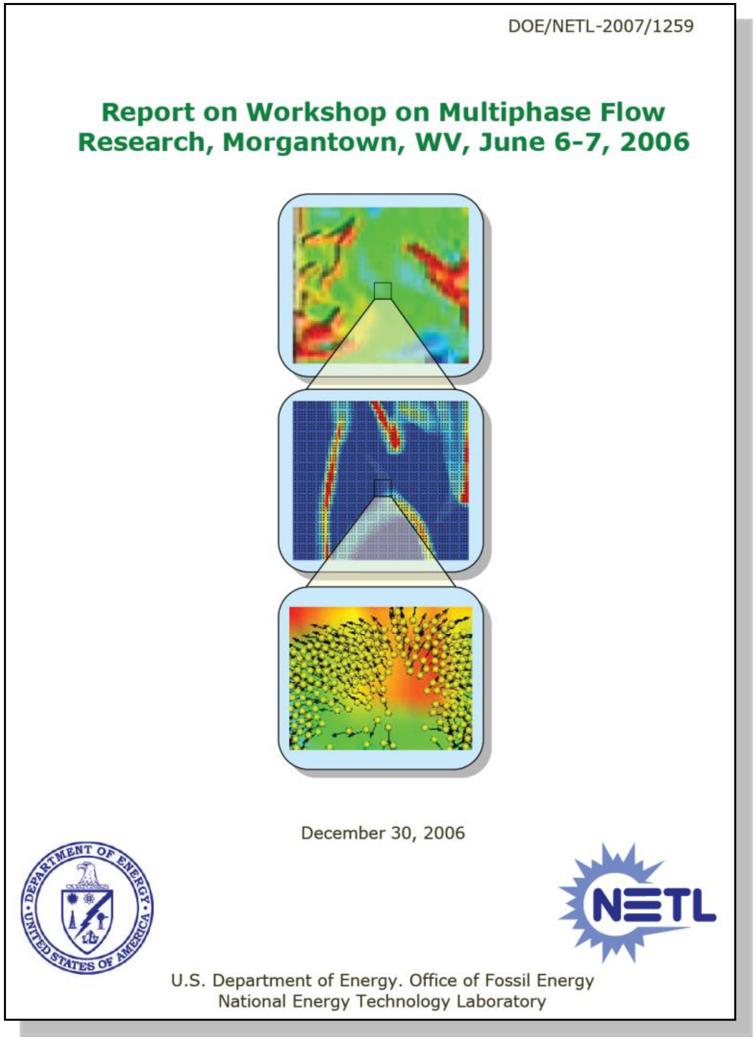


Jet simulation

Validated model

Examples of progress made at NETL

- **Progress on the five areas in the Technology Roadmap**
  - *A. Benchmark Cases*
  - *B. Numerical Algorithm and Software Development*
  - *C. Theory and Model Development*
  - *D. Physical and Computational Experiments*
  - *E. Communication, Collaboration, and Education*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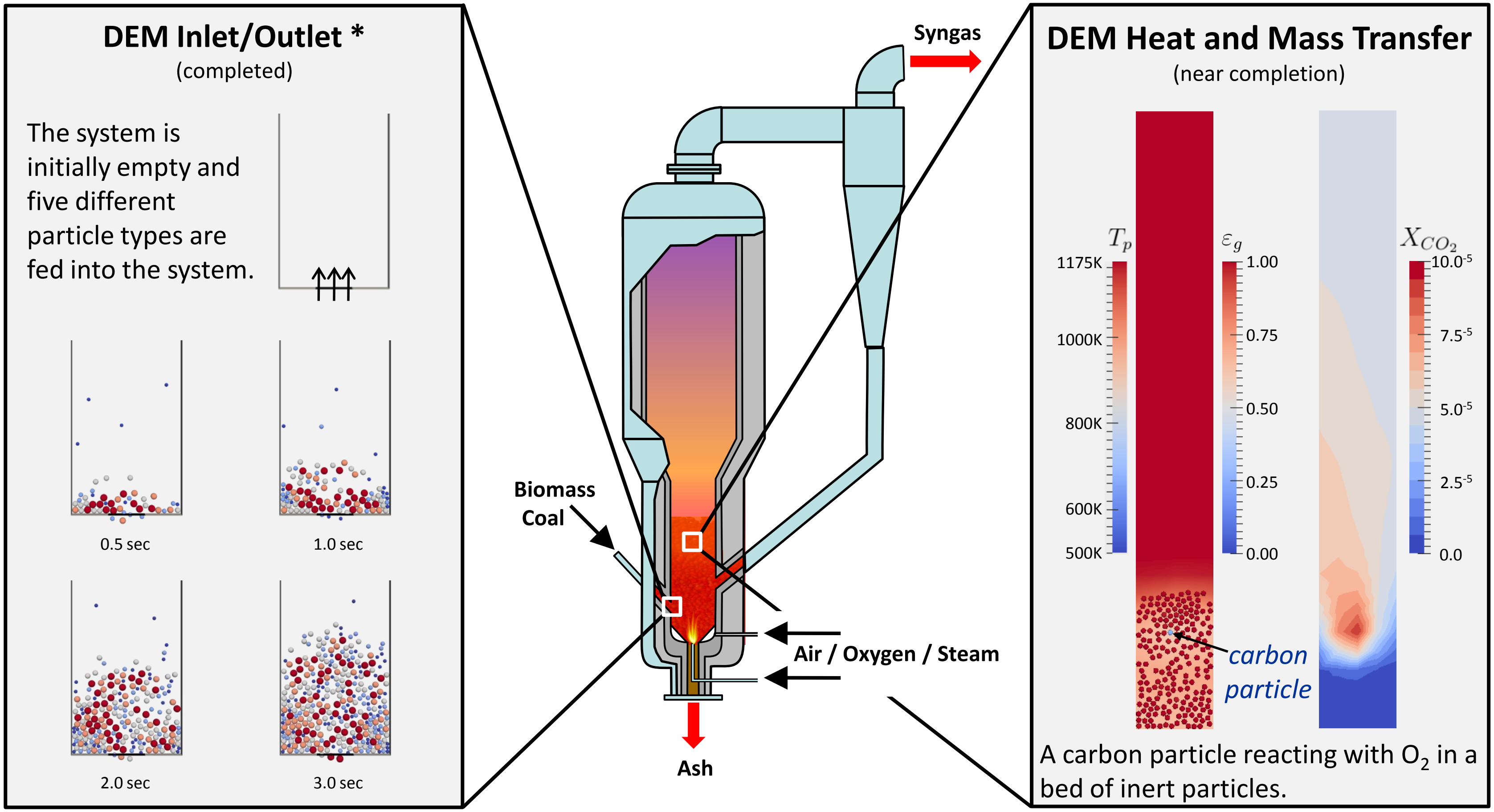
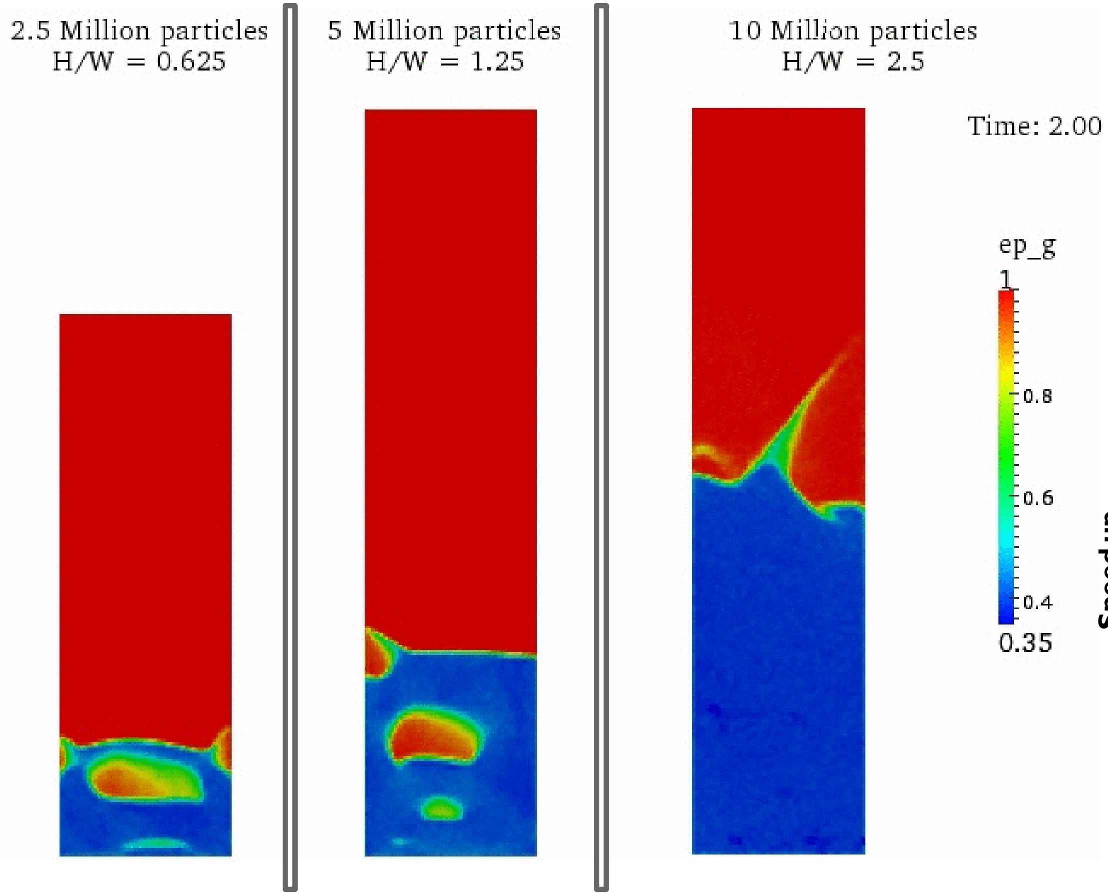
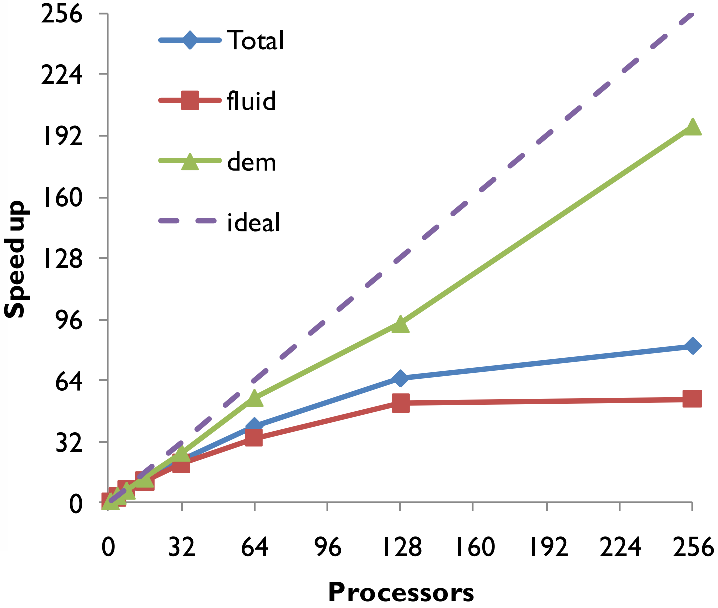
Gas-solids reactions added to MFIX-DEM



* J. Musser, M.A. Clarke, J. Galvin, 2011, Development of a discrete mass inflow boundary condition for MFIX, Journal of Systemics, Cybernetics and Informatics, 9(1), pp. 94-98.

Parallelization speeds up MFIX-DEM





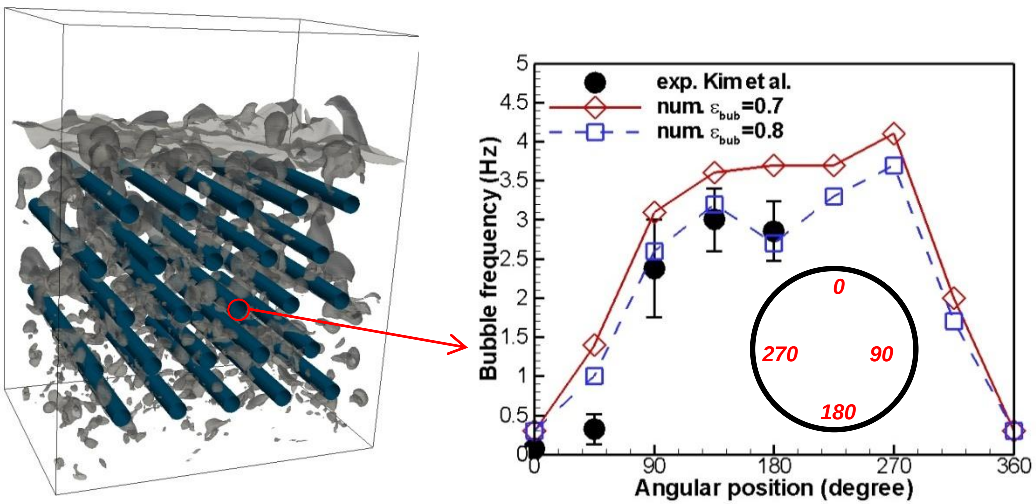
Void fraction at the center of a square bed

For 2.5 M particles/82 K cells/256 cores the speed up is 81

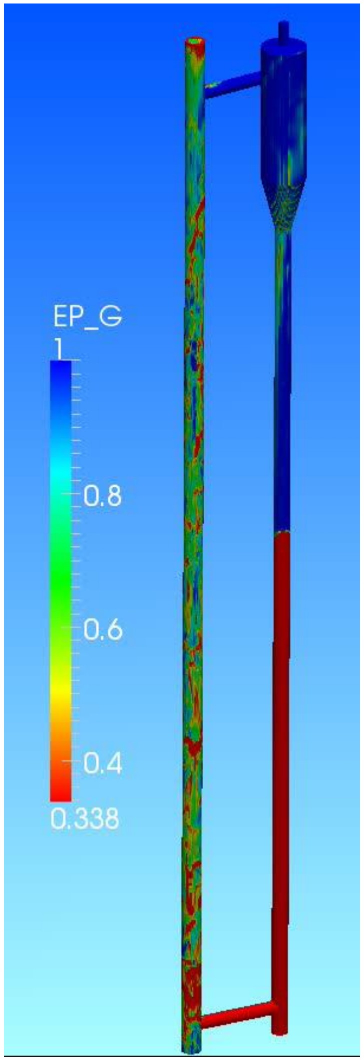
Gopalakrishnan, P., Tafti,D.K., "Large Scale Coupled Eulerian-Lagrangian Simulation of Fluidized Bed", accepted for presentation at AIChE 2011, Minneapolis, MN, October 16-21,2011.

Capability for complex geometry developed

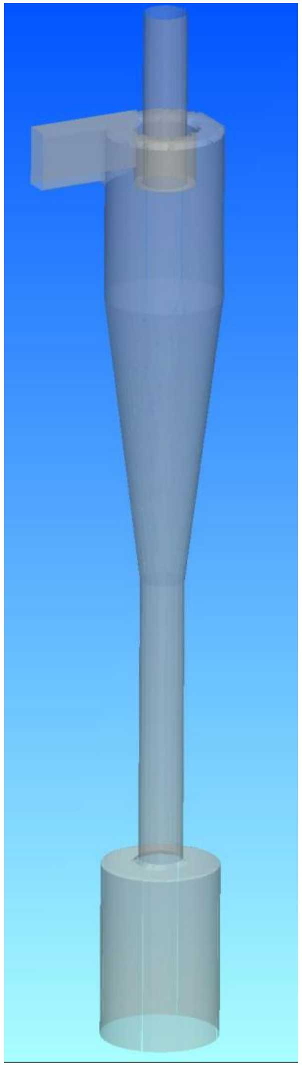
- Cut-cell technique implemented in MFIX to represent complex geometries
- Examples: Tube bundle in bubbling bed [1], full loop simulation of CFBs [2]



- Implementation in Eulerian-Lagrangian solver is underway [2]



EE simulation of NETL CFB (Challenge problem)

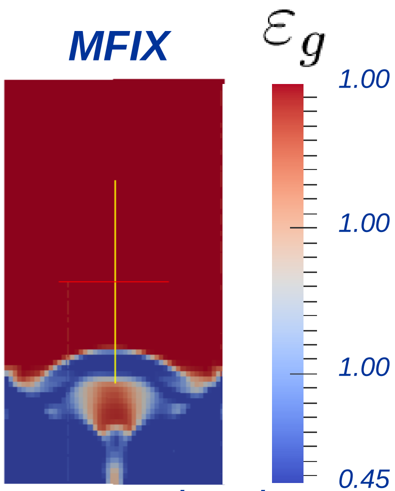


MPPIC cyclone simulation

[1] Li, T., Dietiker, J.-F., and Zhang, Y., "Cartesian grid simulations of bubbling fluidized beds with a horizontal tube bundle", submitted to Chemical Engineering Sciences, May 2011.
[2] Dietiker, J.-F., Li, T.,Garg, R., and Shahnam M.,"Cartesian Grid Simulations of Gas-Solids Flow Systems with Complex Geometry", accepted for presentation at AIChE 2011, Minneapolis, MN, October 16-21, 2011.

Multiphase ROM under development

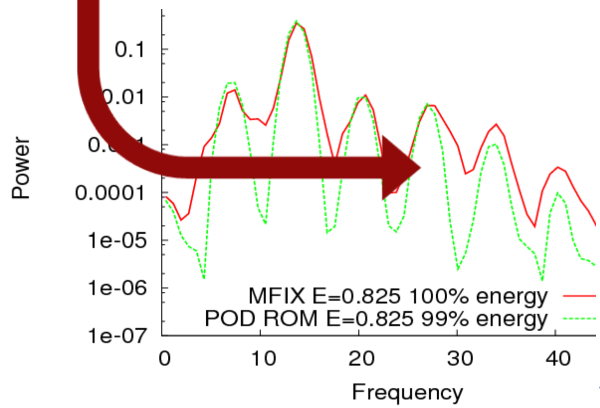
MFIX



Computational Time: >9 h

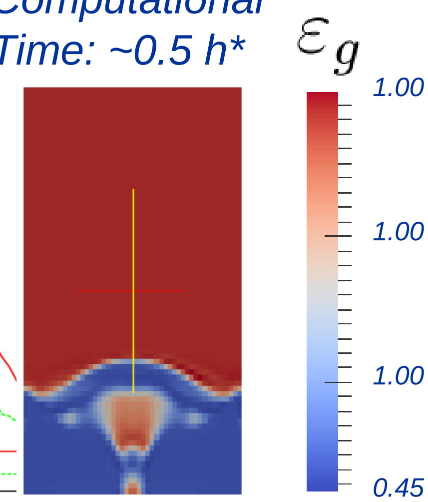
$$\iint_{D_x D_y} \frac{\partial}{\partial t}(\varepsilon_g \rho_g)\begin{bmatrix}U_{xg}\\ U_{yg}\end{bmatrix}\varphi_z \, dy\, dx + \int_{D_x} \varepsilon_g \rho_g U_{yg}\begin{bmatrix}U_{xg}\\ U_{yg}\end{bmatrix}\varphi_z \, dx \cdots$$

$$\iint_{D_x D_y} \frac{\partial}{\partial t}(\varepsilon_s \rho_s)\begin{bmatrix}U_{xs}\\ U_{ys}\end{bmatrix}\varphi_z \, dy\, dx + \int_{D_x} \varepsilon_s \rho_s U_{ys}\begin{bmatrix}U_{xs}\\ U_{ys}\end{bmatrix}\varphi_z \, dx \cdots$$



ROM

*Computational Time: ~0.5 h**

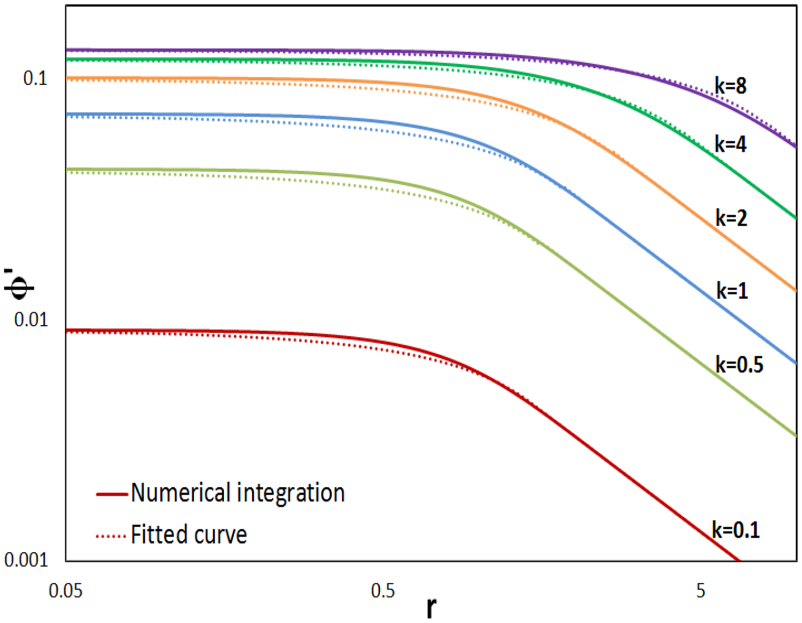


** using 30 processors with output at 0.2 Hz*

Beck Roth, S. Reduced order model of a spouted fluidized bed utilizing proper orthogonal decomposition. WVU Dissertation, August 2011.

Specularity coefficient expressed as function of physical parameters

- **Specularity coefficient in Johnson-Jackson boundary condition expressed as a function of**
  - particle-wall restitution coefficient
  - frictional coefficient
  - normalized slip velocity at the wall

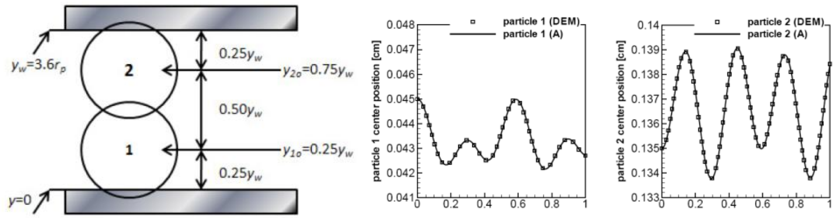


$$\phi' = \begin{cases} -\frac{7\sqrt{6\pi}\left(\phi'_0\right)^2}{8k} r + \phi'_0 & r \le \frac{4k}{7\sqrt{6\pi}\phi'_0} \\ \frac{2}{7}\frac{k}{r\sqrt{6\pi}} & \text{otherwise} \end{cases}$$

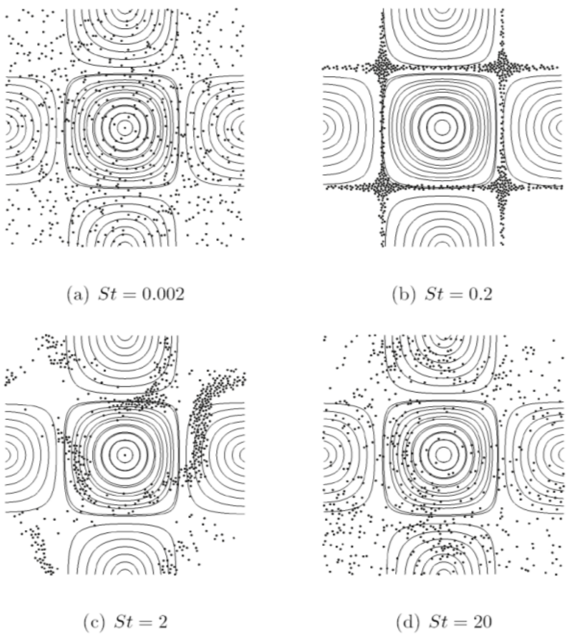
$$r = u_{slip} / \sqrt{3\Theta} \qquad k = \frac{7}{2}\mu(1+e_w)$$

T. Li, and S. Benyahia, Revisiting Johnson and Jackson boundary conditions for granular flows, AIChE Journal, doi: 10.1002/aic.12728.

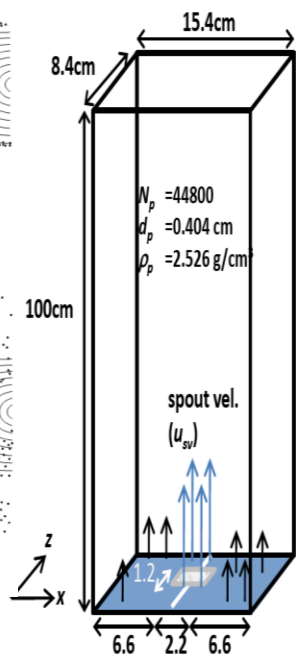
MFIX-DEM verification and validation

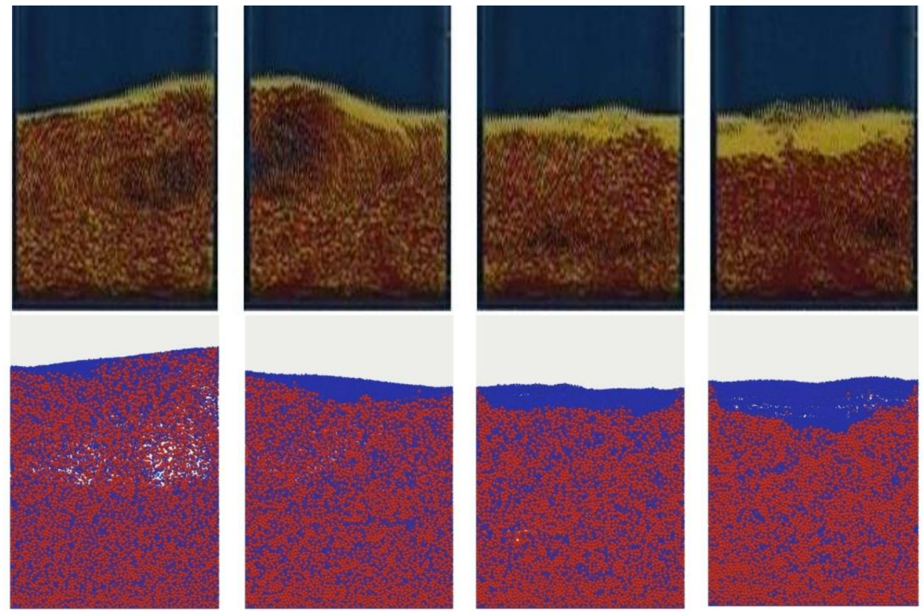


Two stacked particles

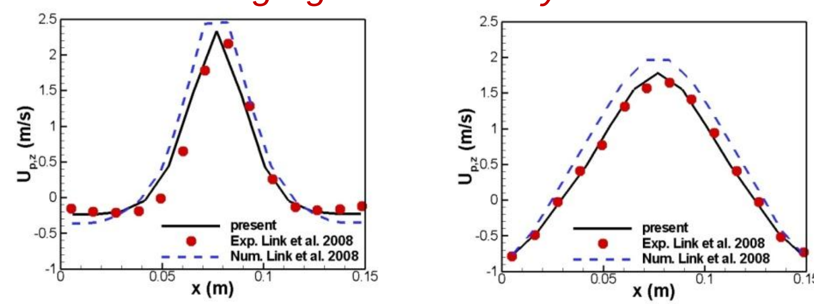


Particle motion in a Taylor-Green vortex





Segregation of binary mixture

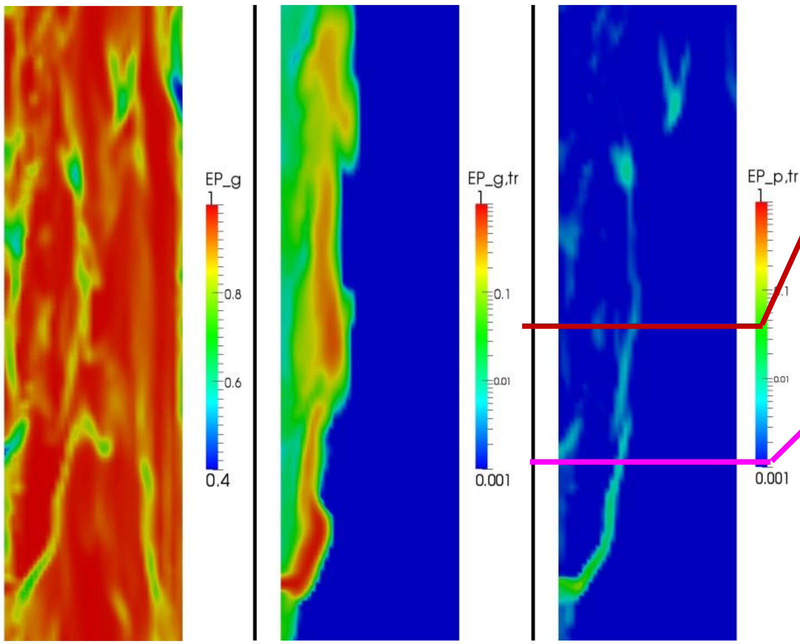


Spout-fluid bed

R. Garg, J. Galvin, T. Li, and S. Pannala, Open-source MFIX-DEM software for gas-solids flows: Part I – verification studies, submitted to Powder Technology, Oct. 2010.

T. Li, R. Garg, J. Galvin, and S. Pannala, Open-source MFIX-DEM software for gas-solids flows: Part II – validation studies, submitted to Powder Technology, Oct. 2010.

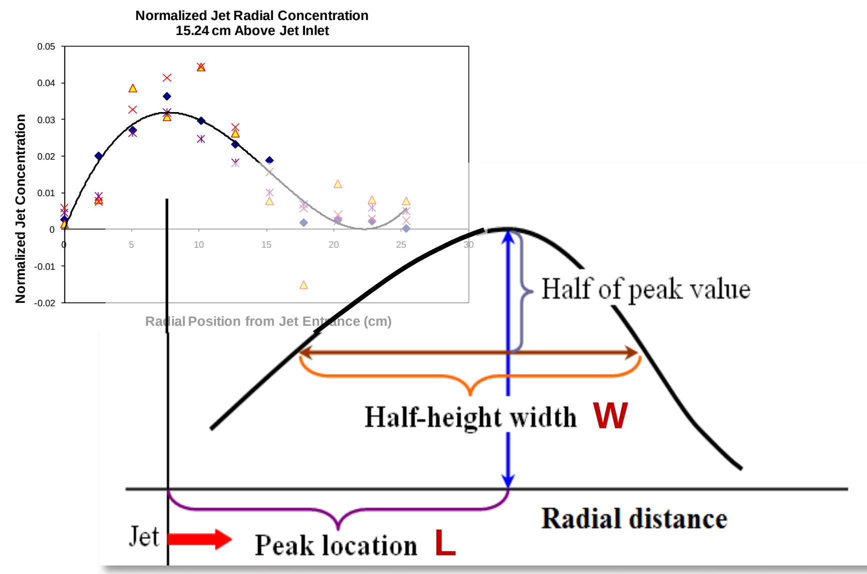
Validation of gas-solids jet in riser flow



Distributions of voidage, tracer particle and tracer gas in the riser flow with gas-solids jet U_j=37m/s

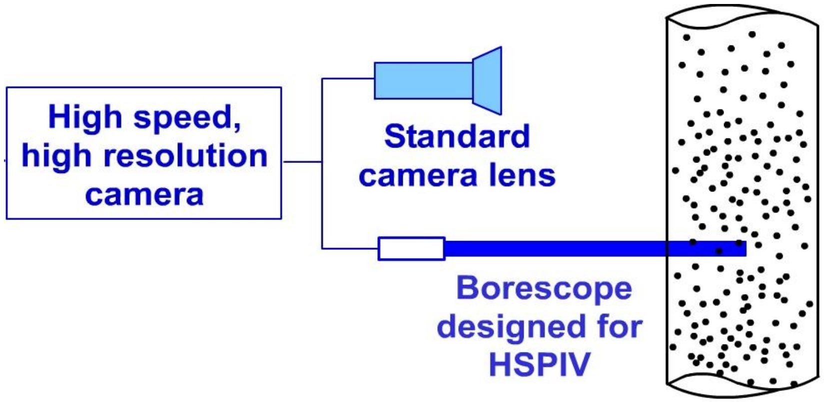
30 cm above distributor	L (cm)	W (cm)
Simulation [1 a, b]	15	7.2
Experiment [2]	14	17

15 cm above distributor	L (cm)	W (cm)
Simulation [1 a, b]	12.8	6.4
Experiment [2]	13	18

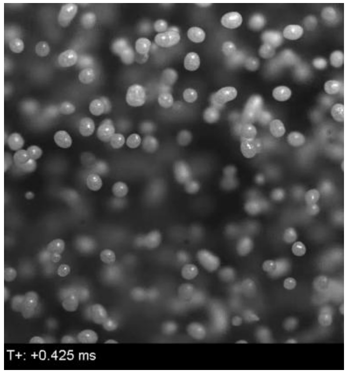


[1 a] T. Li, and C. Guenther, A CFD study of gas-solids jet in a riser flow, AIChE Journal, doi: 10.1002/aic.12619.
[1 b] T. Li, and C. Guenther, High-resolution simulations of gas-solids jet penetration into a high density riser flow, CFB10, Engineering Conference International, Brooklyn, pp. 281-288, 2011.
[2] Shadle L, Ludlow JC, Spenik J, Seachman S, Guenther C. Jet penetration into a riser operated in dense suspension upflow: experimental and model comparisons. In: Circulating Fluidized Bed IX. eds. Werther J Hamburg, Germany: Tutech Innovation, 2008; 307-312.

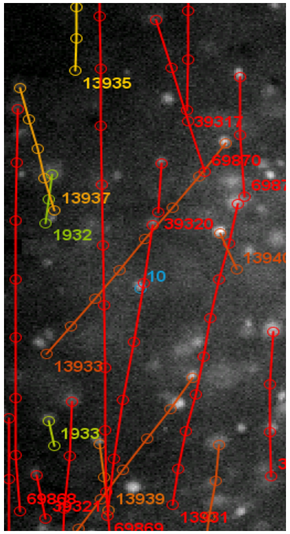
HSPIV used to extract detailed data on particle flow in CFBs



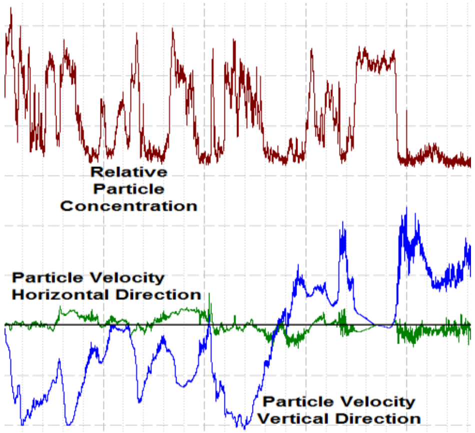
High speed particle image velocimetry (HSPIV)



High speed flow visualization

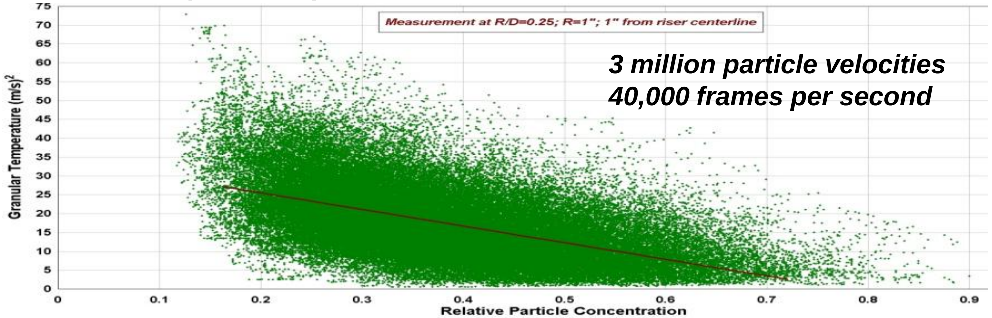


Automatic analysis
(patent pending)



Particle velocity and concentration

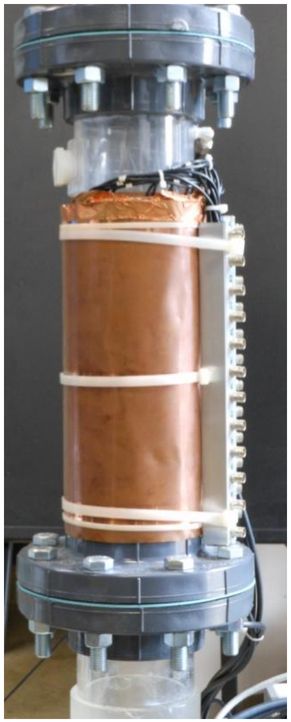
Granular Temperate vs particle concentration PSRI CFB Riser, 70 micron FCC



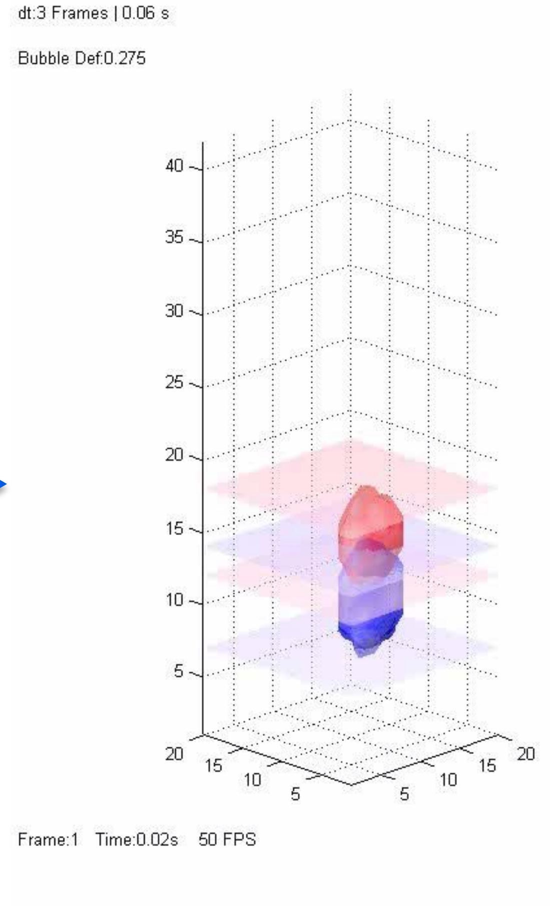
Direct comparison with key modeling parameters

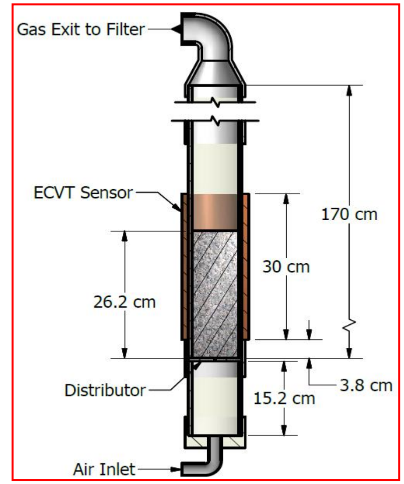
(1) Shaffer, F., "Method of particle trajectory recognition in particle flows of high particle concentration" U.S. Patent Application no 116,773.
(2) B. Gopalan and F. Shaffer, "A New Method for Decomposition of High Speed Particle Image Velocimetry Data," Accepted for publication in Powder Technology, 2011.

ECVT enables measurement of transient, 3D volume fraction data

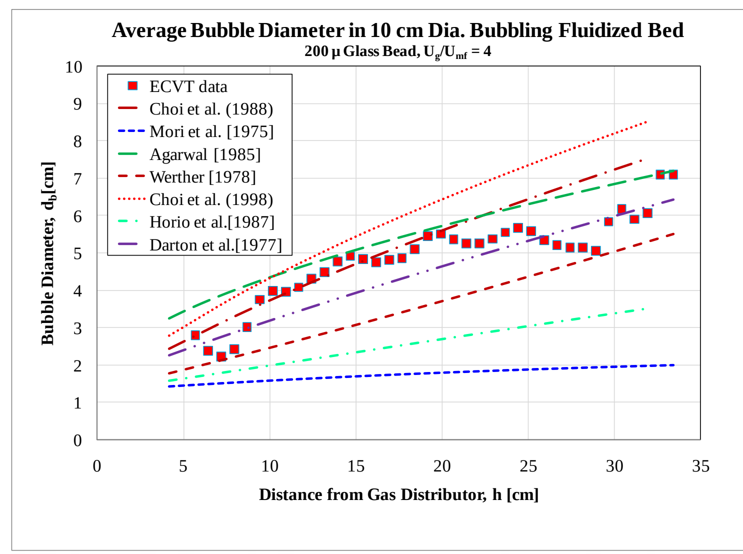


Electrical Capacitance Volume Tomography (ECVT) Sensor

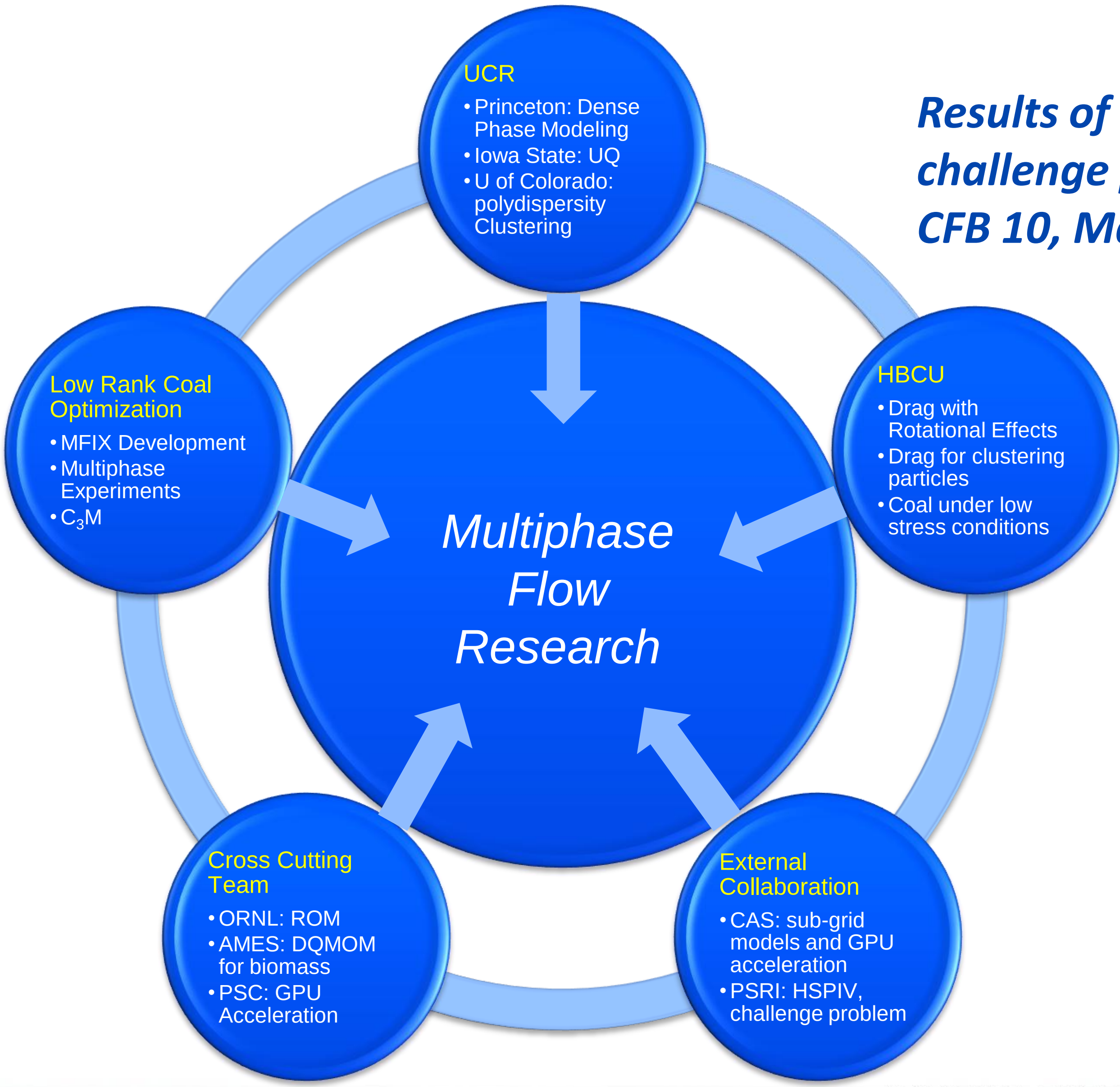




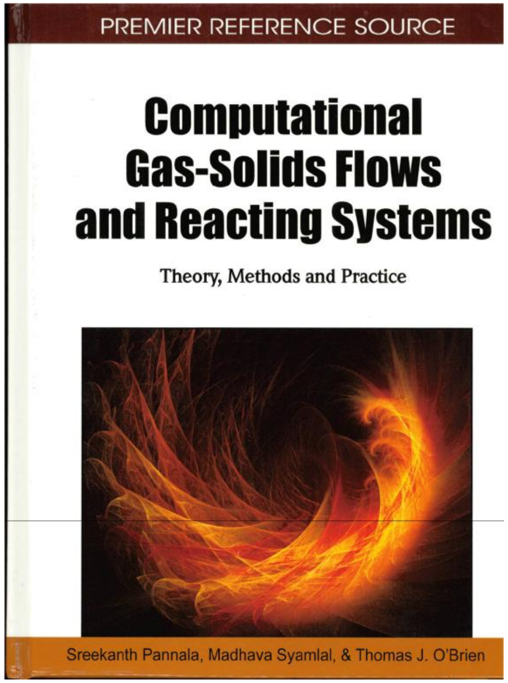
3D volume fraction data



Communication and collaboration

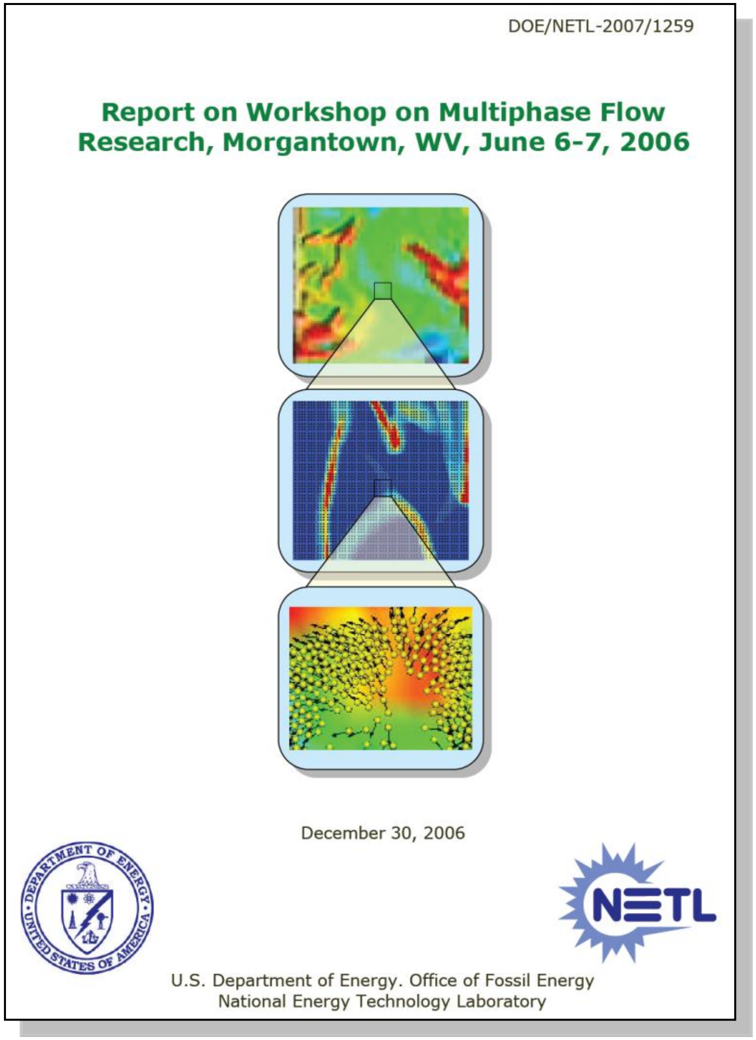


Results of NETL-PSRI Fluidization challenge problem presented at CFB 10, May 2011



The path forward

- A mid-term goal in the Technology Roadmap is *"High-fidelity, transient, 3-D, two-phase with PSD (no density variations), hydrodynamics with heat and mass transfer simulation of transport reactor at a scale of at least 12.5 MW (or 5,000 kg/h coal feed rate) to run on 2012 computer cluster overnight."*
- Focus so far has been on increasing speed, accuracy, and capabilities
- We now need to answer
  - what is meant by "High-fidelity"
  - how high should the fidelity be to realize the vision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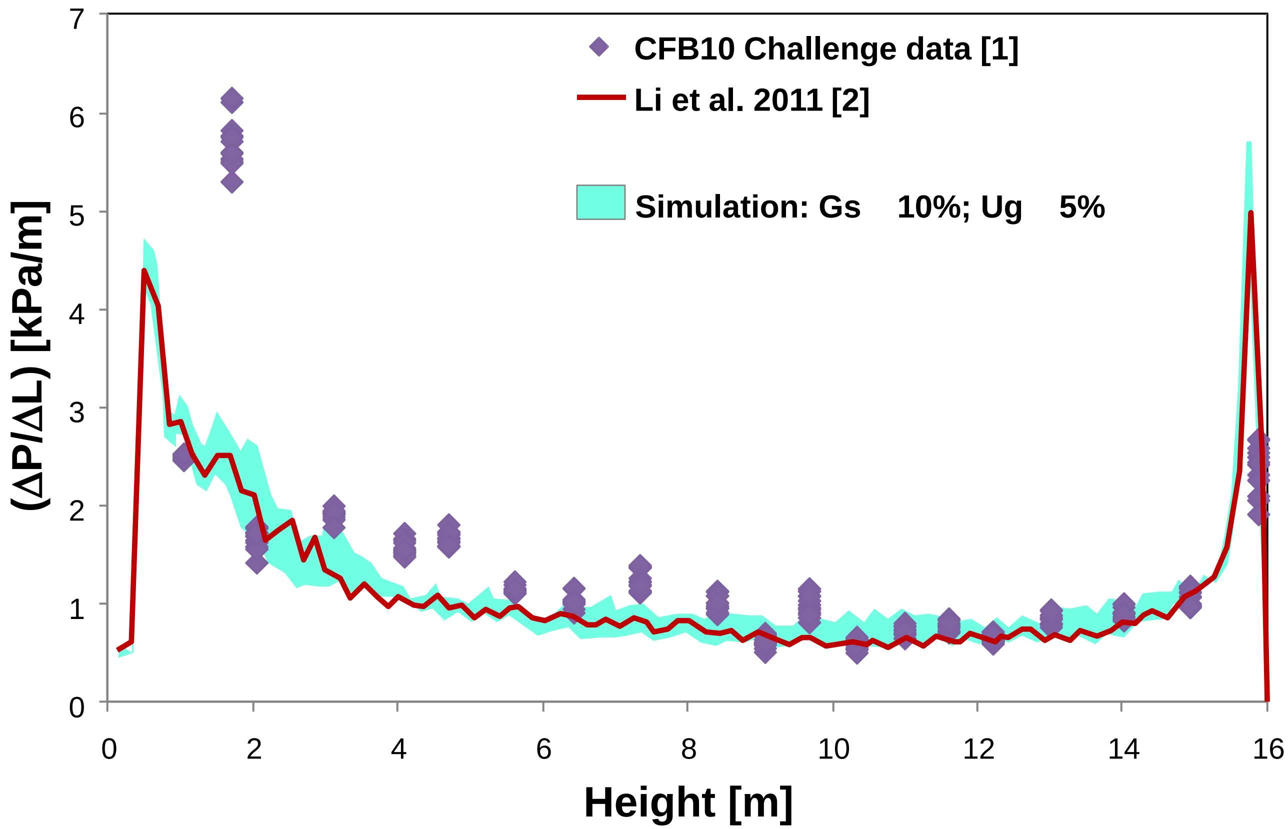
Workshop report at http://tinyurl.com/c9r7ux

Example of current state of model validation



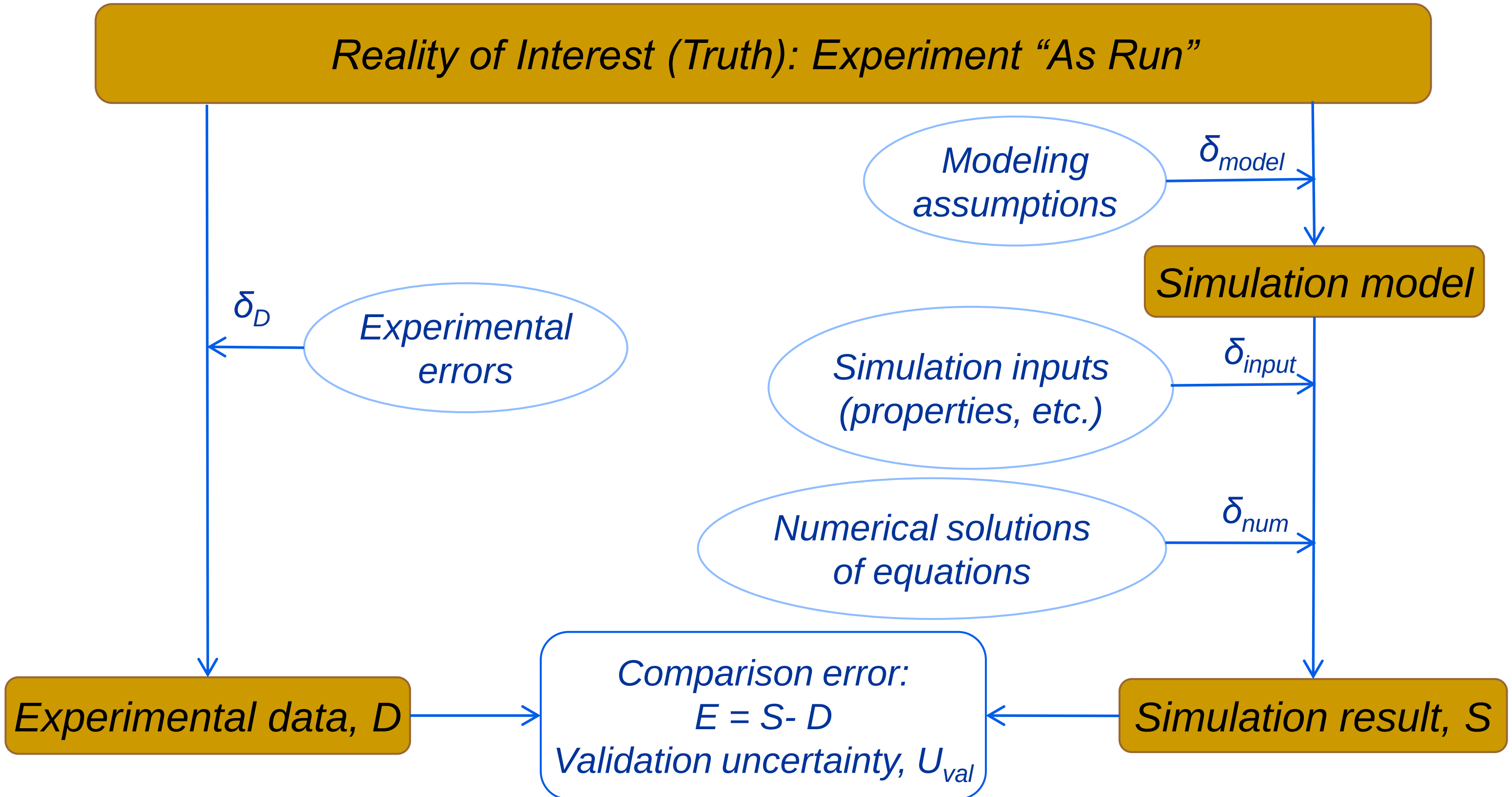
"… the actual agreement between CFD model predictions and experimental data … is often presented in an overly favourable light, for example suggesting that agreement is "good" when at best one might call it fair."
Grace and Taghipour (2004)

[1] L. J. Shadle, J. Spenik, R. Cocco, J. C. Ludlow, R. Panday, A. Issangya, R. Dastane, F. Shaffer, C. Guenther and E. Johnson (2010) Circulating Fluidized Bed Challenge Problem Experimental Test Results, 2010 AIChE Annual Meeting Conference Proceedings, Salt Lake City, UT, November 7-12, manuscript # 297i, pp.10. (https://mfix.netl.doe.gov/challenge/index.php.)

[2] T. Li, J. Dietiker, M. Shahnam, Numerical simulation of PSRI/NETL challenge problems. Poster at CFB10, May 1~5, 2011, Sunriver, Oregon.

What should be the objective of validation?

Error sources according to ASME V&V20-2009 Standard



$$\delta_{model} = E \quad U_{val}$$

$$U_{val} = \sqrt{U_{num}^2 + U_{input}^2 + U_D^2}$$

"The objective of the validation exercise is to estimate δ_{model} to within an uncertainty range."

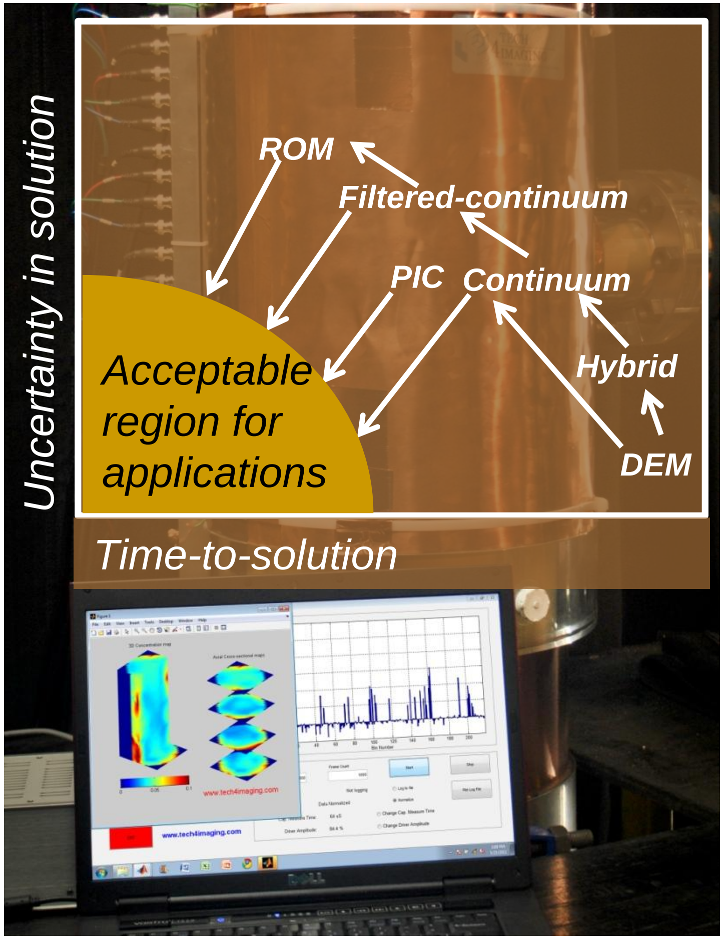
Uncertainty Quantification in multiphase CFD being initiated

- **Quantify the degree of confidence in the simulation results used for design support**
- **Assess probability of failure for technical risk analysis**
- **Identify and prioritize validation experiments and model development**
- **…**

Summary: Reducing uncertainty and time-to-solution are the primary needs

- **Support of open-source MFIX suite of codes: DEM, Hybrid, PIC, Continuum, Filtered-continuum, ROM**
- **Generation of accurate validation data from physical and numerical experiments**
- **Development of constitutive models for hydrodynamics and chemistry**
- **Quantification of uncertainty associated with CFD models of *reacting gas-solids* flows**

MFiX www.mfix.netl.doe.gov



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