Overview of Multiphase Flow Science at NETL

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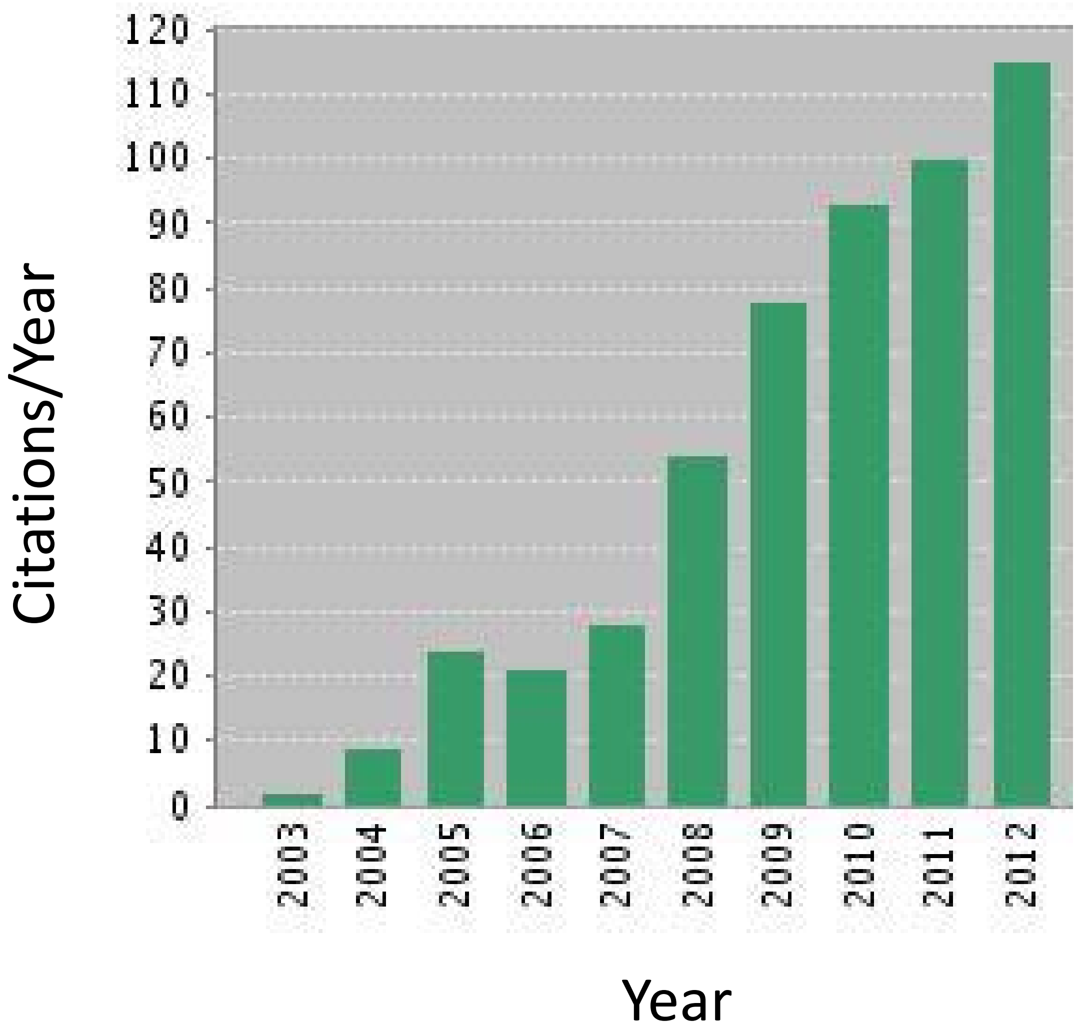
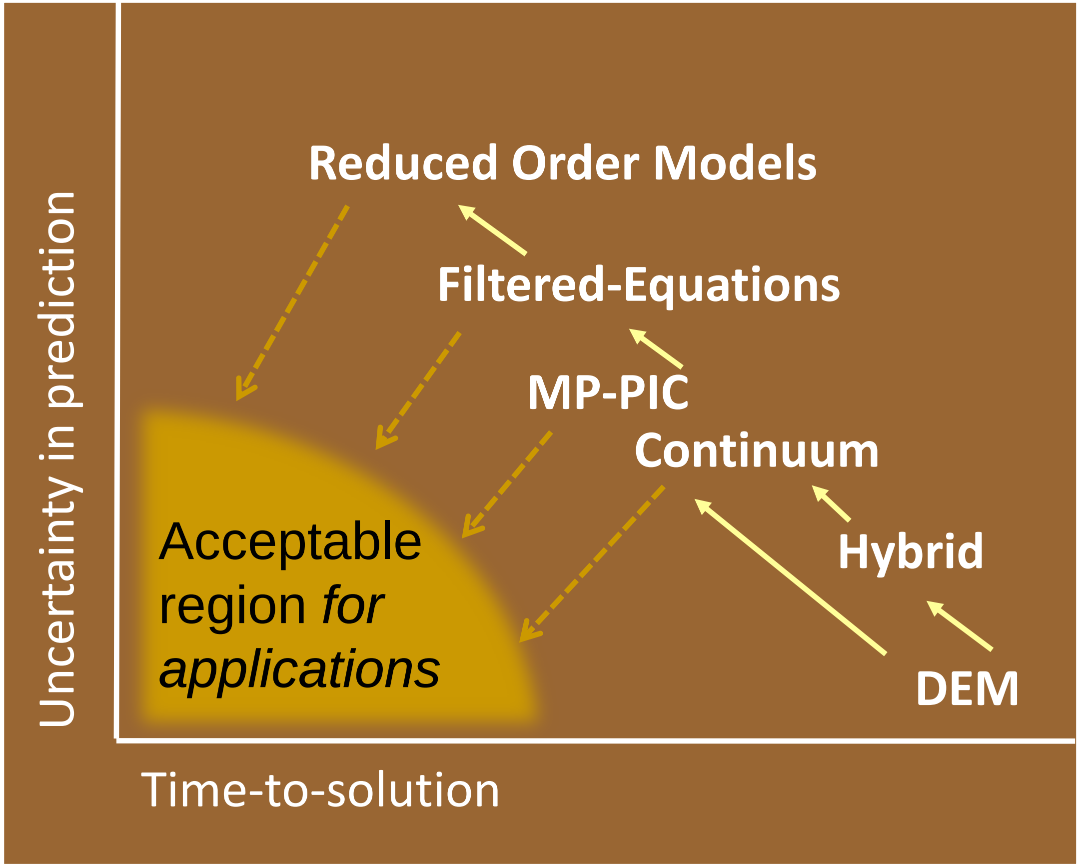
MFIX citations exceed 100/year



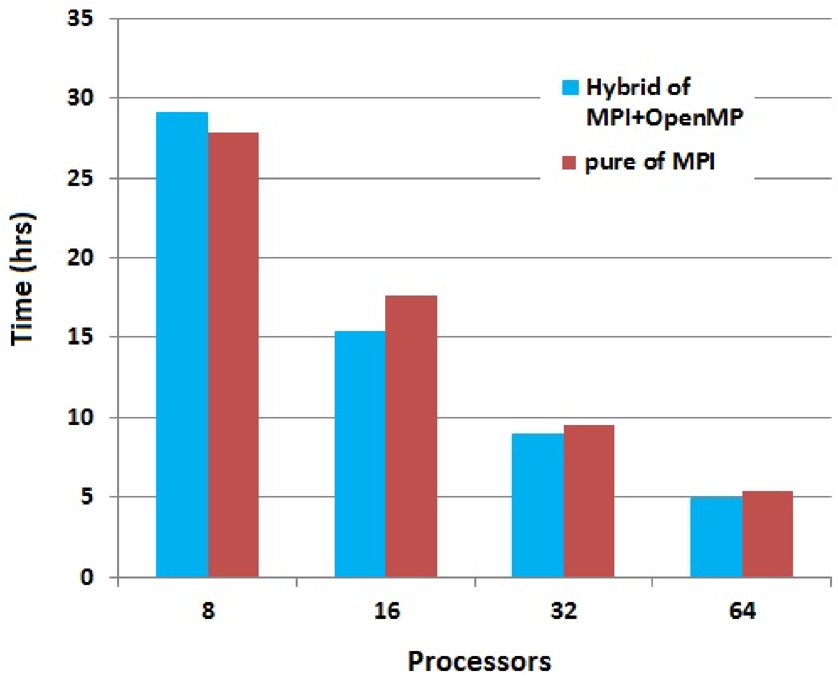
2006

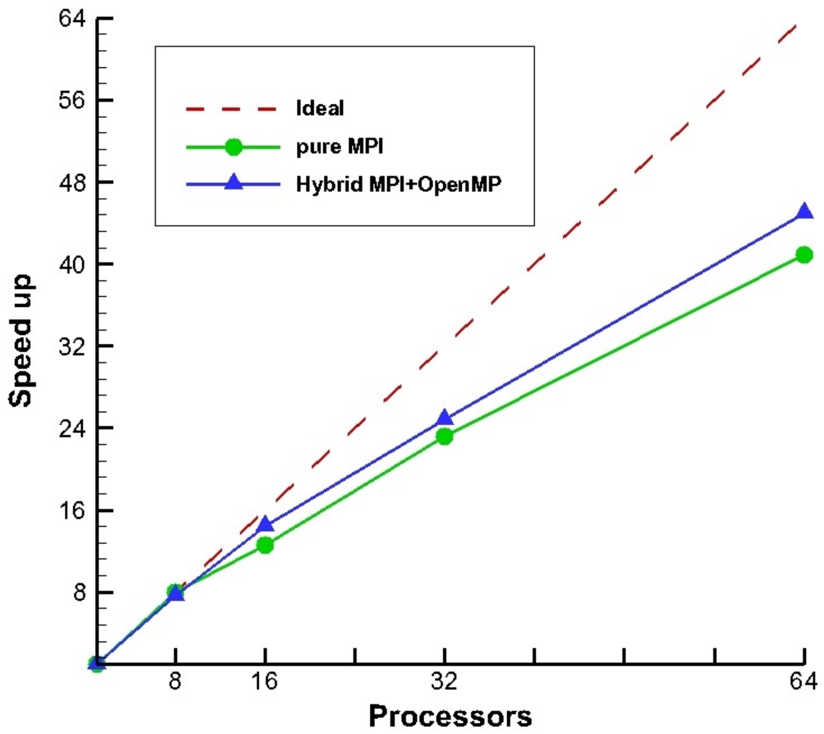
2007

Reduce uncertainty and time-to-solution in multiphase-CFD for energy applications



40x speed up of MFIX-DEM on 64 processors





Hybrid parallelism

- **4 OpenMP threads plus**
- **2, 4, 8 and 16 MPI processes for a total of**
- **8, 16, 32 and 64 processors**

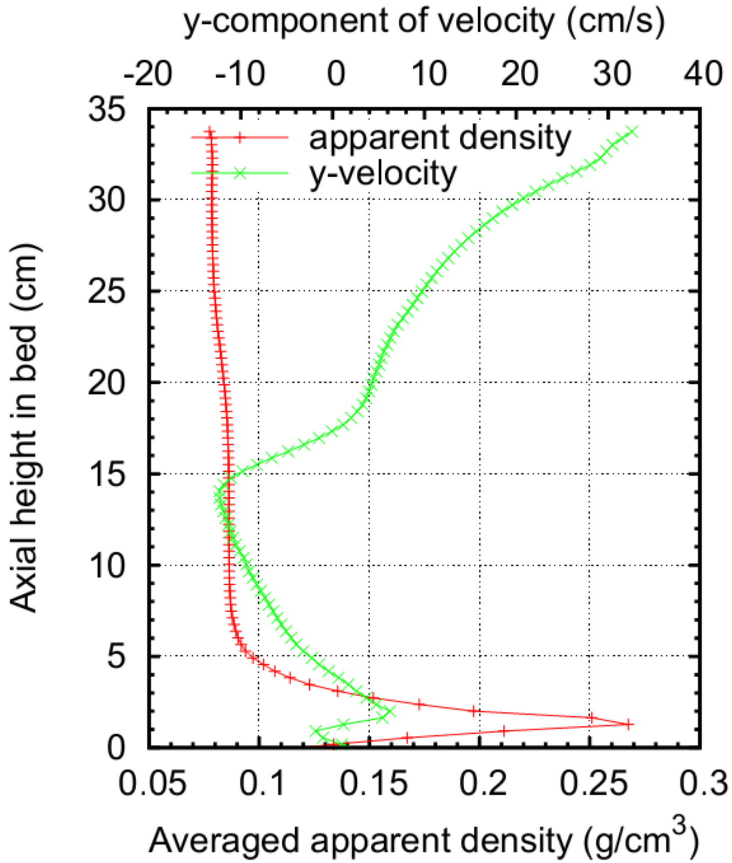
Liu, H., Tafti, D. Summary Report for MFIX Acceleration on New Code. March 2013. Project Title: MFIX acceleration (number: 683.232.001).

VirginiaTech Invent the Future

NETL

Stiff chemistry solver and variable solids density model incorporated into MFIX-TFM

- **Stiff chemistry solver handles the much smaller oxidation reaction time-scale in comparison to the flow time-scale.**
- **Solids density allowed to vary as a function of solids composition (e.g., reacting coal particle).**
- **Capabilities will be released to MFIX community in the next maintenance release**



Xue, Q., Dalluge, D., Heindel, T.J., Fox, R.O., Brown, R.C. (2012) , Experimental validation and CFD modeling study of biomass fast pyrolysis in fluidized-bed reactors, *Fuel* 97, 757-769.

The Ames Laboratory
Creating Materials & Energy Solutions

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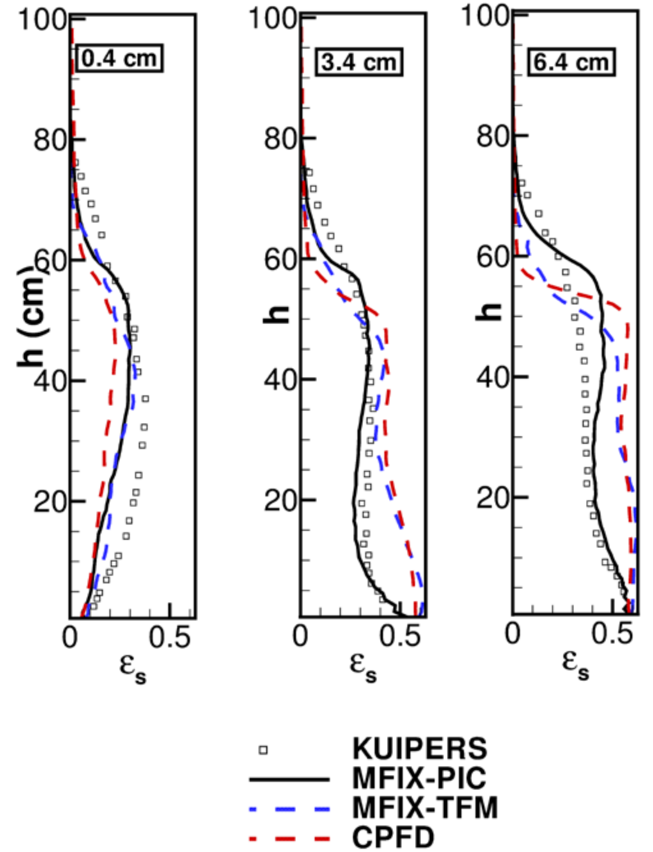
MFIX-PIC model released on March 2013

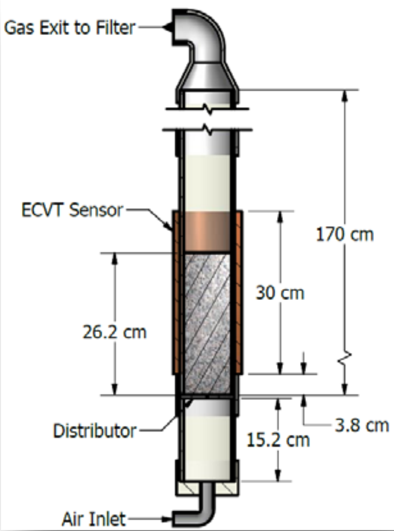
- Possibly the first open-source version of MP-PIC method
- Development guided by the trade off between numerical stability and physics for three problems
- Reasonable agreement with data and other codes for bubble frequency and void fraction distribution
- Pressure drop is under predicted by 15%, however
- Single-core comp. time (min):
  - TFM – 400
  - MP-PIC – 80



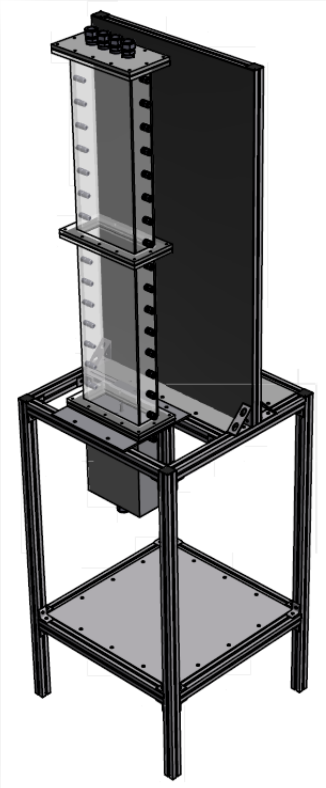
Bubbling fluidized bed simulation

Experimental facilities at various scales

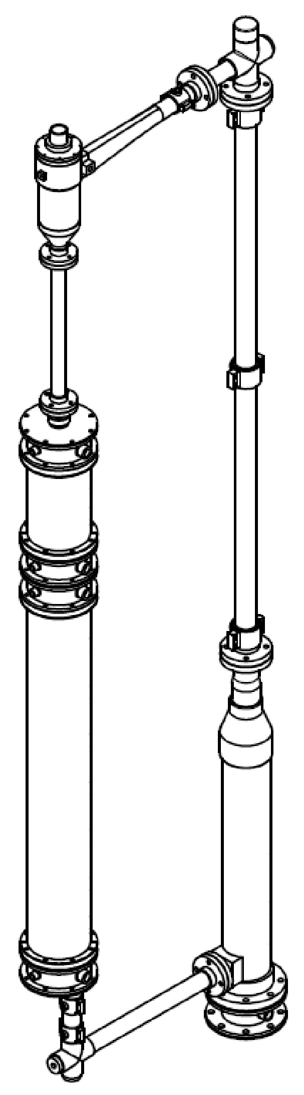
- Moving, spouted, fluidized, turbulent, and circulating fast fluid and transport regimes



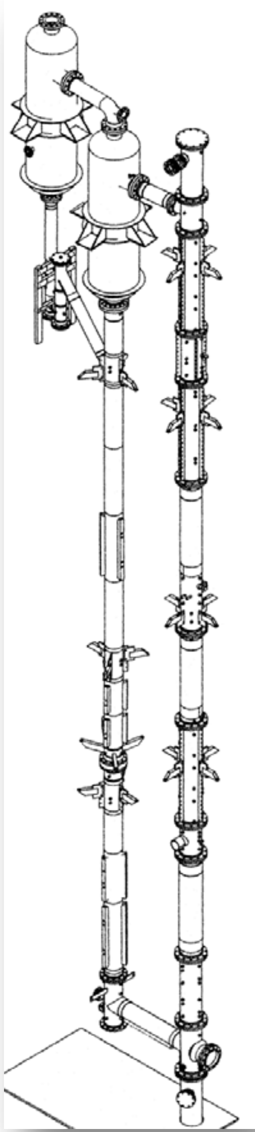
BFB (10-cm diam.)



Rectangular FB (7.5x23x122 cm)



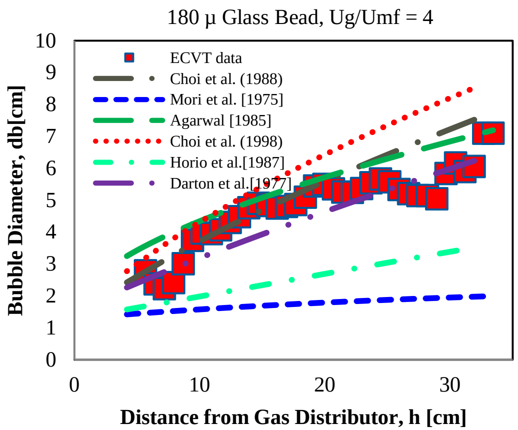
CLR (5 cm dia x 5 m tall)

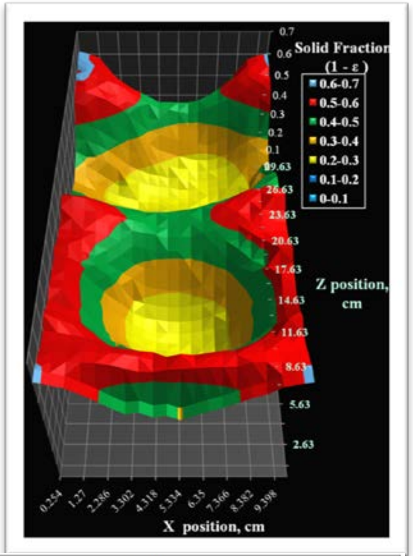


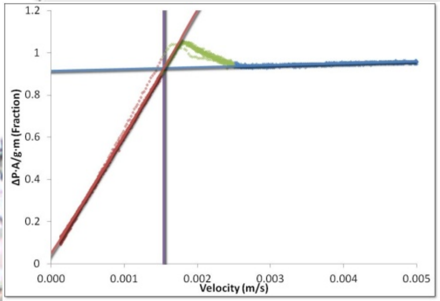
CFB (30 cm dia x 15 m tall)

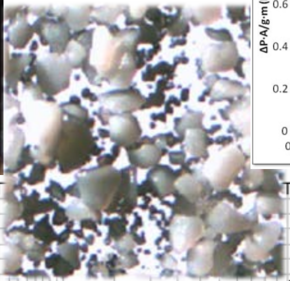
Measurement techniques

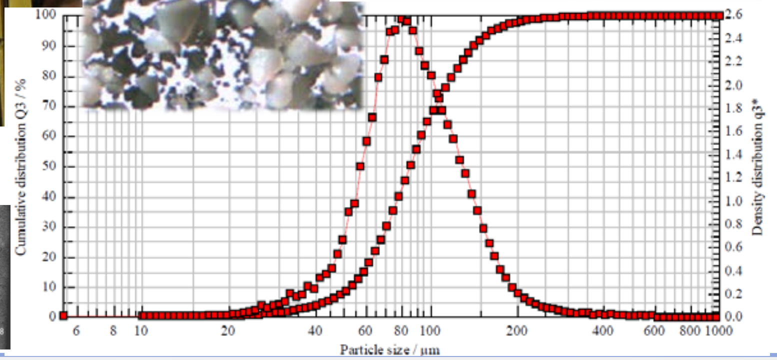
- **Electro Capacitance Volumetric Tomography (ECVT)**
  - bubble velocity, frequency, diameter
- **High Speed Particle Imaging Velocimetry (HS-PIV)**
  - Particle velocity, trajectories, fluctuations
  - granular temperatures
- **Laser Doppler Velocimetry (LDV)**
  - Gas and particle velocities
- **Gas and solids tracers**
  - Phosphorescent particles (dispersion, solids circulations, flow distribution)
  - He and CO2 gases (velocities, dispersion)
- **Optical particle velocity probes**
  - Particle, bubble, and cluster velocities
- **Local solids flux probe**
  - Core annular flow profiles
- **Particle characterization**
  - Size distribution
  - Minimum fluidization
  - Densities

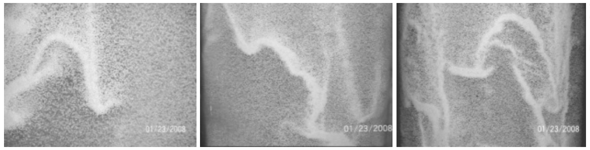






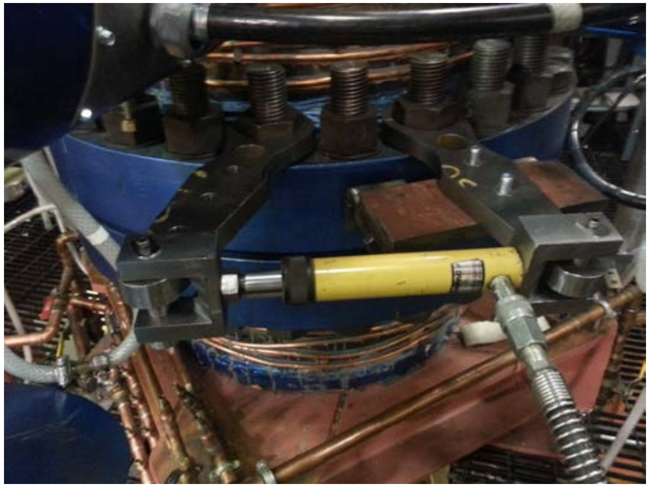




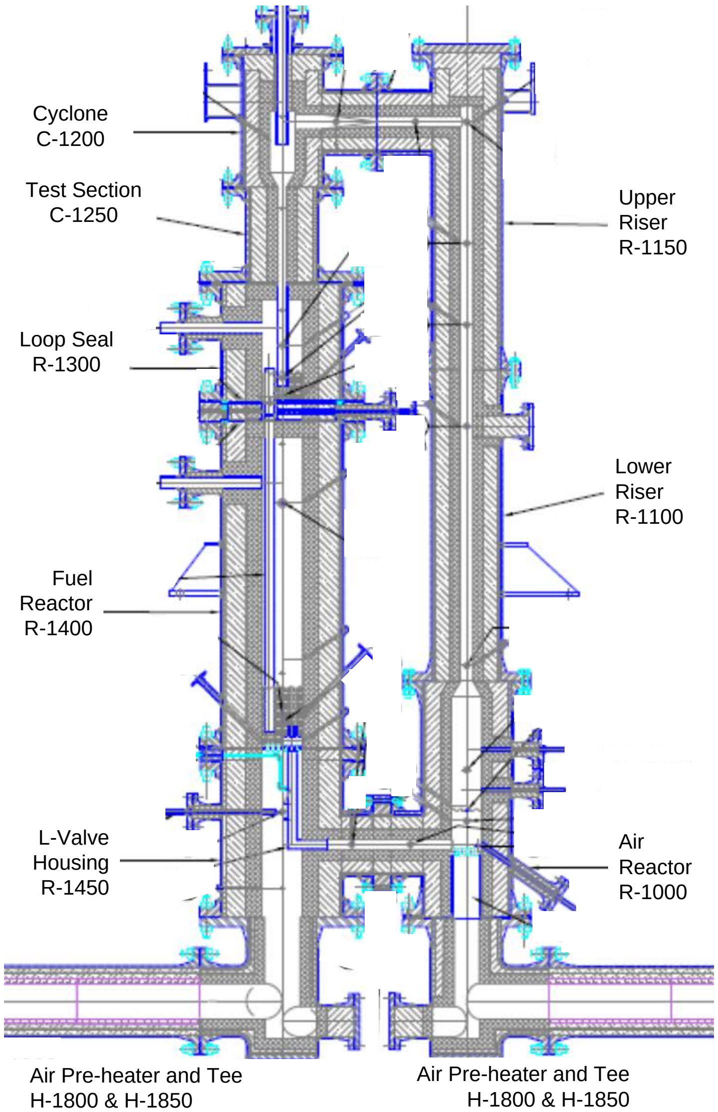


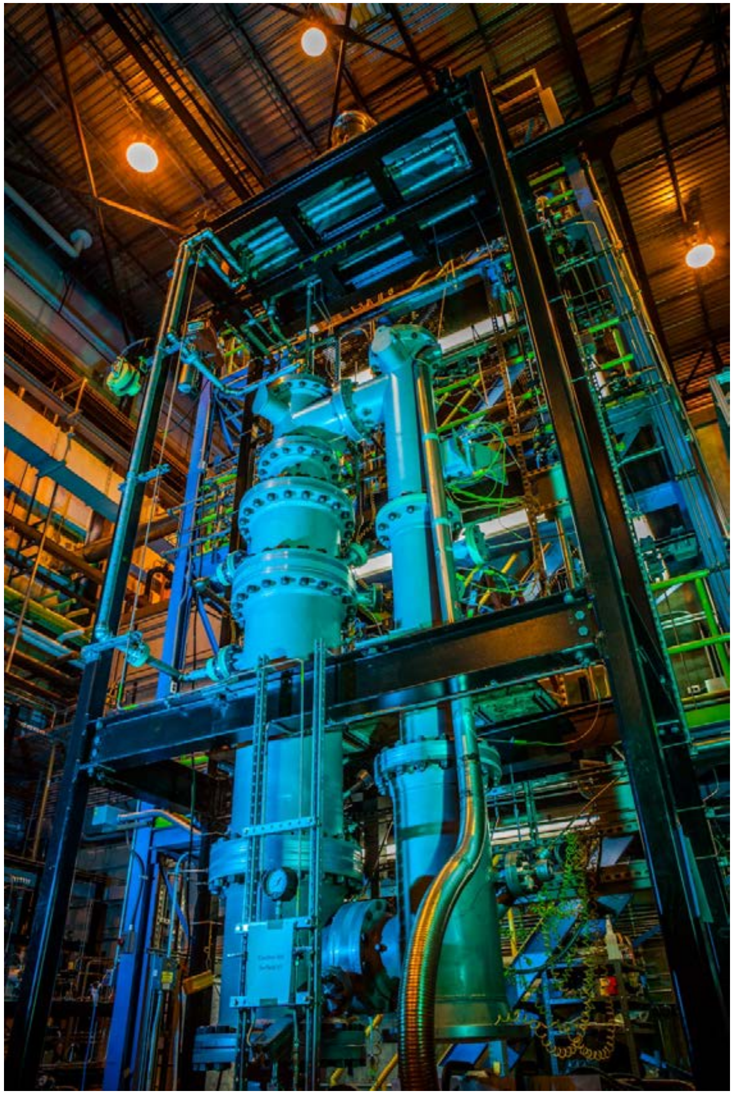
High-pressure entrained flow gasifier

- **Organic and inorganic transformations in fuels (coal, biomass, coal & biomass blends) under pyrolysis, gasification, and combustion conditions**
- **Kinetics of pyrolysis and gasification**
- **Kinetics of mineral transformations to validate ash deposition/viscosity models**
- **Slag refractory interactions by using reaction tubes made of different compositions.**



Chemical looping hot unit

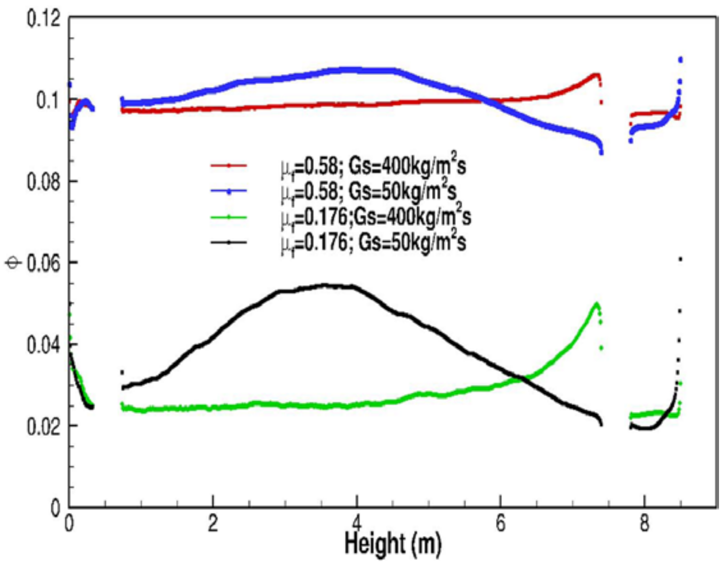




Improved partial slip boundary condition implemented

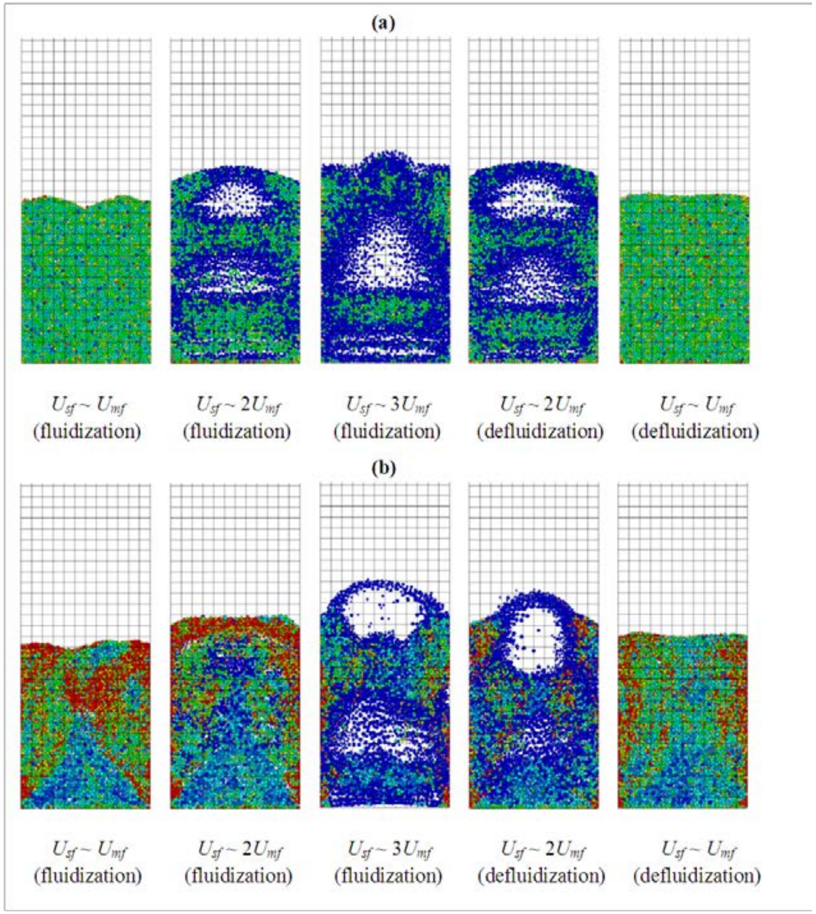
- **Variable specularity coefficient model[1] for Johnson & Jackson BC implemented in MFIX**
- **Tested for both bubbling and circulating fluidized beds[2]**

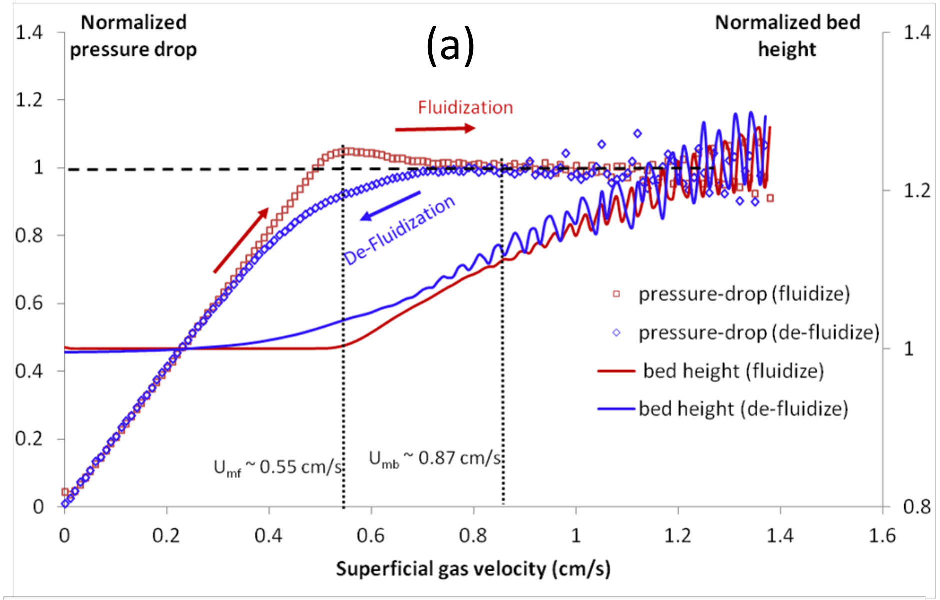
Variation of mean specularity coefficient along riser wall for different friction coefficients and solids circulation rates

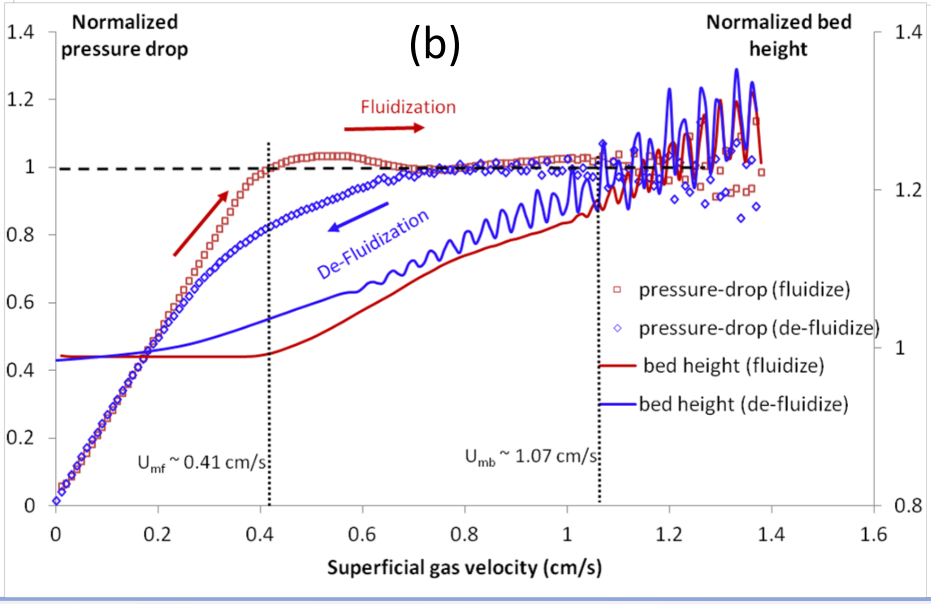


1. T. Li & S. Benyahia, Revisiting Johnson and Jackson boundary conditions for granular flows, *AIChE J.*, 2012, 58, 2058-2068.
2. T. Li & S. Benyahia, Evaluation of wall boundary condition parameters for gas-solids fluidized-bed simulations, 2013, *AIChE J.*, doi: 10.1002/aic.14132.

Cohesive force model in MFIX-DEM



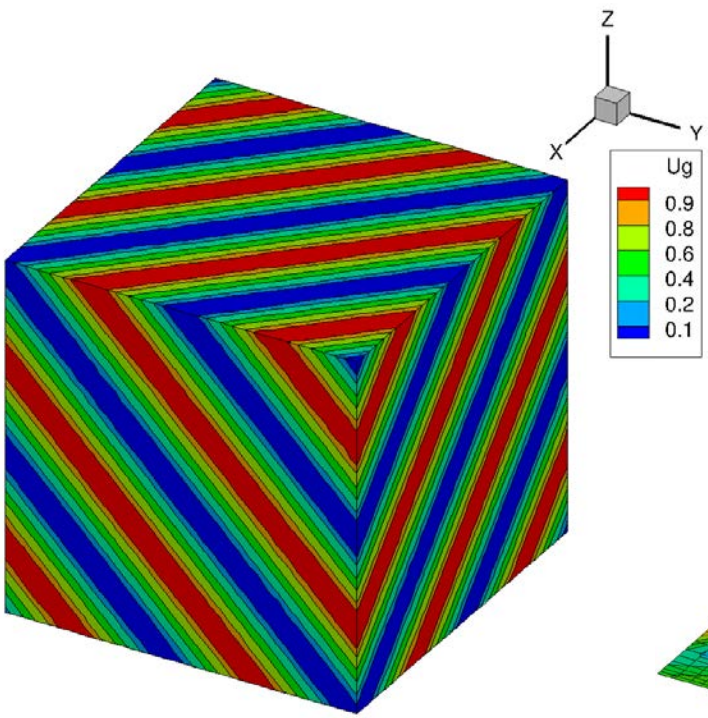




Fluidization/defluidization behavior of aeratable powder. (a) monodisperse and (b) polydisperse

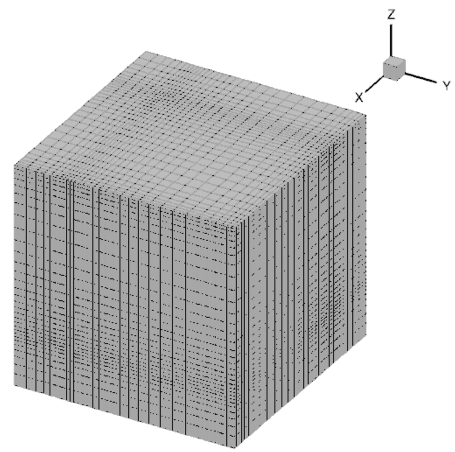
Galvin, JE & Benyahia, S. The Effect of Cohesive Forces on the Fluidization of Aeratable Powders. Submitted to *AIChE J.* (2013).

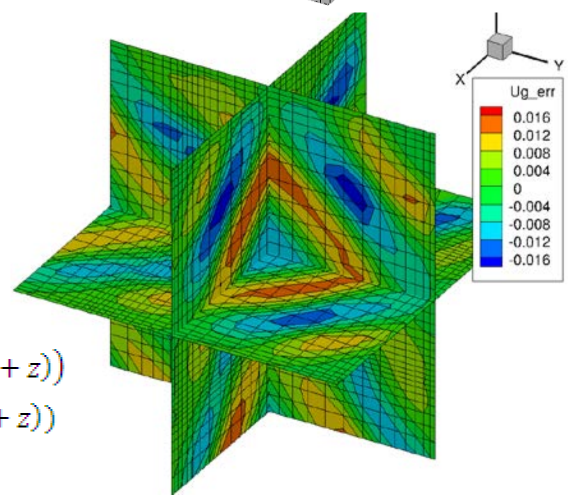
Verified MFIX for single-phase 3D unsteady flow on stretched Cartesian grids

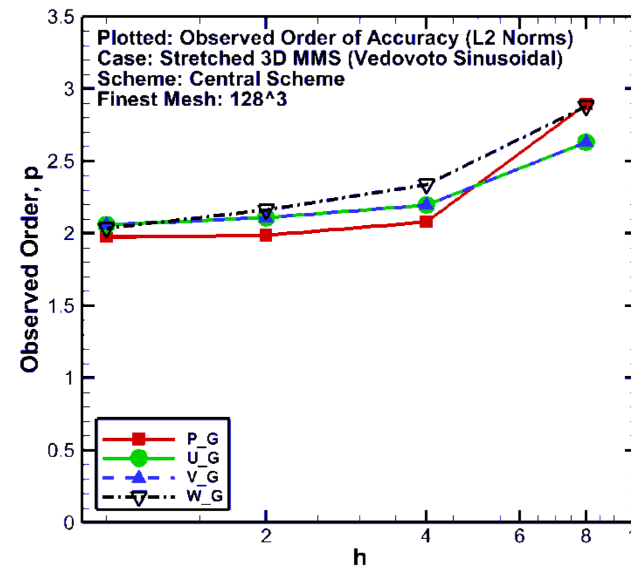


$$u = \sin^2\left(2\pi(x+y+z)\right) \quad v = \cos^2\left(2\pi(x+y+z)\right)$$

$$w = 1 \quad p = \cos\left(2\pi(x+y+z)\right)$$





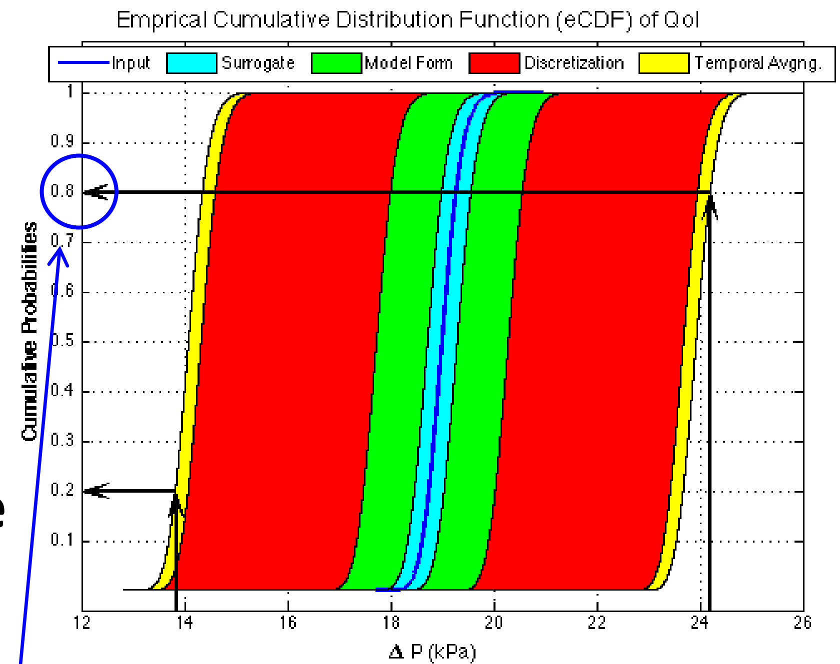


VirginiaTech Invent the Future

Choudhary, A. and Roy, C.J., "Code Verification of Multiphase Flows with MFIX," Presented at the ASME 2013 Verification and Validation Symposium, Las Vegas, NV, May 22-24, 2013.

UQ analysis demonstrated for 3D transient fluidized bed riser simulation

- Predictive Total Uncertainty Quantification: Accounts for various sources of uncertainties with the UQ framework
- The CDF plot provides answers to questions such as, for example:
  - What is the probability that the fluid bed pressure drop could exceed 24.2 kPa?
  - Answer: (1-0.8) => at most 20 %



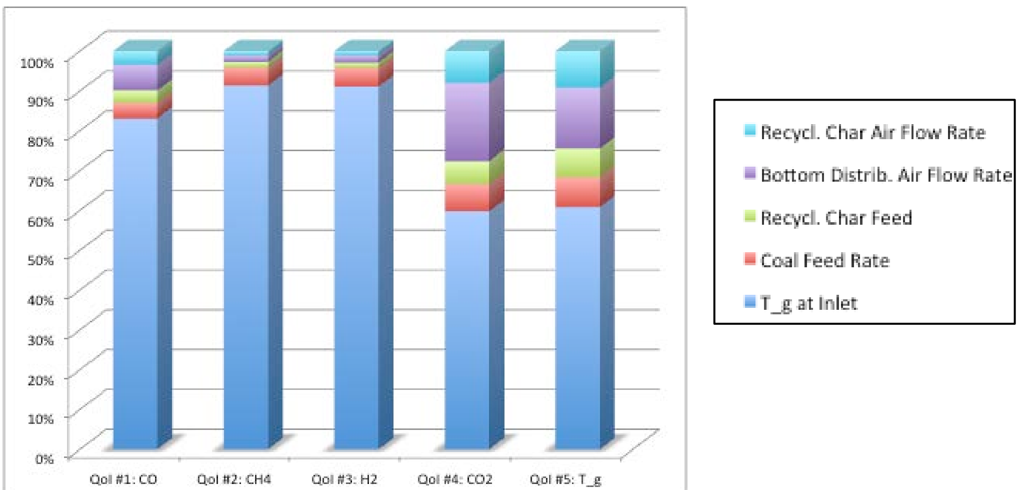
Total uncertainty quantification performed in validation domain

Gel, A., Li, T., Gopalan, B., Shahnam, M., Syamlal, M., "Validation and Uncertainty Quantification of a Multiphase CFD Model", *Industrial & Engineering Chemistry Research*, 2013 http://pubs.acs.org/doi/abs/10.1021/ie303469f.

Sensitivity analysis demonstrated for 2D transient gasifier simulation

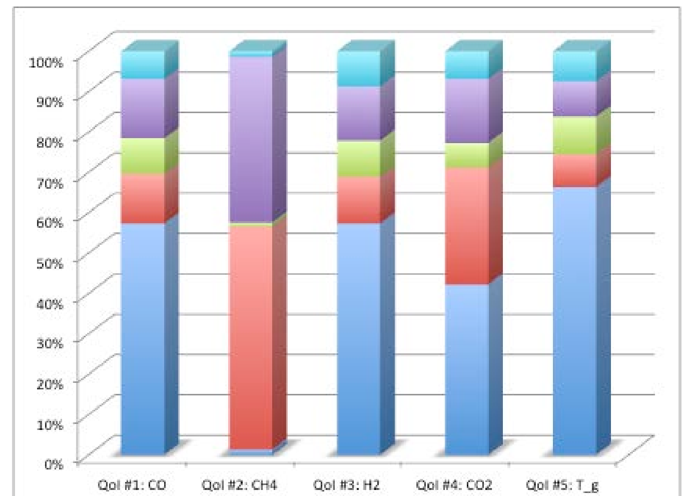
Sobol Total Sensitivity Indices Analysis: How much each input contributes to the observed variability in output?

MGAS Pyrolysis Kinetics



Inlet temperature is the primary & most dominant contributor to all QoI variability

PCCL Pyrolysis Kinetics

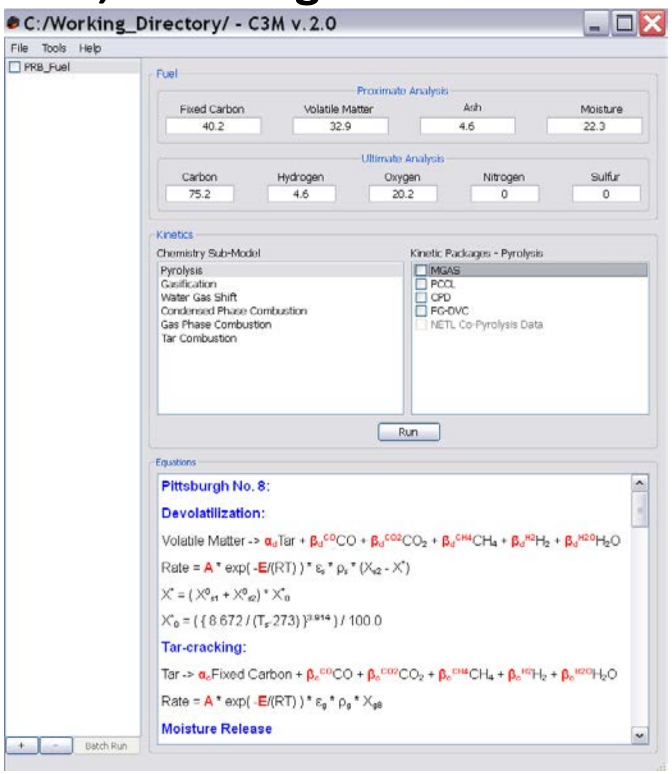


For CH_4 production, coal flow rate is the primary contributor to observed variability

1. Gel, A., Chaudhari, K., Turton, R., and Nicoletti, P., "Application of Uncertainty Quantification Methods for Coal Gasification Kinetics in Gasifier Modeling Part 1: Coal Devolatilization", accepted for publication in *Powder Technology*, 2013.
2. Gel, A., Garg, R., Tong, C., Shahnam, M. and Guenther, C., "Applying Uncertainty Quantification to Multiphase Flow Computational Fluid Dynamics", *Powder Technology*, 2013, 242, 27-3939.

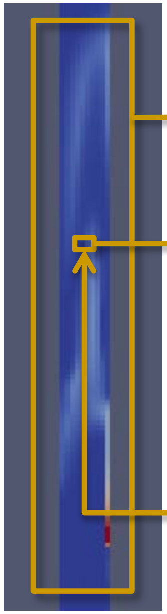
Advances in Carbonaceous Chemistry for Computational Modeling

New, more logical User Interface



C3M™
Carbonaceous Chemistry for Computational Modeling

High Fidelity Surrogate Models



Average T_s in domain to get T_R

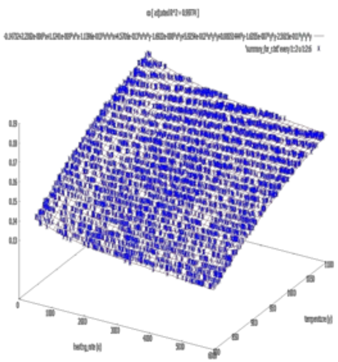
Calc HR from Energy Balance

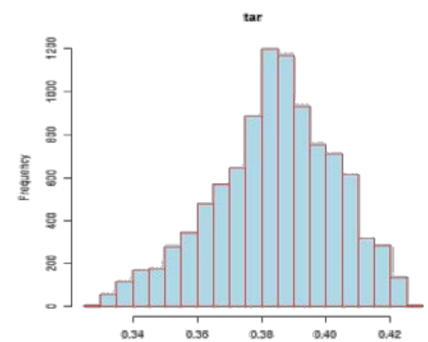
$$X_{char} = 1 - \frac{(1 - m_{ash})|_{cell,dry}}{(1 - m_{ash})|_{initial,dry}}$$

$$X_{Final} = E(HR, T_R)$$
$$A_{Tot} = F(HR, T_R)$$
$$Ea_{Tot} = G(HR, T_R)$$
$$\beta_i = H(HR, T_R)$$

$$r_i = r_{Tot} Y_i = \rho_s \varepsilon_s m_{char} A_{Tot} e^{-\frac{Ea_{Tot}}{RT_s}} (X_{Final} - X_{char}) \beta_i$$

UQ Toolbox





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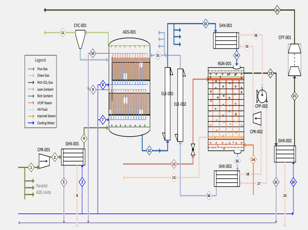
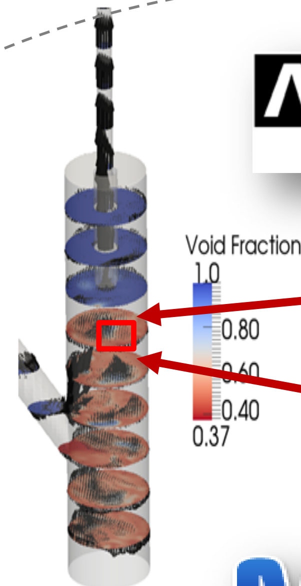
Multi-scale models use multiphase CFD

CCSI Carbon Capture Simulation Initiative

Experimental Validation

Process Models & Optimized Process

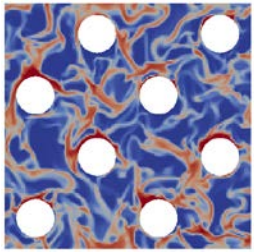




Void Fraction along horizontal planes and velocity vectors

ANSYS FLUENT

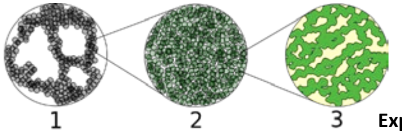
Heat-transfer-tube-scale hydrodynamics

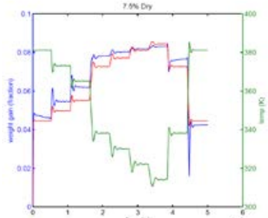


$$f^*_{drag} = \beta^*\left(-v_s^*\left|v_s^*\right|\right)+\gamma^*$$

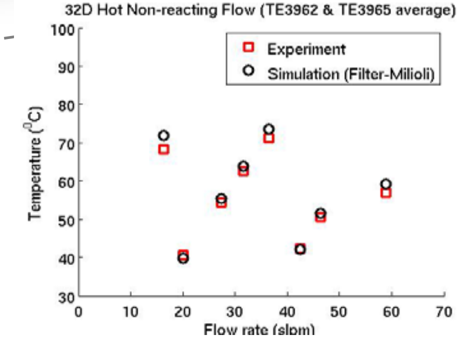
MFiX

SORBENTFIT





Experimental Kinetic/Mass Transfer Data



Miller, D.C., "The U.S. DOE's Carbon Capture Simulation Initiative for Accelerating Commercialization of CCS Technology," presented at the NETL CO2 Capture Technologies Meeting, Pittsburgh, PA, July 9, 2012.