Fluidized Beds: Recent Model Applications

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Outline

- Introduction to NETL Multiphase Flow Science
- The Multiphase Flow Modeling Tools
- Model Application: TRIG™ Gasifier
- Model Application: Lab and Pilot Scale Carbon Capture
- Summary

Why Multiphase Flow Science?
Solids processing poses a big design challenge

An estimated 40% of the value added by the U.S. chemical industry is related to particle technology[1]

"plants processing solids anywhere on the main process train perform more poorly than plants that process only liquids and gases."[2]

	Performance as % of design
Only liquids and gases	84%
Addition of solids	63%

"scale-up of fluidized bed reactors and transfer systems is a daunting task"[3]

Examples of challenges in fossil energy processes

- Erosion of heat transfer tubes in combustors
- 3-10 years for IGCC plants to reach an availability of 80%[4]
- Attrition and loss of fines in a chemical looping system
- Novel CO_2 capture processes require scaling up of fluidized bed reactors

[1]Ennis, B.J., J. Green, R. Davies. 1994. The Legacy of Neglect in the U.S., *Chemical Eng. Progress*, 32-43.
[2]Merrow, E.W. 1985. Linking R&D to Problems Experienced in Solids Processing. *Chemical Engineering Progress*.14-22.; Merrow, E.W. 1986. A quantitative assessment of R&D requirements for solids processing technology. Rand Corp. R-3216-DOE/PSSP.
[3]Knowlton, T.M., S.B.R. Karri, and A. Issangya. 2005. Scale-up of fluidized bed hydrodynamics. Powder Technology, 150(2): p. 72-77.
[4]Mauerstad, O. 2005. An Overview of Coal-Based Integrated Gasification Combined Cycle (IGCC) Technology. MIT Publication No. LFEE 2005-002 WP

NETL Multiphase Flow Science – 30 years of R&D

- **Goal: Ongoing development and support of accurate, validated, practical simulation tools to guide design, operation, and troubleshooting of multiphase flow devices**
  - Emphasis on Fossil Fuel Technology (e.g., coal gasifiers, CO_2 capture devices, Chemical Looping)
  - Promote application to other Industries and Natural Processes

- **The Historical Challenge for Modeling: Managing the tradeoff between accuracy and time to solution**

Tradeoff between uncertainty and time-to-solution leads to models at different of resolutions

Time to Solution

DNS *Direct Numerical Simulation: Very fine scale, accurate simulations for very limited size domain*

MFiX DEM *Discrete Element Method: Track individual particles and resolve collisions*

MFiX Hybrid *Hybrid: Continuum and discrete solids coexist*

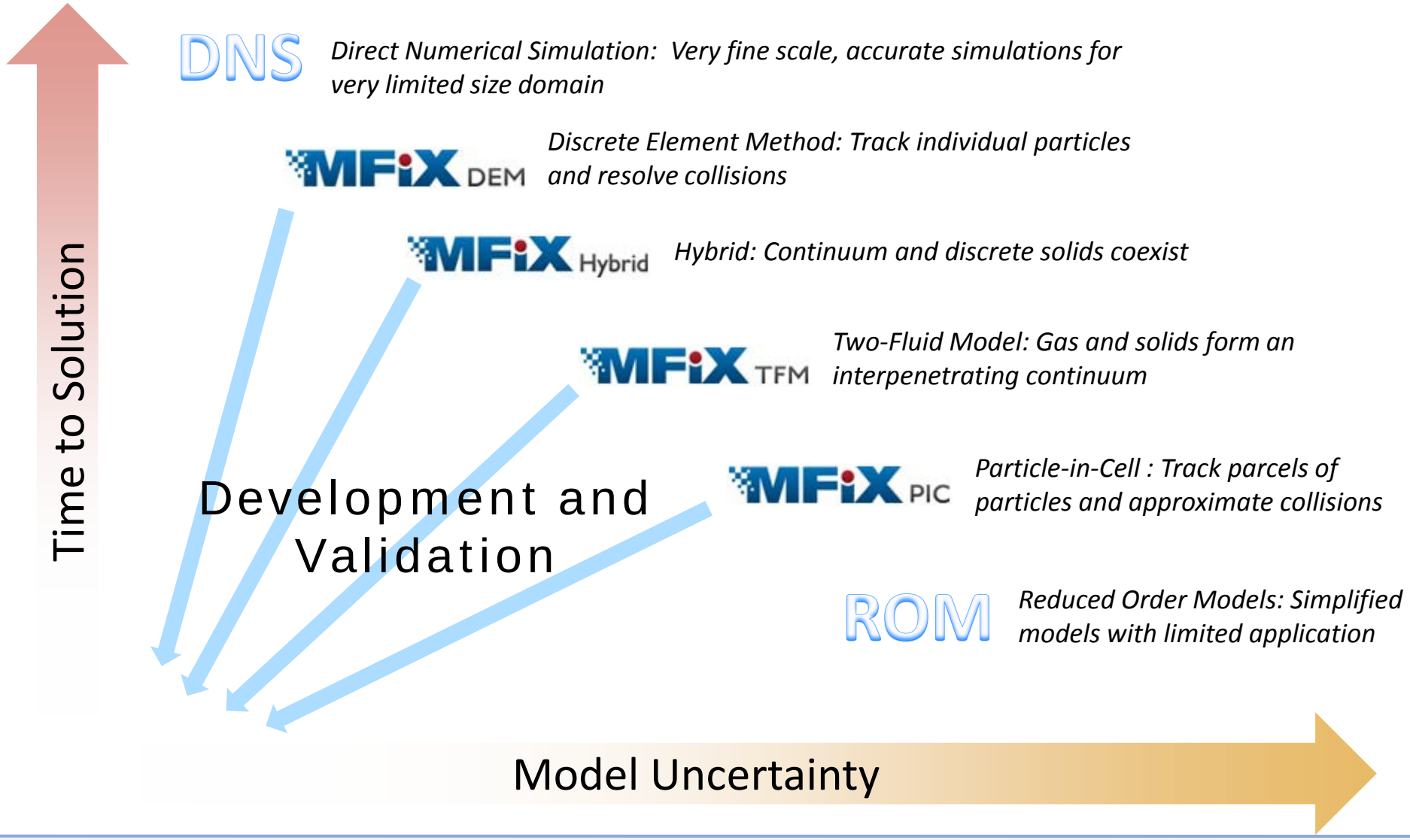
MFiX TFM *Two-Fluid Model: Gas and solids form an interpenetrating continuum*

MFiX PIC *Particle-in-Cell : Track parcels of particles and approximate collisions*

ROM *Reduced Order Models: Simplified models with limited application*

Model Uncertainty

Tradeoff between uncertainty and time-to-solution leads to models at different of resolutions



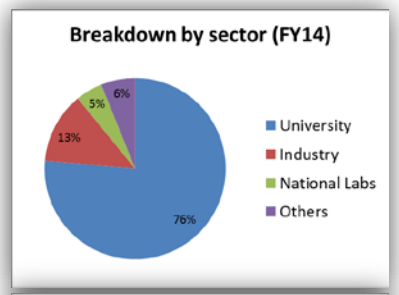
The Modeling Tools

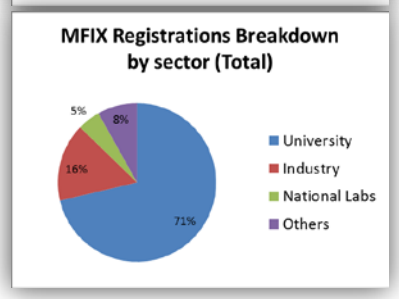
- **The NETL MFiX (*Multiphase Flow with Interphase eXch*anges) Suite of Computational Fluid Dynamics Codes are the basis**
  - MFiX is NETL's open-source CFD software platform for hydrodynamics, heat transfer, and chemical reactions in multiphase systems
  - MFiX provides transient, 3D predictions of pressure, velocity, temperature, and species for all phases
- **The NETL C3M (*Carbonaceous Chemistry for Computational Modeling*) is used for determining the coal reaction mechanism**
  - C3M is chemistry management software focused on computational modeling of reacting systems
  - Provides direct links between kinetic information and CFD
  - Virtual kinetic laboratory – allows evaluation of complex kinetic expressions
- **Simulations are performed on the NETL Supercomputer**
  - Ranked in top 100 supercomputers in the world

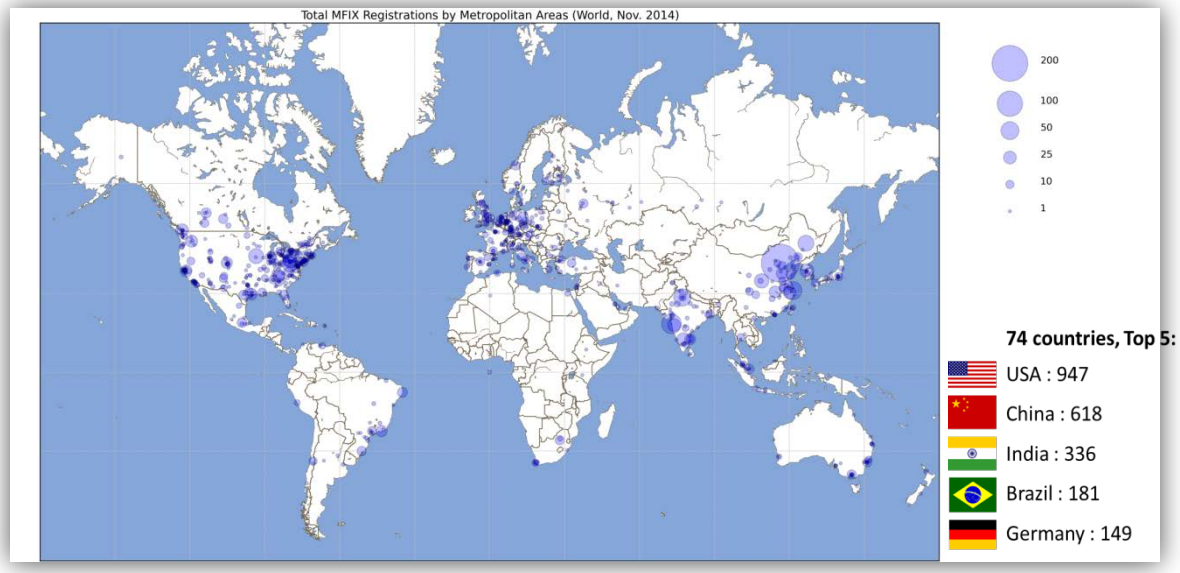
MFiX Use Continues to Grow

- **FY14 new registrations** **229**
  - University 175
  - Industry 29
  - National Labs 11
  - Others 14

- **Total MFIX registrations** **3,513**
  - University 2506
  - Industry 559
  - National Labs 163
  - Other 285

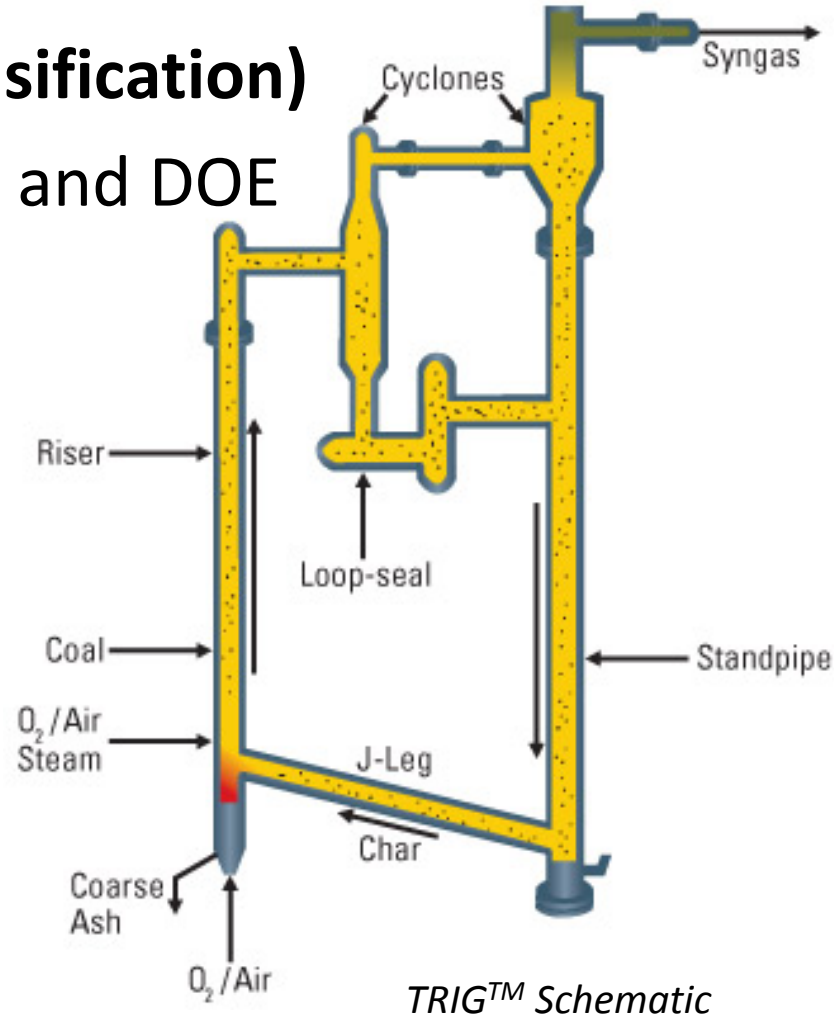






Model Application: Transport Integrated Gasifier (TRIG™)

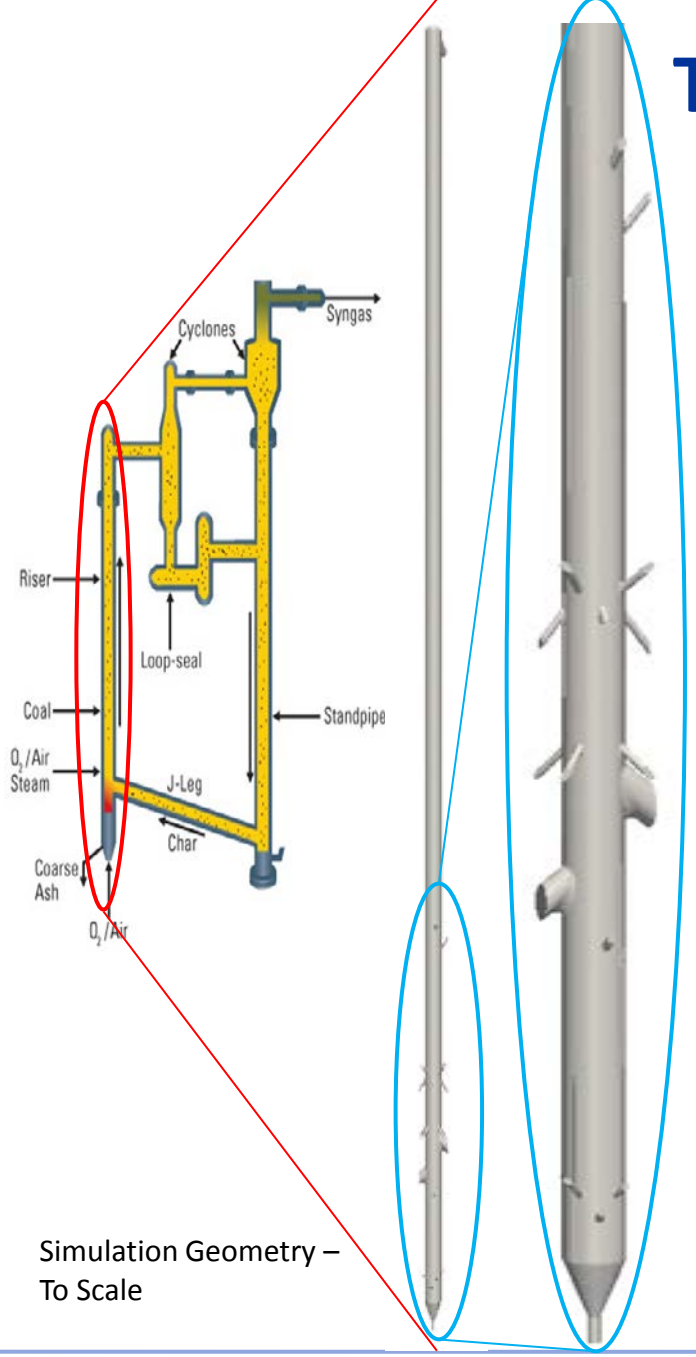
- **TRIG™ (Transport Integrated Gasification)**
  - Developed by KBR, Southern, and DOE
    - Based on KBR FCC technology
  - Air- and oxygen-blown
  - Good for low-rank coal
  - Major components:
    - Mixing zone
    - Riser
    - Cyclone/disengage, loop-seal
    - Standpipe, J-leg



TRIG™ Schematic

www.kbr.com

The MFIX Model Setup



Simulation Geometry – To Scale

Detail of Inlets

- **Simulation with Detailed Setup**
  - Fine grid: 1.3 Million Computational Cells
  - Well-resolved inlets & outlet for all streams
  - Two solid "phases" used for coal and recycled ash with different sizes & densities
  - Although high geometric fidelity, model is expensive to run
    - long simulation time
    - large datasets to manipulate
- **Created Simplified Setup**
  - Compared this to Detailed Setup results to verify acceptable accuracy
  - Now able to do more simulations over a range of operating conditions

The MFIX Model Setup

- **Simplified Setup**
  - Coarse grid: 400,000 computational cells
    - Major inlets & outlets are still well resolved
    - Point sources near walls used to capture smaller inlet flows
  - Single representative solid phase for coal and recycled ash
  - A 'filtered' model used for momentum, heat & mass transfer to capture subgrid-scale physics
  - Resultant model is much less expensive to run – still retains the major flow features
  - Comparison to Detailed Case is very good
    - Temperature and outlet composition are close

- **Li et al. Energy & Fuels, 2013, 27, 7896-7904.**

Chemical Kinetics

- **Detailed coal devolatilization and gasification reaction kinetics were developed for Mississippi lignite**
  - 17 gas-phase species and 4 solids-phase components are tracked
  - Use the ***PC Coal Lab*** database through ***C3M*** to determine rate constants
    - This approach accounts for the effects of local bed conditions and feed stock properties on the kinetics
  - Thermodynamic properties provided by ***C3M*** from standard databases
- **Other reactions included in the scheme**
  - Char combustion: shrinking core model
  - Gas phase combustion: global reaction mechanisms for hydrocarbons
  - Water-gas shift: combination of catalytic and non-catalytic kinetics
- **Chemical kinetics parameters were held constant for all simulations**
  - No 'tweaking' of parameters was done to improve agreement

- **Van Essendelft et al. Advanced Chemistry Surrogate Model Development within C3M for CFD Modeling, Part 1: Methodology Development for Coal Pyrolysis, I&ECR 2014, 53, 7780-7796**
- **Westbrook and Dryer, Simplified Reaction Mechanisms for the Oxidation of Hydrocarbon Fuels in Flames, Combustion Science and Technology, 1981, Vol. 27, pp. 31-43.**

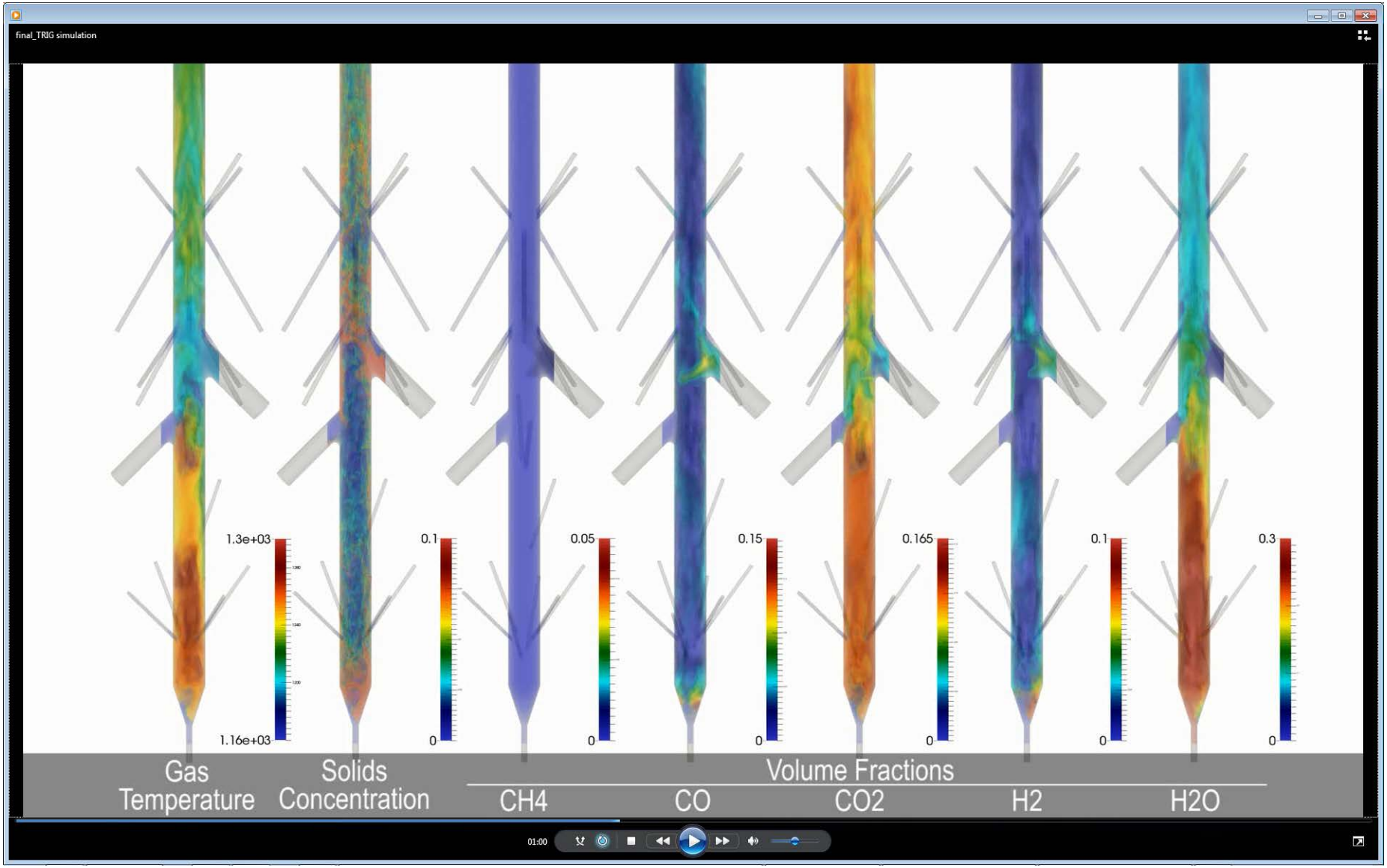
PSDF TRIG™ Tests using Mississippi Lignite

- **Operating conditions that were simulated – 11 Runs**
  - Gasifier temperature (~1600-1750F)
  - Pressure (~191-211 psig)
  - Steam-to-coal ratio (~0.005-0.174)
  - Coal feed rate (~3500-4340 lb/hr)
  - Lignite coal composition used for the simulations (after drying):

Proximate analysis		**Ultimate analysis**	
Fixed carbon (%)	31	Carbon (%)	46
Volatile matter (%)	37.1	Hydrogen (%)	3.5
Moisture (%)	17.1	Oxygen (%)	17.1
Ash (%)	14.8	Nitrogen (%)	1
		Sulphur (%)	0.6

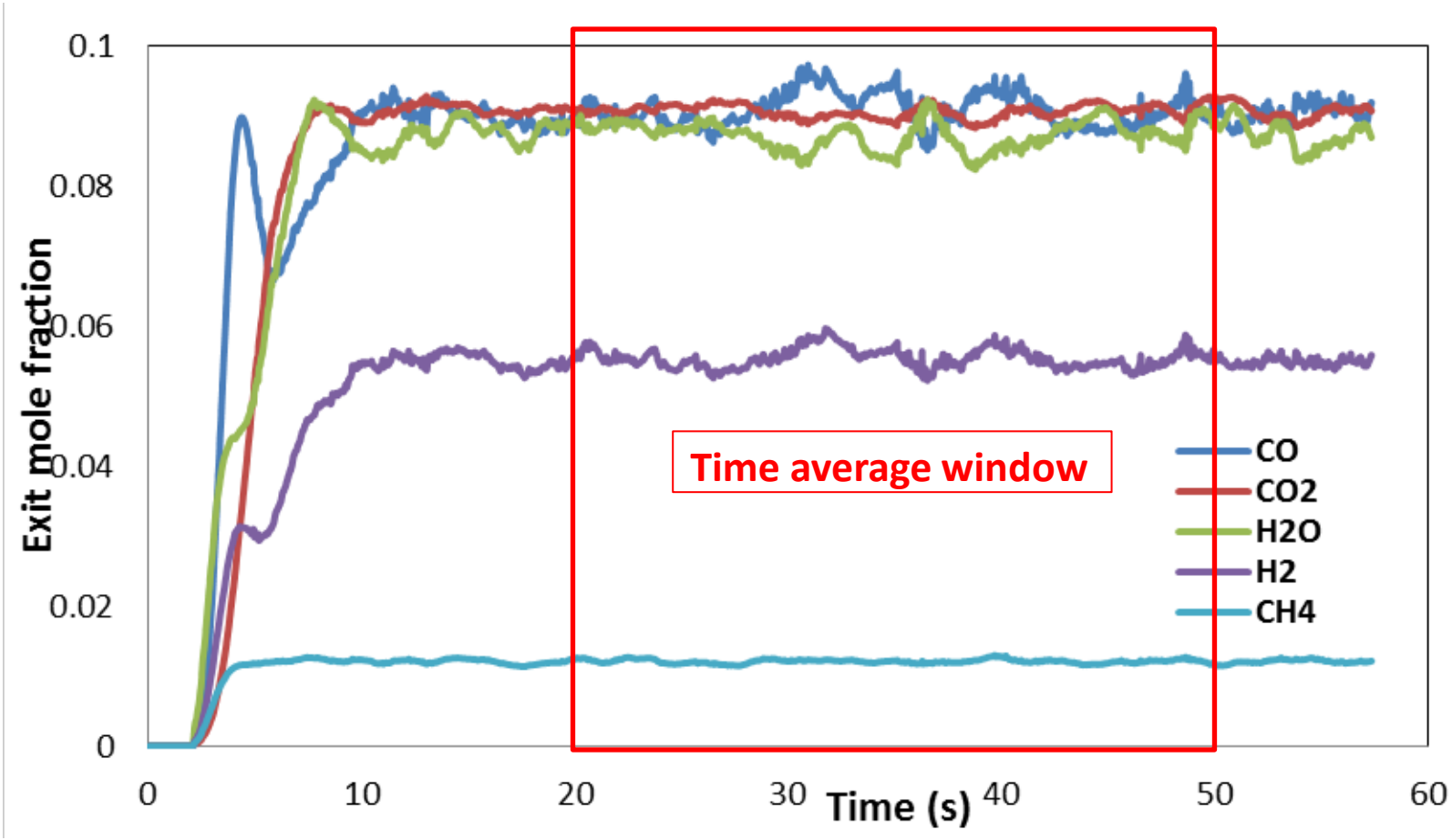
POWER SYSTEMS DEVELOPMENT FACILITY TOPICAL REPORT: GASIFICATION TEST CAMPAIGN TC25, 2008

Visualization of Transient Results



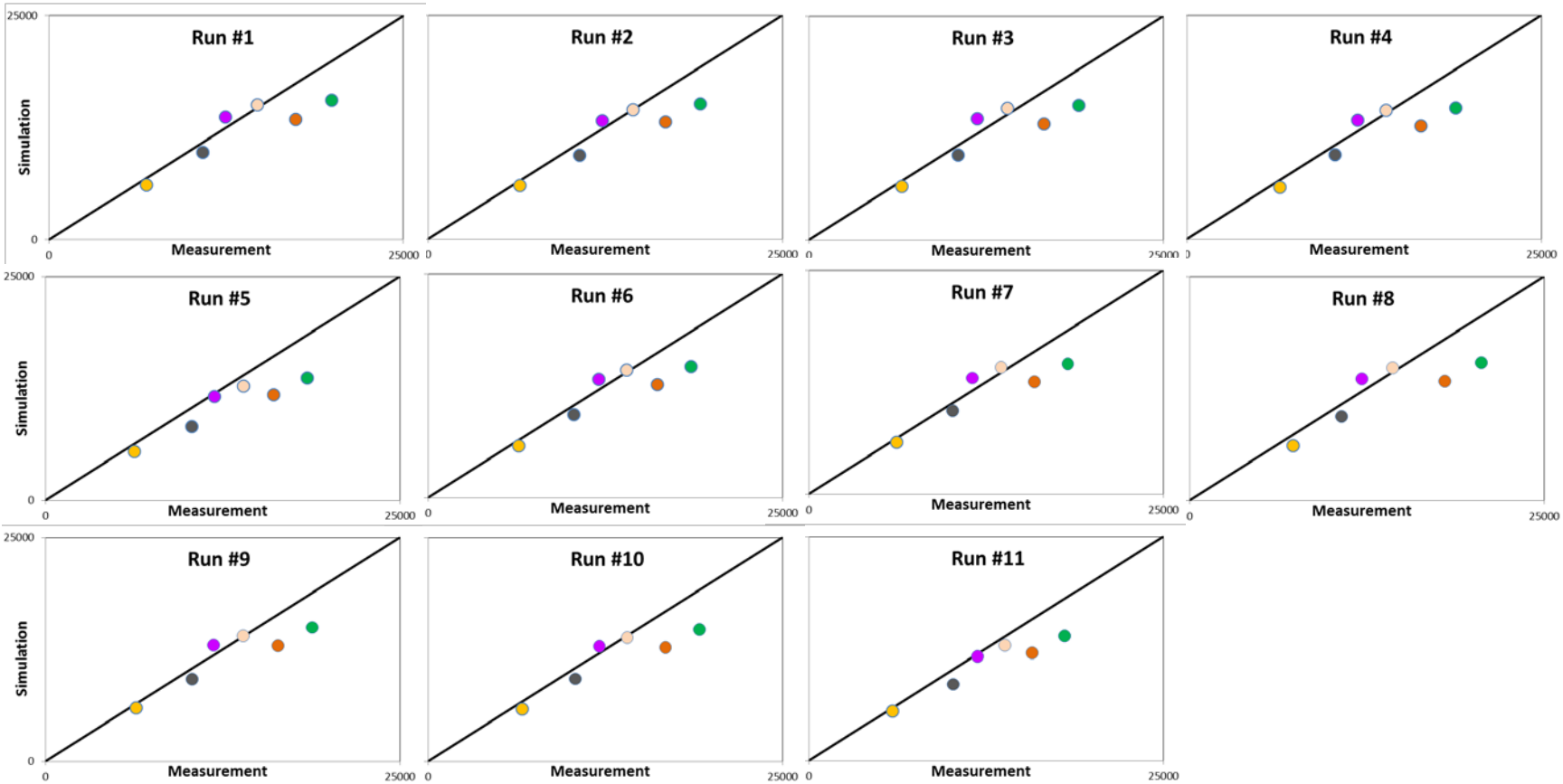
Comparison of Model and Operating Data

- **Time-averaged model predictions were used for comparison with data**
  - e.g. Time history of syngas composition at riser exit for one case

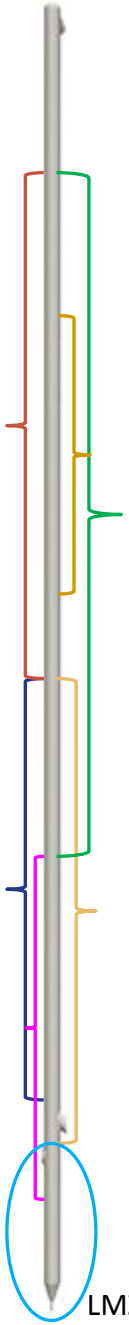


Comparison of Model and Operating Data

- **Time-averaged pressure drop values – parity plots comparing prediction to measurement**

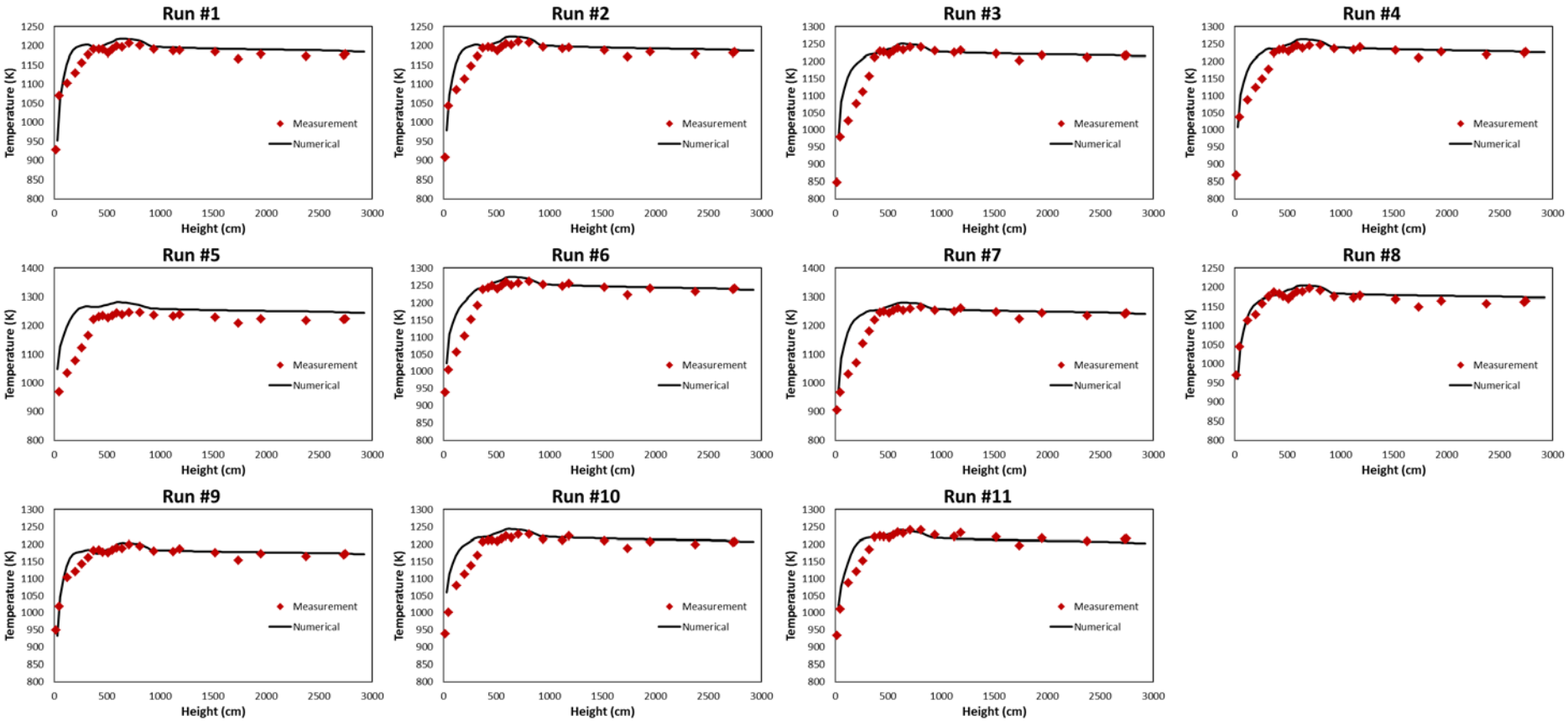


- **Above the Lower Mixing Zone (LMZ), measured and predicted pressure data are in good agreement, with maximum discrepancy < 30%**
- **Pressure drop values for the LMZ are excluded here - the simulation consistently underpredicts pressure drop in LMZ**



Comparison of Model and Operating Data

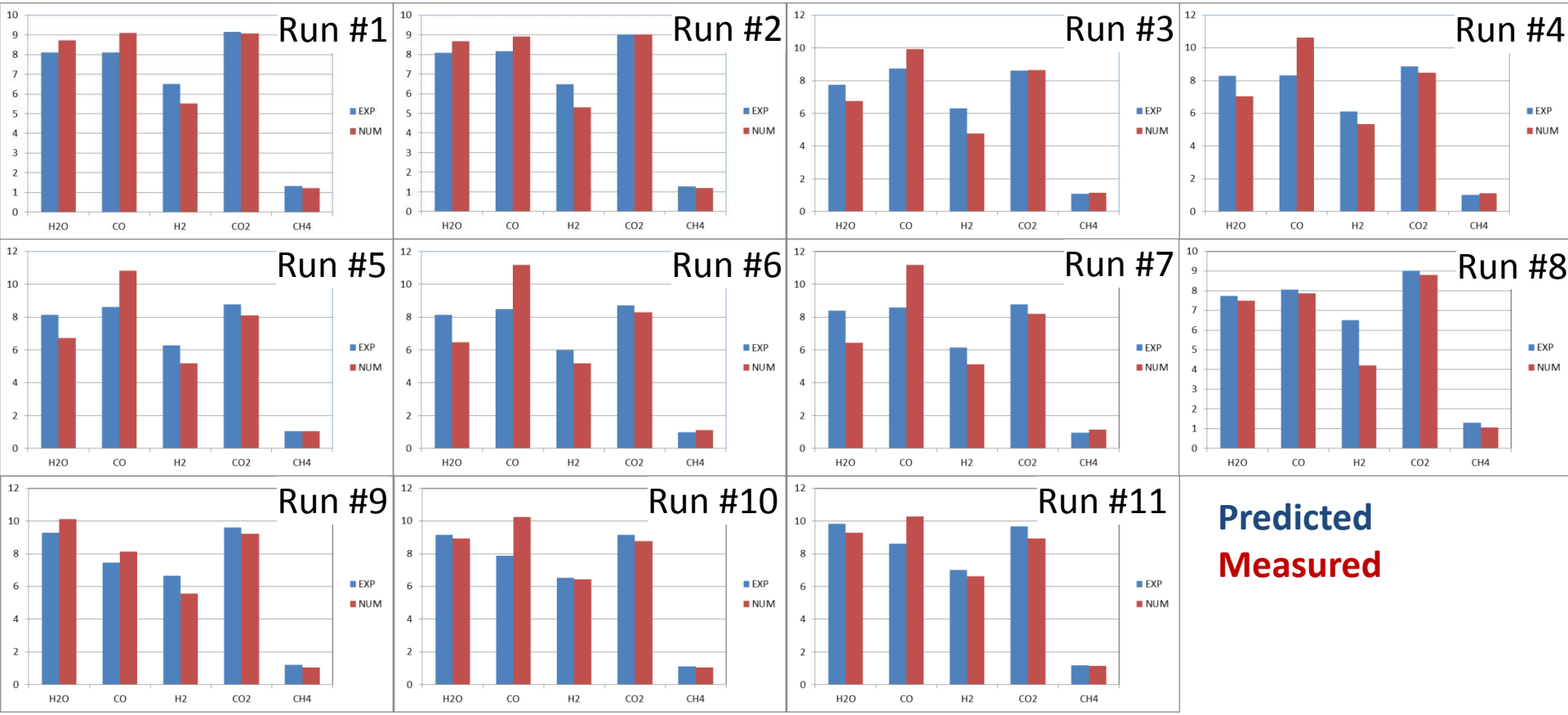
- **Time-averaged Temperature at varying height**



- Temperature profiles are in good agreement with measurements
- Lower Mixing Zone temperatures from the model are slightly higher than data
  - Model overpredicts carbon and resultant combustion in LMZ

Comparison of Model and Operating Data

- **Time-averaged syngas composition at riser exit**

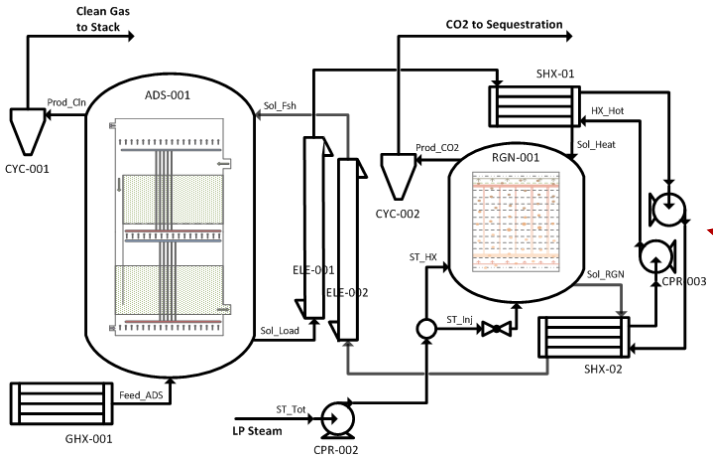


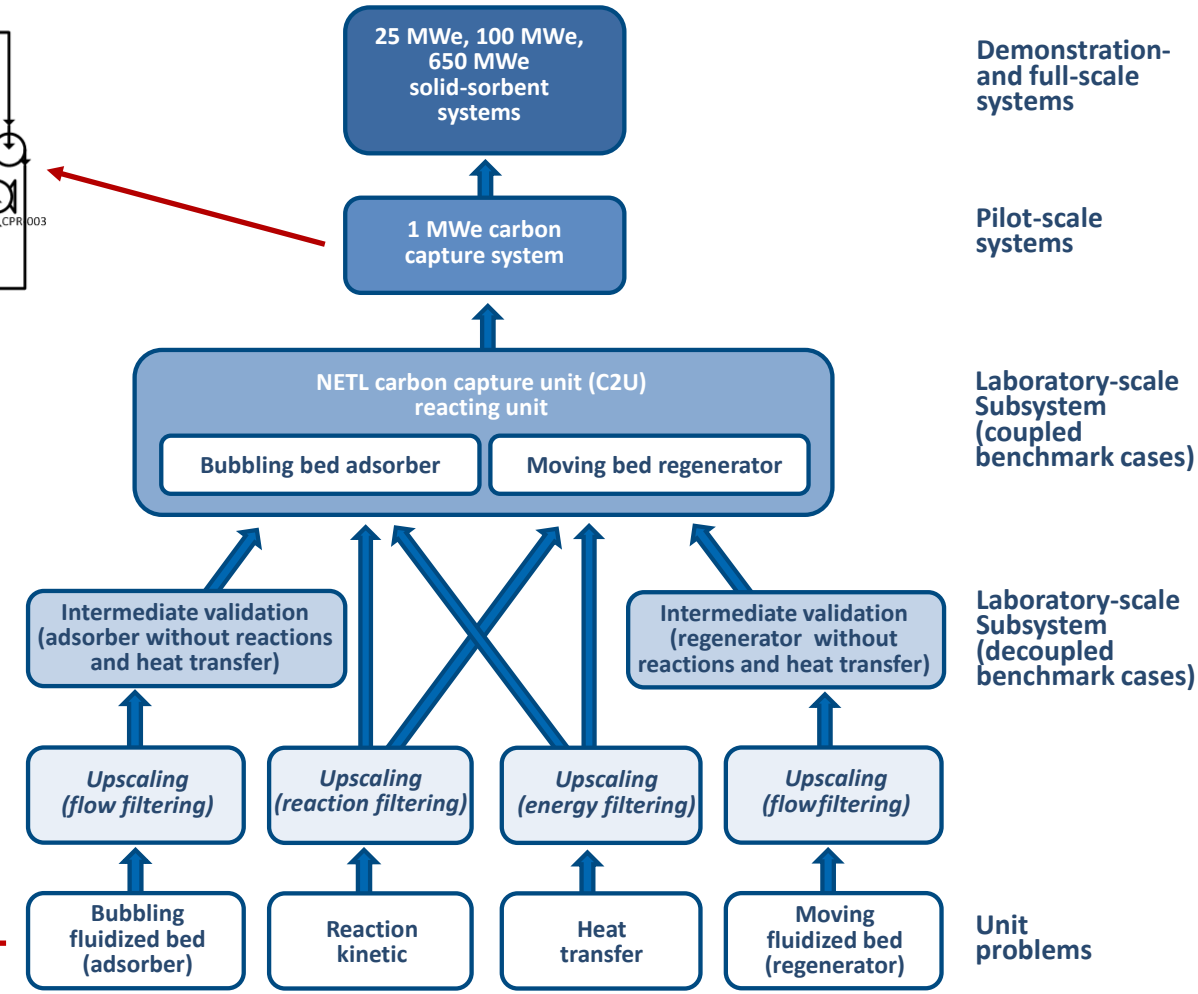
- Predicted exit syngas compositions are in good agreement with measurements - with most discrepancies within 20%.

TRIG™ Model Conclusions

- **The MFIX simulation of the TRIG™ gasifier showed very good agreement with PSDF operating data over a broad range of operating conditions for Mississippi lignite fuel**
  - Syngas composition and temperature profiles are in good agreement with PSDF data
  - Predicted pressure drops for all conditions match data well for most locations - <u>except for the Lower Mixing Zone</u>
    - Model underpredicts the solids loading in the LMZ
- **Use of PC Coal Lab database and C3M software provides accurate devolatilization and gasification kinetics**
  - Kinetic parameters were accurate for all operating conditions
- **Improvement in prediction of LMZ solids loading is needed**
  - May be potential for size segregation - lower mixing zone could accumulate larger size particles from recycle flow
  - Model may need to consider a distribution of sizes to allow for size segregation at the J-leg return

Model Application: Building predictive confidence for device-scale CO_2 capture with multiphase CFD models





Ryan E.M., Montgomery C., Storlie C., Wendelberger J. CCSI validation and uncertainty quantification hierarchy for CFD models. CCSI Tech. Rep. Ser., 2012.

Application to 1MW Pilot Scale CO2 Adsorber

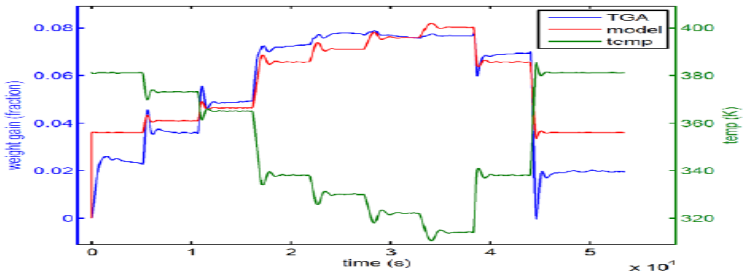
- **Complex process involving solids and gas flow, heat transfer, chemical kinetics of exothermic adsorptions**
- **Validate Adsorption kinetics**
  - Fixed bed tests – adsorption reactions isolated from solids flow and mixing
- **Validate non-reacting solids and gas flow**
  - Bubbling bed tests – no adsorption reactions
- **Validate heat transfer models**
  - Heated bed – no adsorption reactions
- **Validate lab scale adsorption**
  - Fixed bed with reactions
  - Bubbling bed with reactions
- **Apply validated models to pilot scale and compare to data when it comes available.**

Are the reaction kinetics derived from TGA adequate?

- **CCSI sorbent kinetics (Bhat et al., 2012)**

$$2R_2NH + CO_2(gas) \rightleftharpoons R_2NCO_2^- + R_2NH_2^+$$
$$R_2NH + H_2O(phys) + CO_2(gas) \rightleftharpoons HCO_3^- + R_2NH_2^+$$
$$H_2O(gas) \rightleftharpoons H_2O(phys)$$

$$k_i = A_i T exp\left(\frac{-E_i}{RT}\right) \quad K_i = exp\left(\frac{\Delta S_i}{R}\right) exp\left(\frac{\Delta H_i}{RT}\right)/P$$

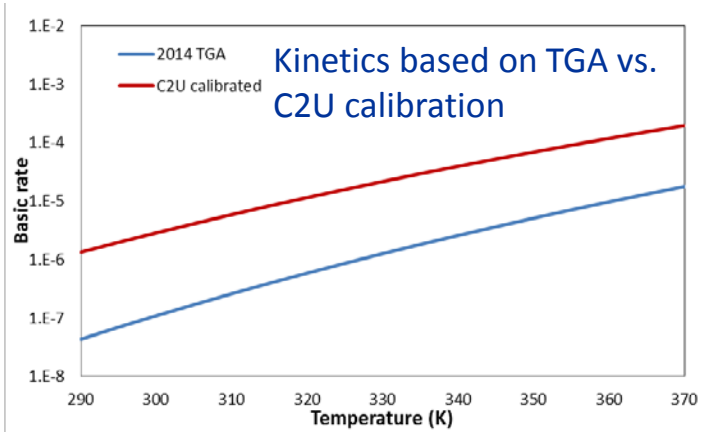


TGA Data → Reaction Rate → Bayesian Calibration → Calibrated Reaction Rate

- The calibrated reaction rate parameters differed considerably from the parameter values obtained from TGA data

- Understand the cause of discrepancy
  - Inherent limitation of rate derived from TGA?
  - Predicted bed hydrodynamics is not correct?

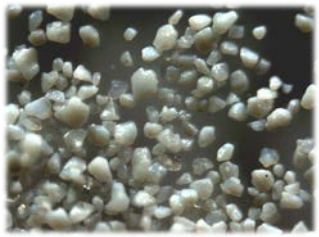
- Simplify the hydrodynamics
  - Remove the heat transfer coil
  - Run fixed to bubbling bed tests



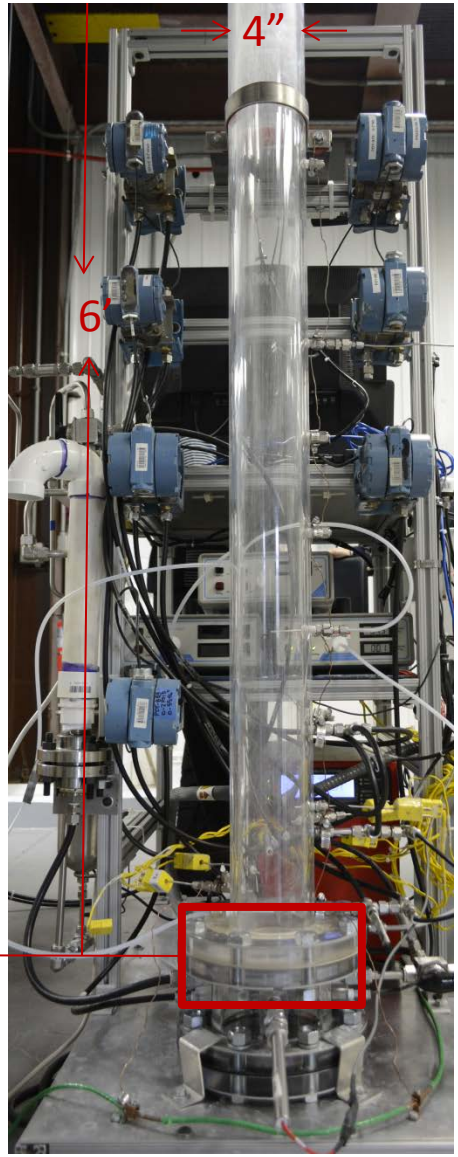
K.S. Bhat, D.S. Mebane, H. Kim, J. Eslick, J.R. Wendelberger, D.C. Miller, LANL Tech. Rep. LA-UR-12-21855, 2012.

Small Scale, Fixed and Bubbling Bed: well controlled experiments

- **Materials**
  - NETL 32D (100µm, 0.48 g/cc)
  - ADA-ES sorbent
- **Cold flow in bubbling beds**
  - Pressure drops, visual observation
  - Experimental runs
    - Static bed heights (4, 6, 8 in)
    - Gas flow: 1, 3, 5, 7 u_{mf}
    - 7 repeats for most conditions
- **Reacting flow in fixed and bubbling beds**
  - Pressure drops, temperature, breakthrough curve
  - Experimental runs
    - Various superficial gas velocity, bed height
    - Different CO_2 concentrations



Sorbent 32D

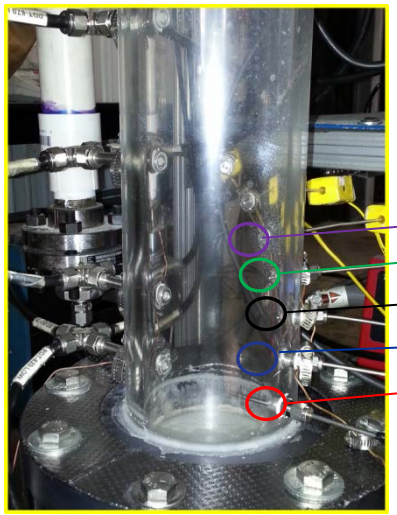


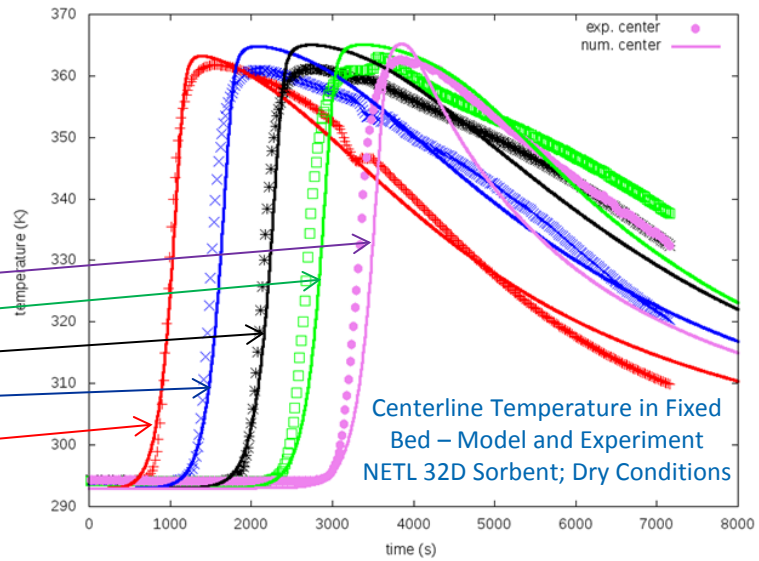
Carefully designed distributor ensures uniform flow in fixed bed.

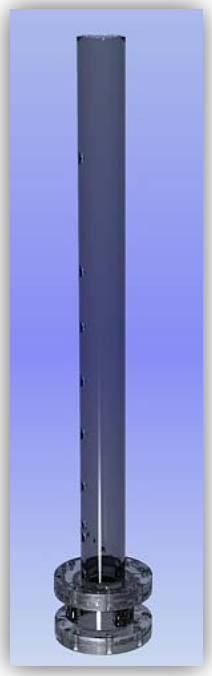
Presented at ***National Lab Day on the Hill***

Small Scale, Fixed and Bubbling Bed: well controlled experiments

- **Model application to experiments performed with CO_2 Sorbent Particles**
  - MFIX model in good agreement with fixed bed tests (no solids phase hydrodynamics) for kinetics





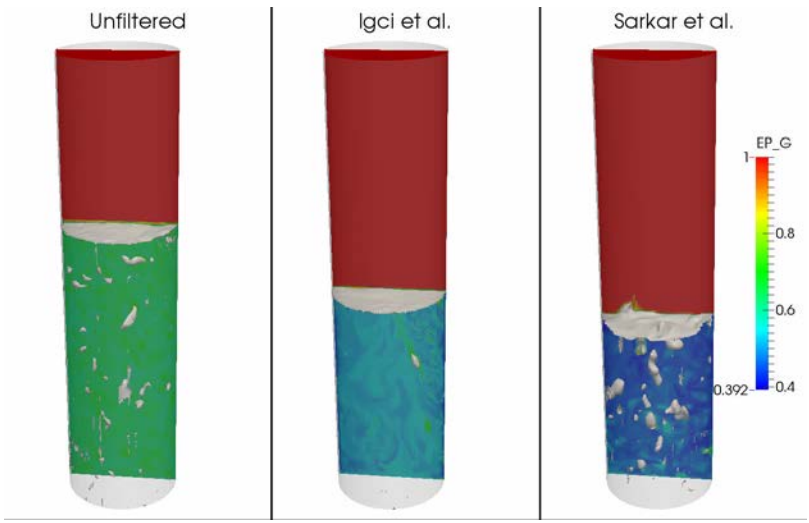


  - Work now underway to compare with bubbling bed tests
  - Need to validate the hydrodynamics

Make sure we get the hydrodynamics right

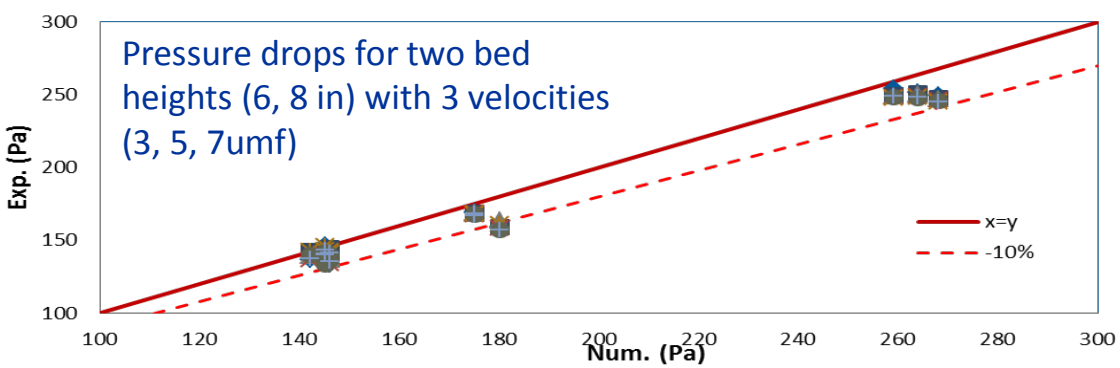
- **Tested three models: Unfiltered model and the filtered models of Igci et al. (2008) and Sarkar et al. (2014)**

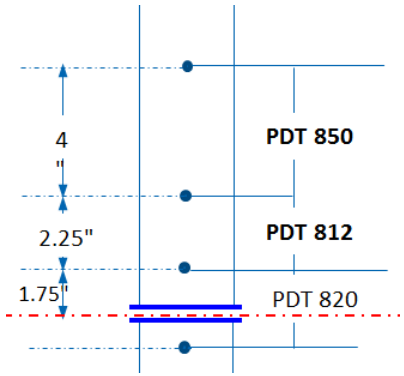
Model	Unfiltered	Igci et al.	Sarkar et al.	Exp.
Bed height (cm)	26	19.8	18	19



- **Selected Sarkar et al. (2014) filtered model**
  - Based on 3D periodic domain simulations
  - Filtered expressions based on two markers (ε_s, V_g-V_s)
  - Predicted bubbling behavior, qualitatively the best

MFiX Simulations

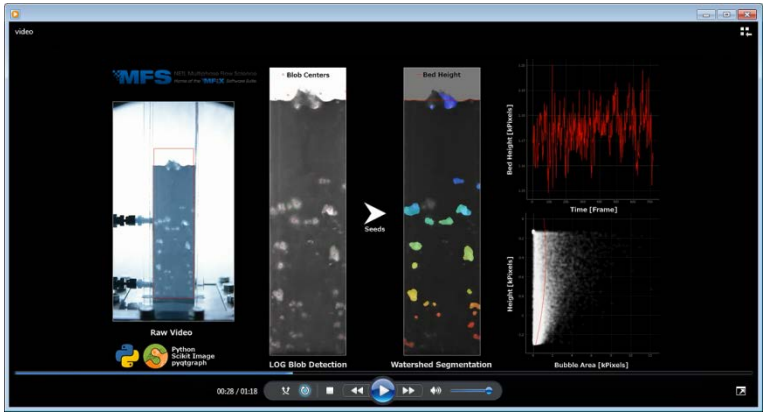


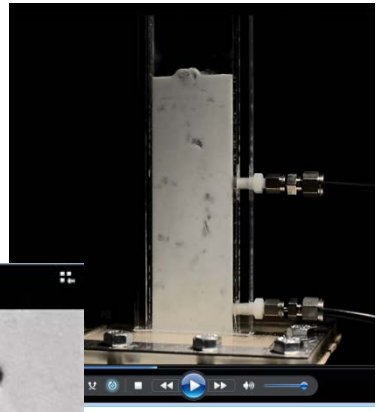


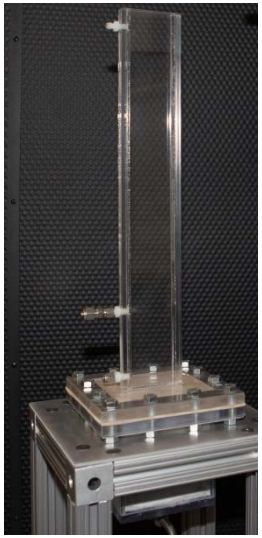
Igci, Y., Andrews, A. T., Sundaresan, S., Pannala, S. and O'Brien, T. AIChE J., 54, 1431–1448, 2008.
Sarkar, A., Sun, X. and Sundaresan, S., AIChE Annual Meeting, Paper 407b, 2014.

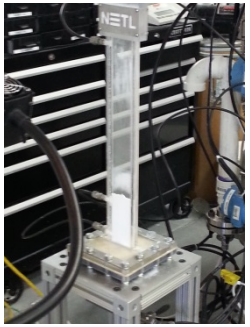
Operation of Small-Scale, Rectangular Fluidized Bed for Code Validation

- **Micro Fluidized Bed has been put into service for validation of model hydrodynamics predictions**
  - Developing techniques to study bubble statistics
  - Work now underway to compare model with bubbling bed tests
  - Need to validate the hydrodynamics for Geldart A sorbent particles









1 MW Pilot Scale CO_2 Adsorber

- **Fundamental model validation work has been performed to support scale up simulations**
  - Small scale, fixed and bubbling beds
  - With and without chemical reactions and heat transfer
- **Validated models are being applied to the pilot scale unit**
- **MFiX Model predictions will be validated with pilot scale data**
- **MFiX Model will be used for scale up to commercial scale**

Summary

- Industrial systems based on solids processing and handling are high risk for not meeting design performance targets
- Improved understanding of the underlying physics and the ability to accurately model and predict their performance is key to reducing this risk
- Multiphase CFD techniques have become a practical tool and are continuing to evolve and improve
- NETL's Multiphase Flow Science program combines expertise in numerical modeling with appropriate physical experiments to advance the field for FE applications
- NETL's coming "Revolutionary Reactors" program will push this forward by using CFD to automate the process of optimizing design and operating conditions for FE devices

Thank you - Questions?

NETL Multiphase Flow Science Team

- Develop and maintain numerical and physical models to promote understanding of multiphase flow physics critical to advanced energy and environmental systems

MFIX Suite of Multiphase Codes

- Open Source Code – available to the public
- Supported and validated
- Over 3800 registered users from 73 countries and 250+ institutions
  - 70% University; 20% Industry; 10% NLs and misc.
- Ongoing Code Development for increased:
  - Accuracy
  - Speed
  - Multiphase physics capability
  - Ease of use
- 2 updates per year on average

Suggestions for Code Capability and Collaboration are Welcome!