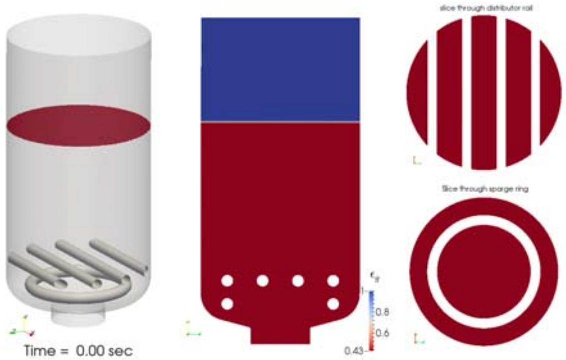
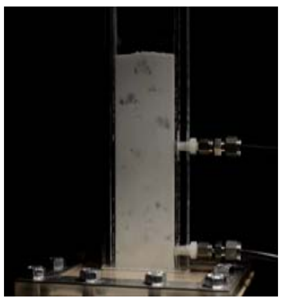
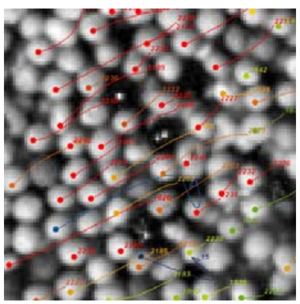
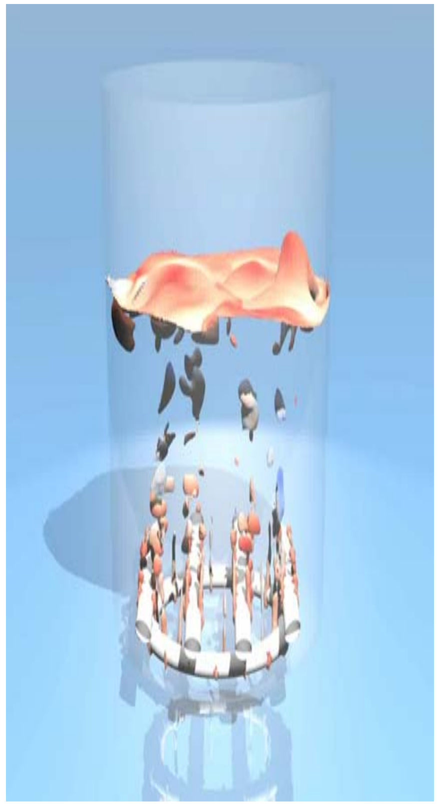
NETL

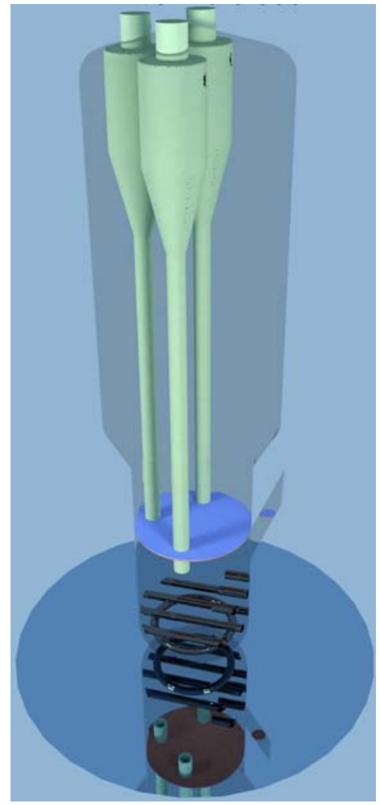
Driving Innovation ♦ Delivering Results

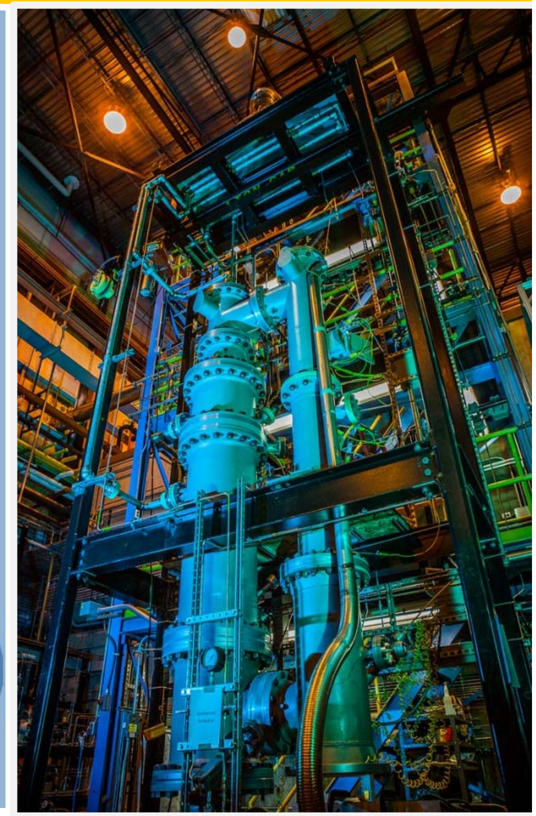












Multiphase Flow Science at NETL

Multiphase Models to Advance Energy Technologies

William A. Rogers, Ph.D., P.E.

Multiphase Flow Sciences Team

August 2015

NETL Multiphase Flow Science – 30 years of R&D

- **Development, Validation, Application and Support of Practical Multiphase Flow Simulation Tools**
  - Tools to guide the design, operation, and troubleshooting of multiphase flow devices
  - Emphasis on Fossil Fuel Technologies (e.g., coal gasifiers, CO_2 capture devices, Chemical Looping)

- **30+ Engineers and Scientists on the team**
  - Open-source Software Tools
    - **MFiX Suite** of Multiphase CFD Software
    - **C3M** Multiphase Chemistry Management Software
  - Multiphase experimentation for model development and validation
    - High quality data made available to the public
  - Funded research with universities and industry
    - University and Industrial stakeholders help to guide MFS program
    - Access to university capability
    - Access to industrial applications

MFiX Suite - managing the tradeoff between accuracy and 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*

Time to Solution

Development
VV&UQ

Model Uncertainty

MFiX Suite

- **MFiX Suite – State of Development**
  - Goal is to have all codes with full set of capabilities

MFiX TFM

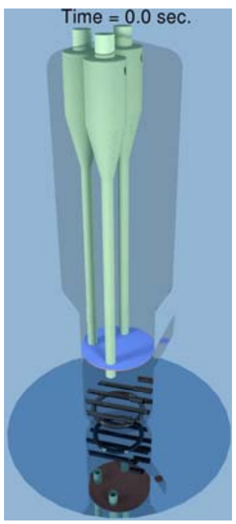
	Serial	†DMP	‡SMP
Momentum Equations	●	●	●
Energy Equations	●	●	●
Species Equations	●	●	●
Chemical Reactions	●	●	
Cartesian cut-cell	●	●	□

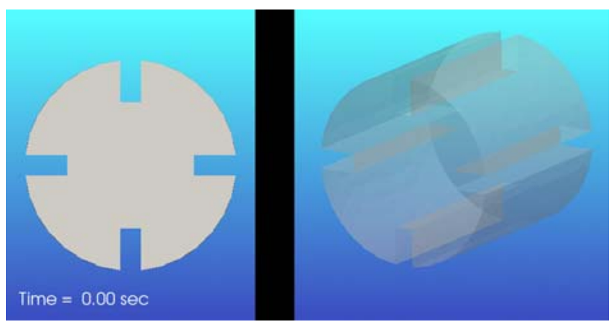
MFiX DEM

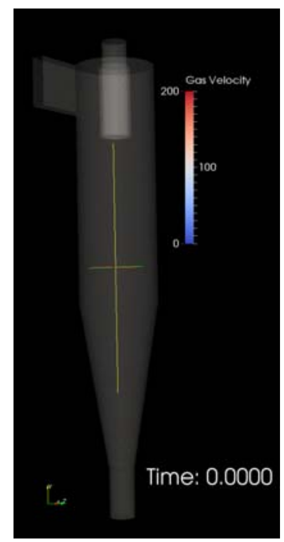
	Serial	†DMP	‡SMP
Momentum Equations	●	●	●
Energy Equations	●		
Species Equations	●		
Chemical Reactions	●		
Cartesian cut-cell	○	○	

MFiX PIC

	Serial	†DMP	‡SMP
Momentum Equations	●		○
Energy Equations			
Species Equations			
Chemical Reactions			
Cartesian cut-cell	○		□



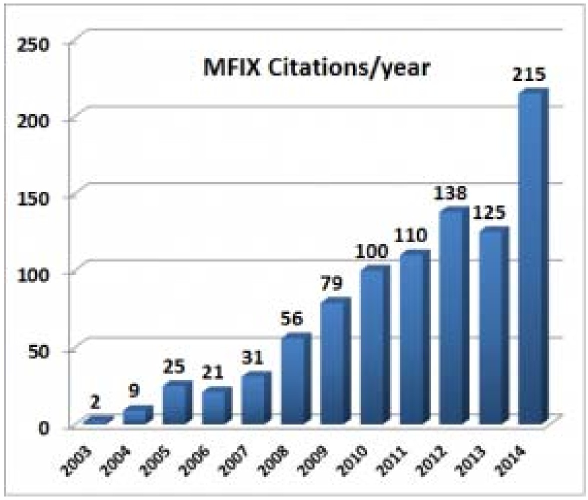


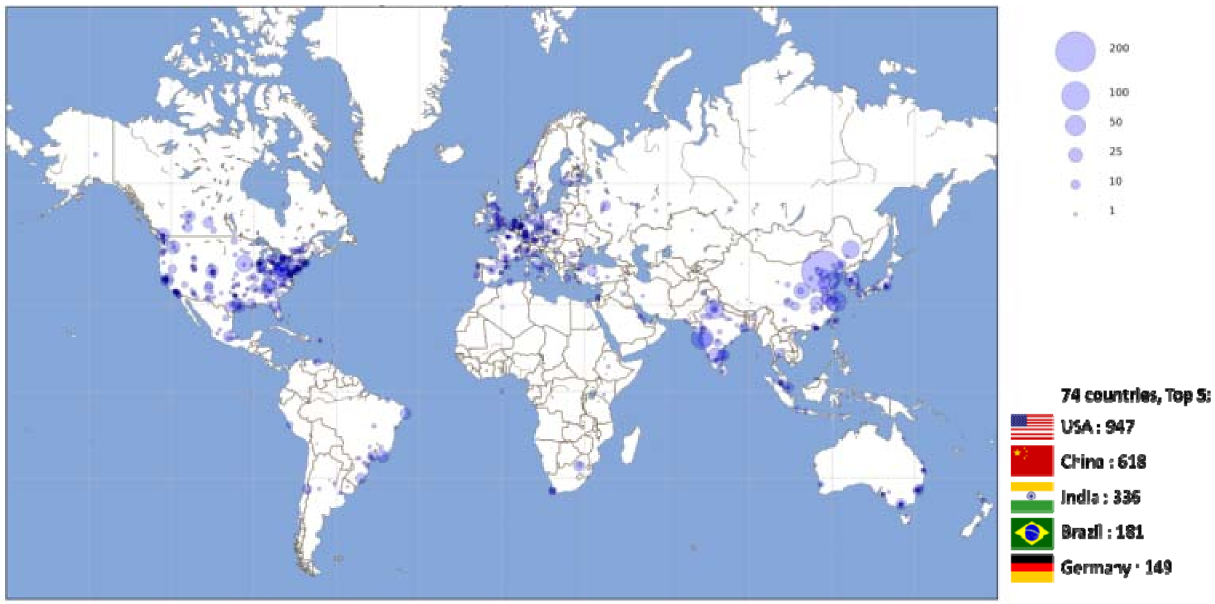


● – implemented and fully tested
○ – implemented with limited testing
□ – not tested or status unknown

MFiX Suite – Open Source Toolset

- **MFiX Suite of software has a large (>3500) user base**



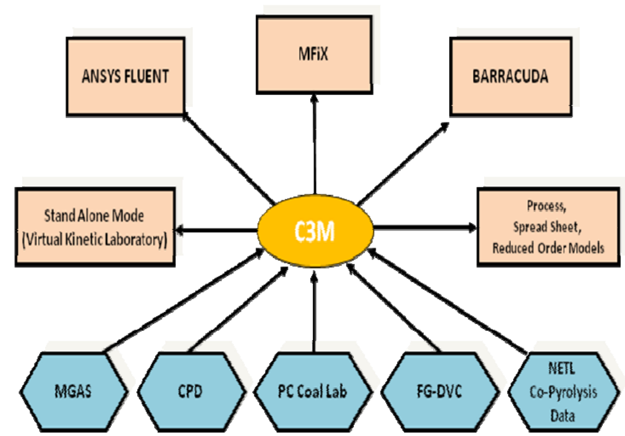


FY14 new registrations		**229**
–	University	175
–	Industry	29
–	National Labs	11
–	Others	14
Total MFIX registrations		**3,513**
–	University	2506
–	Industry	559
–	National Labs	163
–	Other	285

C3M – Chemistry Support for CFD

What Does C3M Bring to the User?

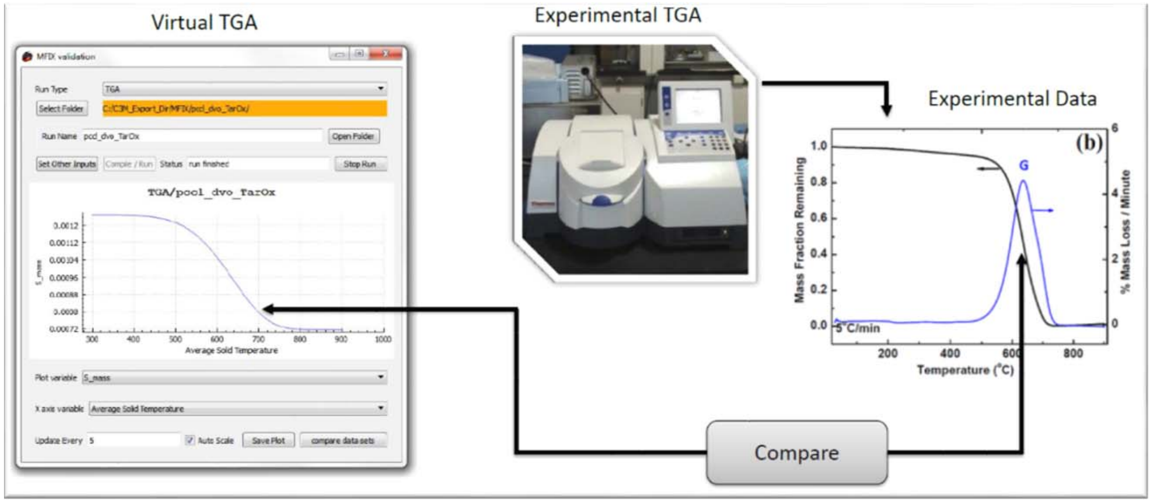
- Easy, Intuitive, Reliable, and Graphical User Interface
- Comprehensive interface between reliable sources of kinetic data and reacting, multi-phase CFD models
- “Virtual Kinetic Laboratory” for quickly assessing the validity of a chemical equation sets before going to full scale, expensive models
- Seamless formatting and units management for code specific implementation
- Advanced Chemistry Analysis and Development Tools
- Open source for collaboration and development



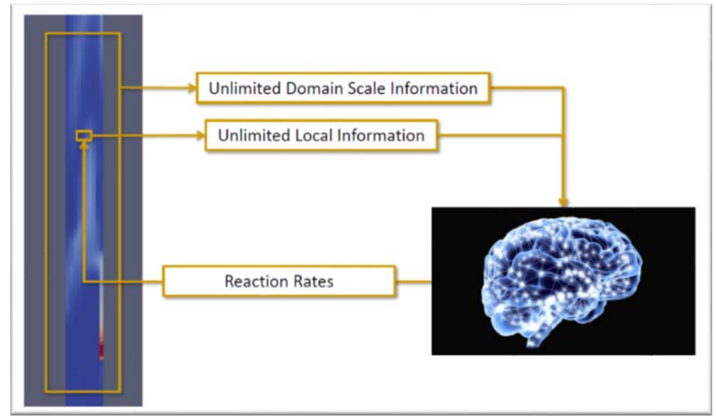
136+ User Downloads
96+ Version 4.0 Downloads (300% increase)
Version 5.0 Coming Soon!

Recent Developments in C3M

Virtual Experimental Capability (TGA/Drop Tube)

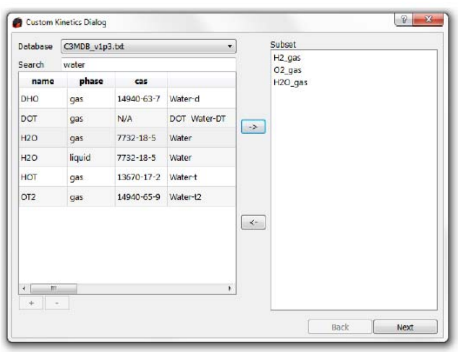


Neural Network Surrogates

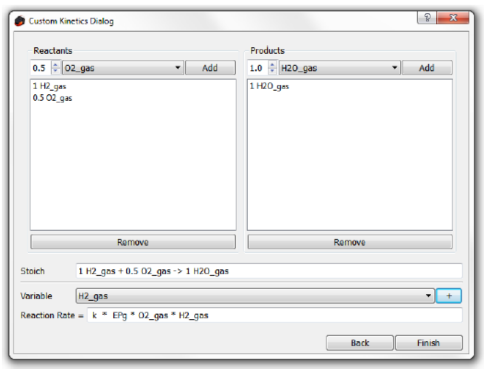


User-Defined Chemistry

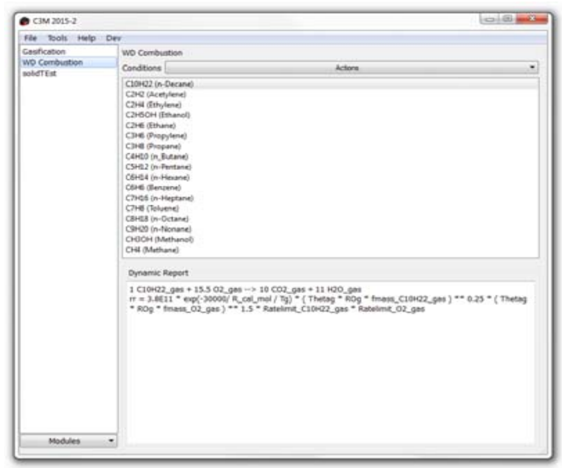
1) Select Species



2) Define Chemistry



User Defined Modules



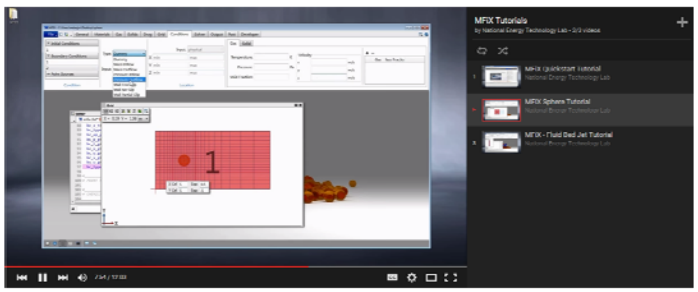
MFiX Graphical User Interface

Makes MFIX Easy to Use

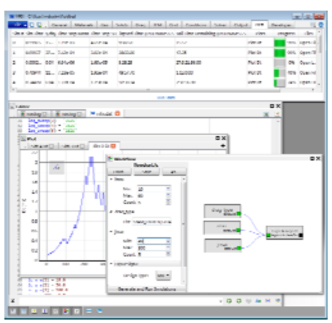
- Providing intuitive tools to create, compile, run, and post process MFIX models.
- Cross platform, binaries available (Windows, Linux).
- Written in Python.
- Integration with MFIX website (download mfix).

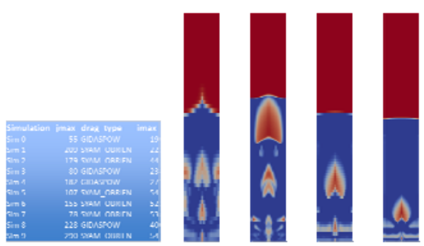
Download Today: mfix.netl.doe.gov

Tutorials on YouTube

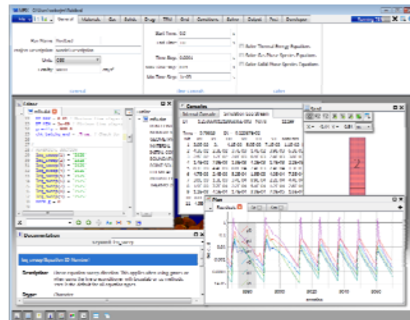


Next Release: Workflow – Automating Design of Experiments

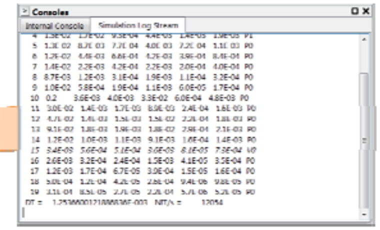




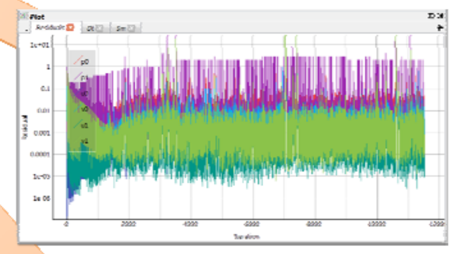
The GUI



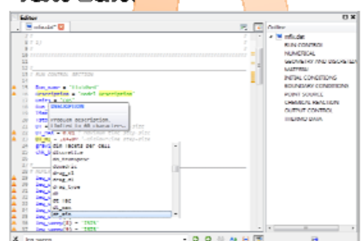
Internal Console



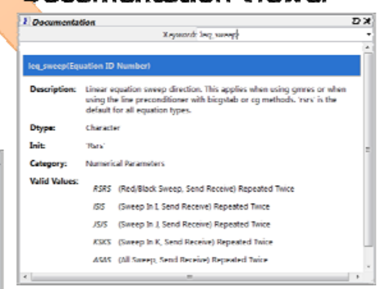
Plot



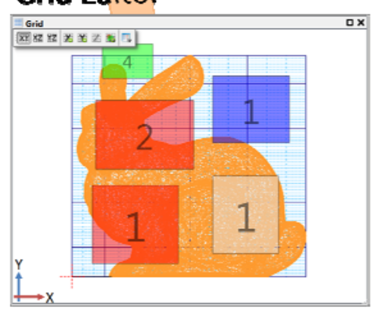
Text Editor



Documentation Viewer



Grid Editor

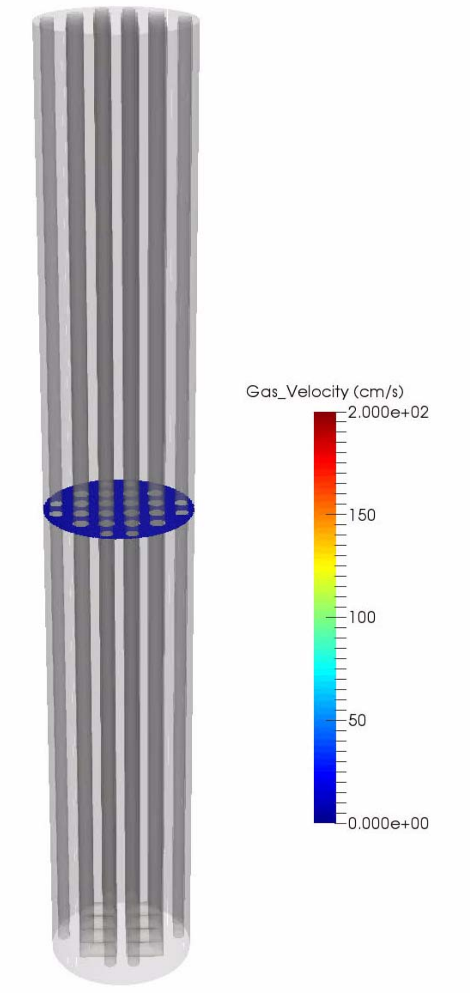


MFS support of the Gasification Program

- **Development of Reacting Multiphase Models for Advanced Gasification Processes**
  - Model Development and Optimization
  - Verification, Validation, and Uncertainty Quantification Tools and Processes for Multiphase Flow
  - Physical Sub-Models, Pre- and Post-Processing Tools for Model Enhancement
  - Model Application And Validation
- **Experimentation for Model Development and Validation**
  - Operation of Small-Scale Fixed, Bubbling, and Circulating Fluidized Beds for Validation

MFS support of the Gasification Program
Model Development and Optimization

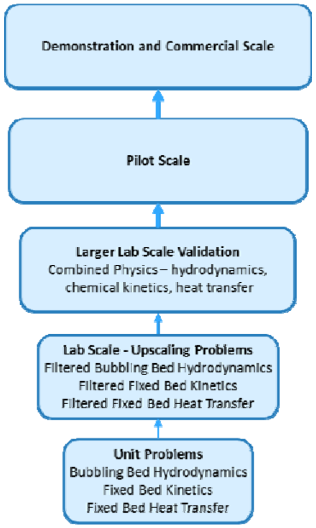
- **Speed and accuracy improvements to MFiX-TFM for industrial scale gasification application**
- **Enhancement to MFiX-DEM for large-scale reacting flows**
  - Efficiency
  - Improved parallel performance
- **Enhancement to MFiX-PIC for industrial scale gasification application**
  - Reacting flow capability
  - Complex geometry
- **Optimization of all codes for new supercomputer architectures**



MFS support of the Gasification Program

Verification, Validation, Uncertainty Quantification

- **Implementation of "Method of Manufactured Solutions" for MFiX Verification**
- **Verification "Test Harness" executed daily to monitor code development process and ensure code quality**
- **Multiphase Flow Validation Problem Set**
  - Validation Hierarchy
- **Develop and Demonstrate Methodologies to Quantify Uncertainty in Model Predictions**
  - Develop and distribute a UQ Toolset
- **Multiphase Flow CFD "Best Practices"**



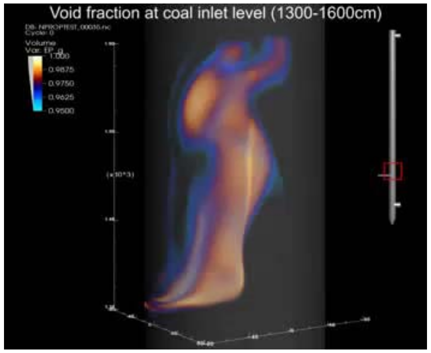
Validation Hierarchy

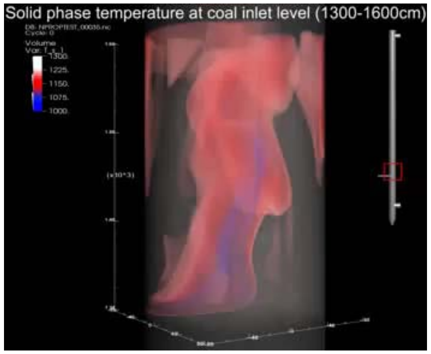
Sources of Uncertainty in Model Predictions

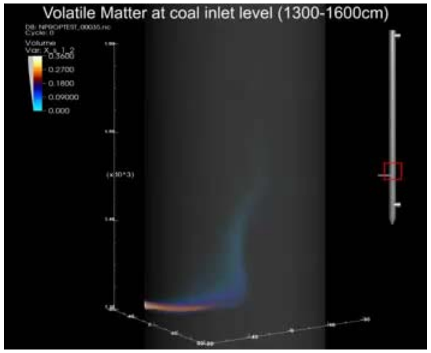
- Input parameter
- Surrogate model
- Model form
- Experimental data;
- Spatial discretization
- Time Averaging

MFS support of the Gasification Program
Physical Sub-Models, Pre- and Post-Processing Tools

- **Enhance C3M Capabilities**
- **Enhance MFiX GUI Capabilities**
- **“Filters” for capturing small-scale effects for more accurate scale-up**
- **Particle size distribution**
- **Cohesion/Agglomeration**
- **Improve heterogeneous chemistry**
- **Improve radiative heat transfer modeling**
- **Bring all codes in the MFiX Suite to same level of capability**



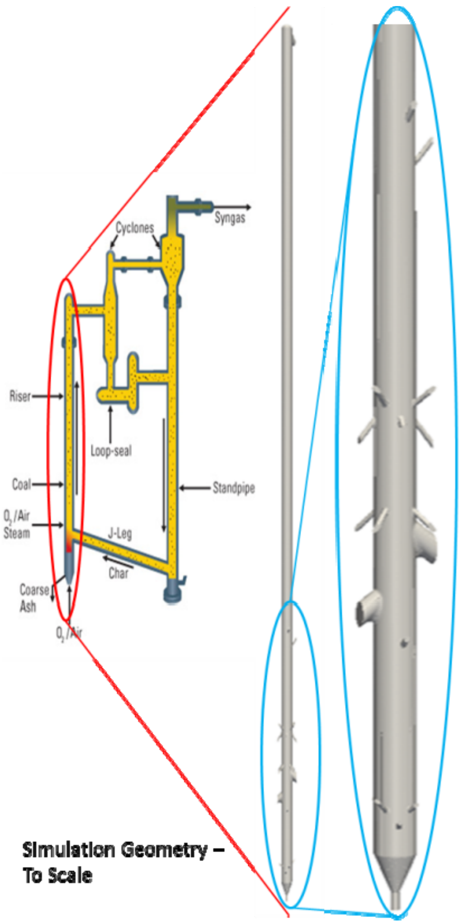


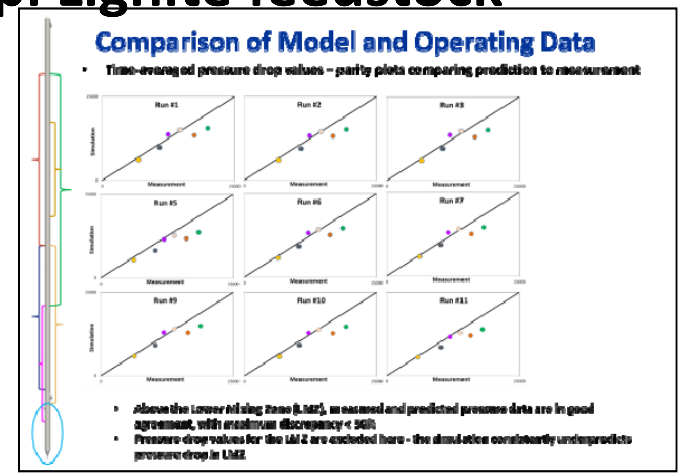


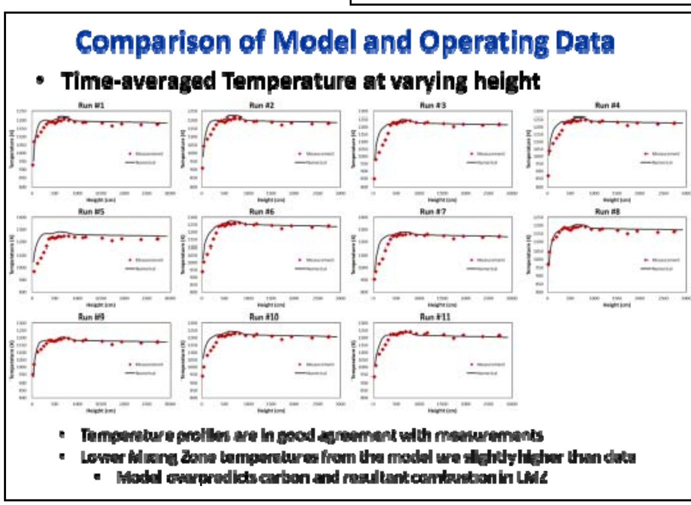
MFS support of the Gasification Program

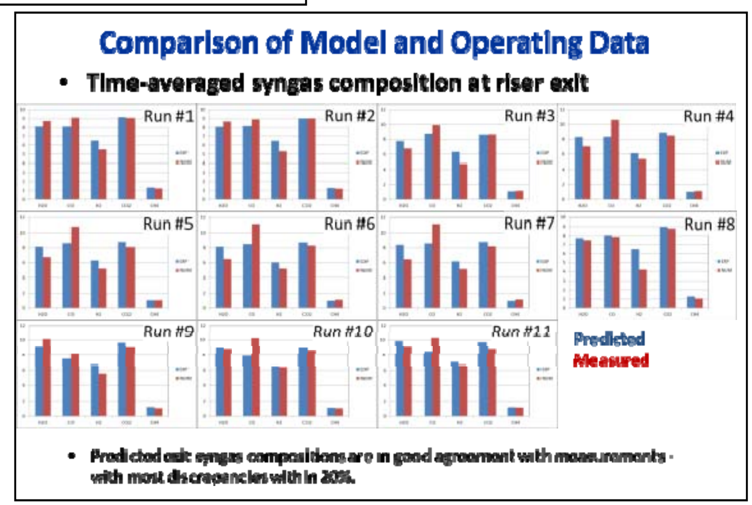
Model Application and Validation

- **Application to TRIG™ Gasifier Riser and Validation with Plant Data for Mississippi Lignite feedstock**







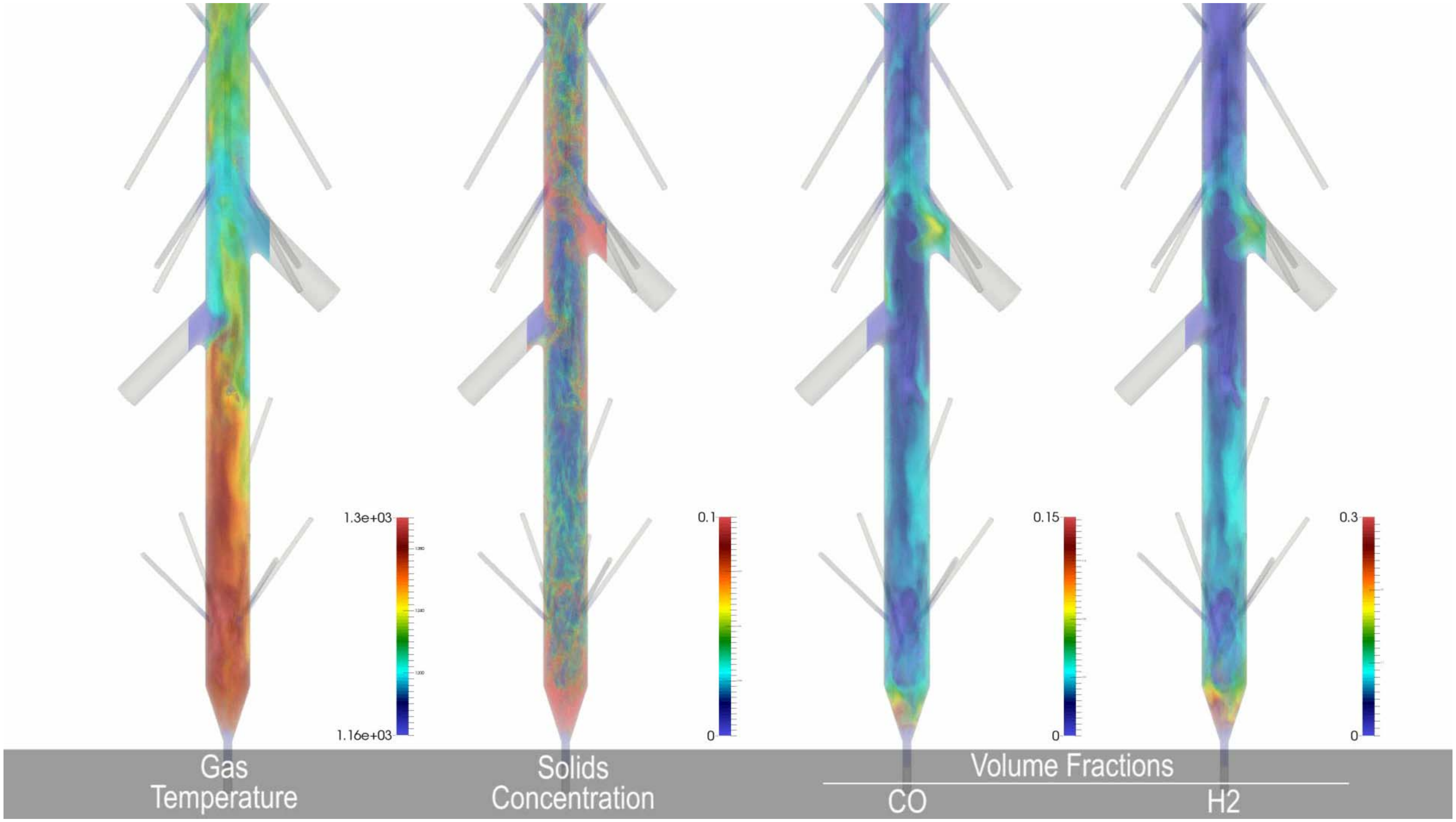


Tingwen Li , William Rogers , Douglas McCarty, Jenny Tennant 2014 Computational Fluid Dynamic Simulations of a Pilot-Scale Transport Gasifier Using Mississippi Lignite Feedstock, Gasification Technologies Conference, Washington DC.

MFS support of the Gasification Program

Model Application and Validation

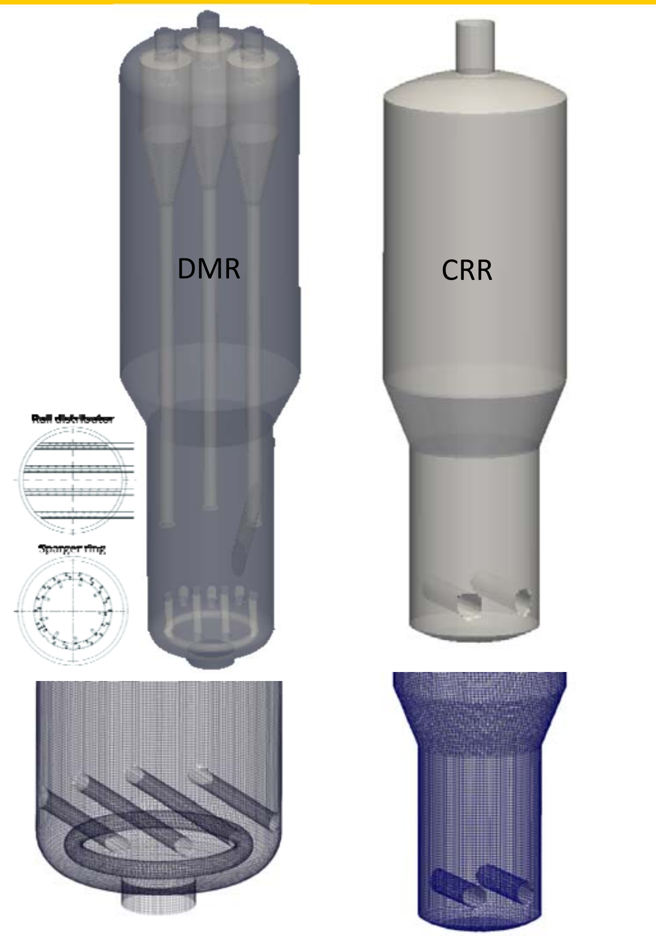
- **Application to TRIG™ Gasifier and Validation with Data for Mississippi Lignite feedstock**



Tingwen Li , William Rogers , Douglas McCarty, Jenny Tennant
2014 Computational Fluid Dynamic Simulations of a Pilot-Scale Transport Gasifier Using Mississippi Lignite Feedstock, Gasification Technologies Conference, Washington DC.

MFS support of the Gasification Program
Model Application and Validation

- **Application to Integrated Waste Treatment Unit Gasifiers – Idaho National Lab**
  - Develop and validate MFiX-TFM models of the Denitration Mineralization Reformer (DMR) and and Carbon Reduction Reformer (CRR).
    - Validate with DMR (mock up) pressure data for cold flow conditions
    - Validate with CRR gas composition data for reacting conditions
  - Provide model-based information to better understand chemistry and hydrodynamics of the vessels

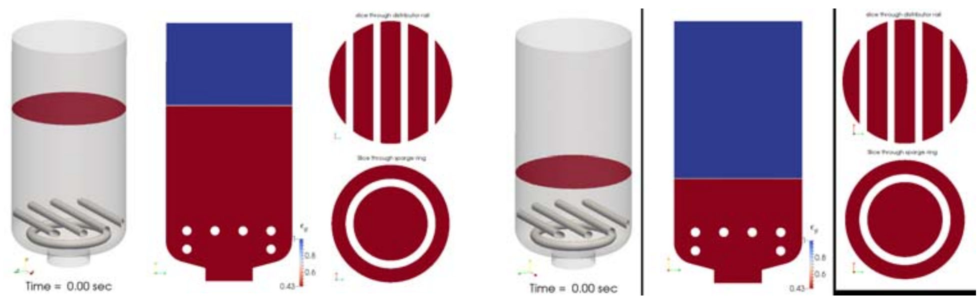


36 orifices for sparger ring
44 orifices for the distributor rails

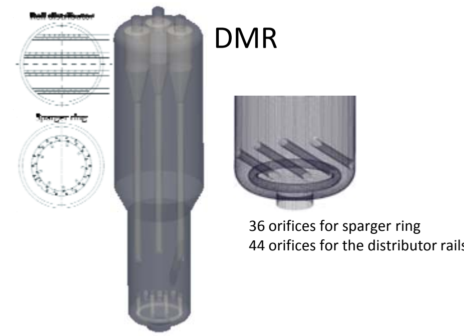
30 nozzles for the 2 distributor rails
18 nozzles on side walls

MFS support of the Gasification Program
Model Application and Validation

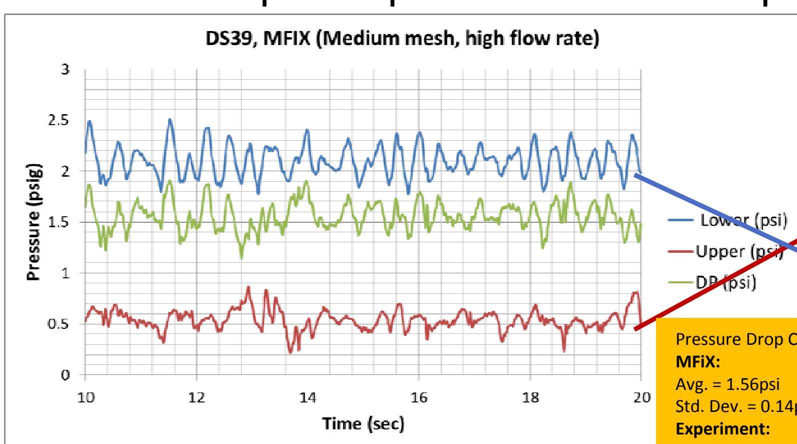
- **Validate with DMR pressure data for cold flow conditions**



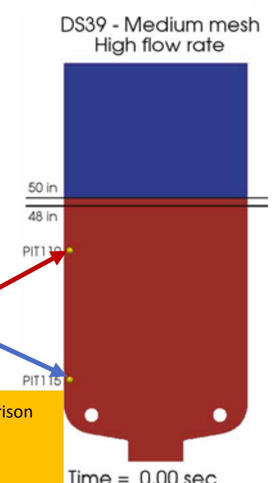
Effect of Bed Height on Bubble Behavior

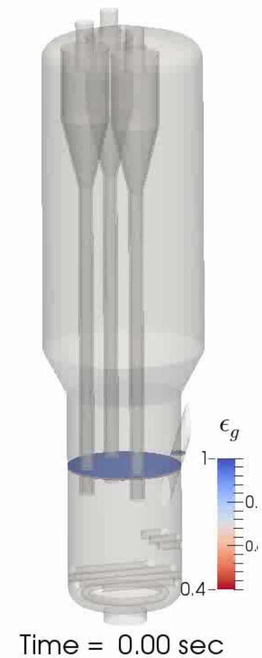


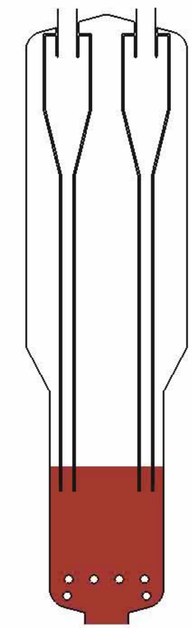
Pressure Drop in Experimental Mock-up



Pressure Drop Comparison
MFiX:
Avg. = 1.56psi
Std. Dev. = 0.14psi
Experiment:
Avg. = 1.52psi
Std. Dev. = 0.23psi







MFS support of the Gasification Program
Model Application and Validation

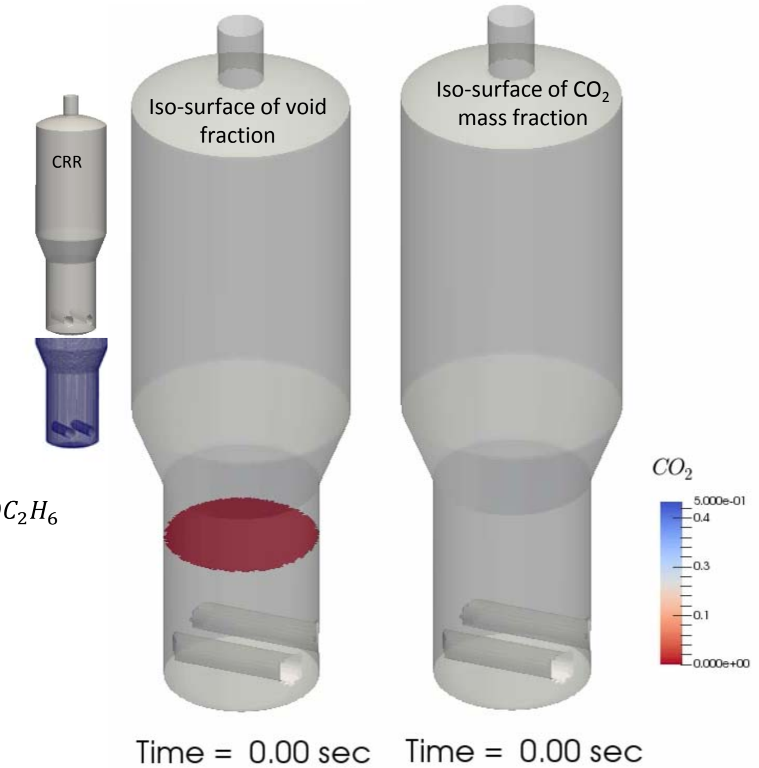
- **Validate with CRR gas composition data for reacting conditions**

- **Composition**
  - 10 gas species (Soot, O_2, CO, CO_2, CH_4, H_2, H_2O, N_2, HCN, C_2H_6)
  - 2 solids phases: coal (C, volatile matter, moisture, ash) and Bauxite
  - Total of 30 transport equations (continuity, momentum, energy, species)

- **Heterogeneous chemical reactions:**
  - Coal moisture release : $H_2O_{(l)} \rightarrow H_2O_{(g)}$
  - Pyrolysis: $VM \rightarrow 1.3788CO + 0.48148CH_4 + 2.87373H_2 + \ 0.128615HCN + 0.0128449C_2H_6$
  - Steam gasification: $C + H_20 \leftrightarrow CO + H_2$
  - CO_2 gasification: $C + CO_2 \leftrightarrow 2CO$
  - H_2 gasification: $C + 2H_2 \leftrightarrow CH_4$
  - Char combustion: $C + O_2 \leftrightarrow CO_2$

- **Homogeneous chemical reactions:**
  - Water gas shift: $CO + H_20 \leftrightarrow CO_2 + H_2$
  - CO combustion: $C0 + \frac{1}{2}O_2 \leftrightarrow CO_2$
  - H_2 combustion: $H_2 + \frac{1}{2}O_2 \leftrightarrow H_20$
  - CH4 combustion: $CH_4 + 2O_2 \leftrightarrow CO_2 + 2H_20$

Kinetics implemented with C3M



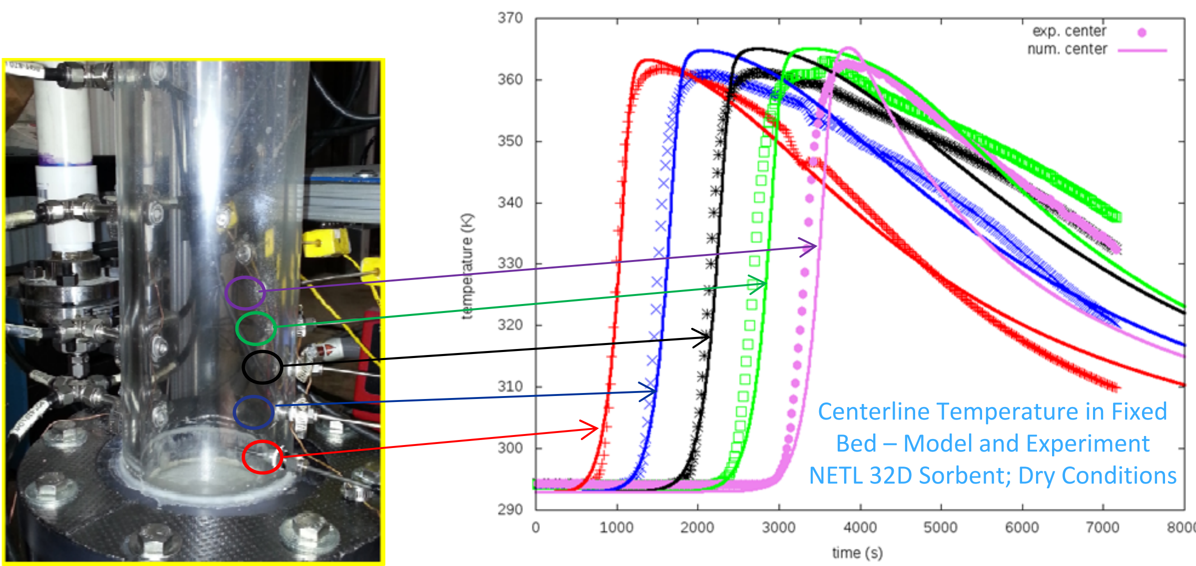
	Flow rate	O_2	CO_2	H_2O	N_2
Exp.	Nominal	5.03%	23.67%	34.48%	36.83%
MFiX	Nominal	5.39%	23.00%	34.95%	36.66%
MFiX	0.25xNominal	0.00%	20.98%	37.59%	34.43%
MFiX	0.10xNominal	0.00%	18.58%	38.81%	33.82%
MFiX	2.00xNominal	15.98%	17.83%	27.27%	38.93%

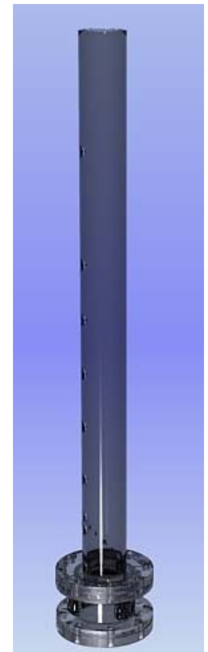
MFS support of the Gasification Program

- **Experimentation for Model Development and Validation**
  - Operation of Small-Scale Fixed, Bubbling, and Circulating Fluidized Beds for Validation
    - Small Fixed Bed for heat transfer, kinetics (1in Dx 6 in H)
    - Bubbling Fluidized Bed (4in D x 72in H)
    - Rectangular 2-D bed (2in x 0.125in x 18in H)
    - Small Scale Circulating Bed (1in D x 48in H)
  - Pilot-Scale Cold Flow Circulating Bed (12in D x 60 ft H)
  - Flow control, measurement, diagnostics
    - High Speed PIV
    - LDV
    - Low and High Speed Pressure
    - High Speed video
    - Image analysis
    - Tracer gas

Experimentation for Model Development and Validation

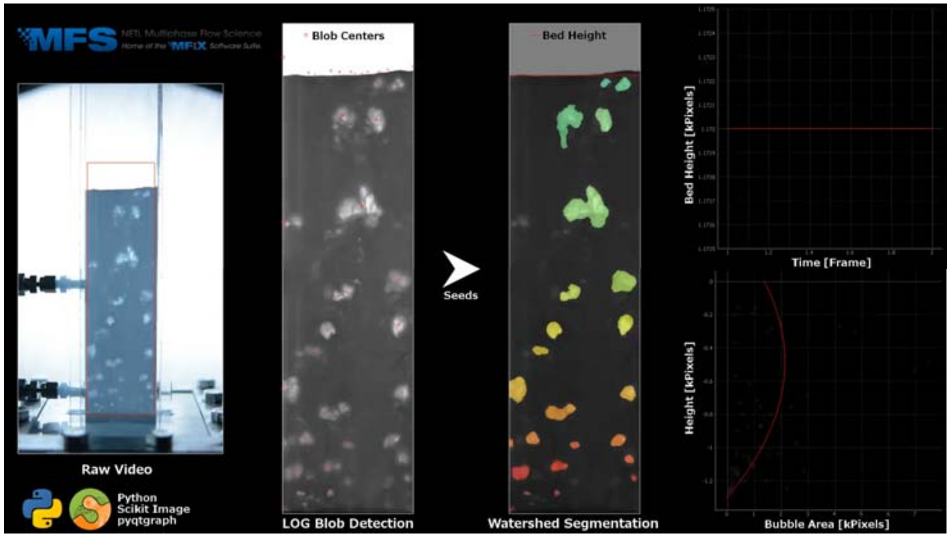
- **Small-Scale Bubbling Bed experiments performed with NETL CO_2 Sorbent Particles to validate MFiX-TFM**
  - excellent agreement with fixed bed tests

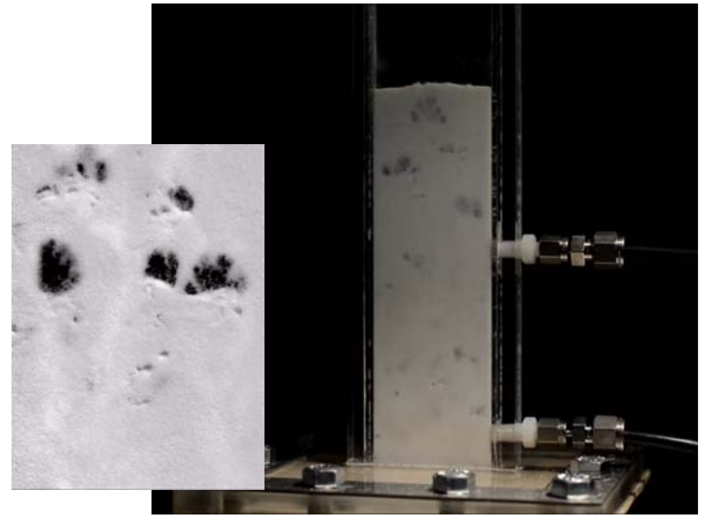


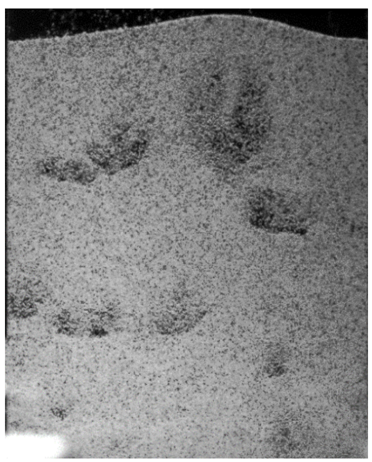


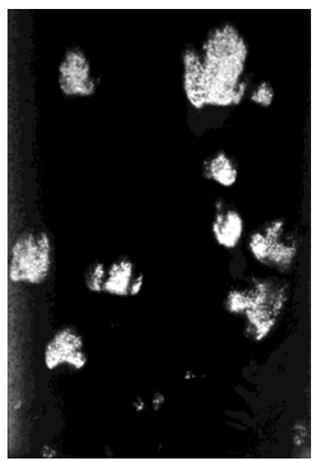
Experimentation for Model Development and Validation

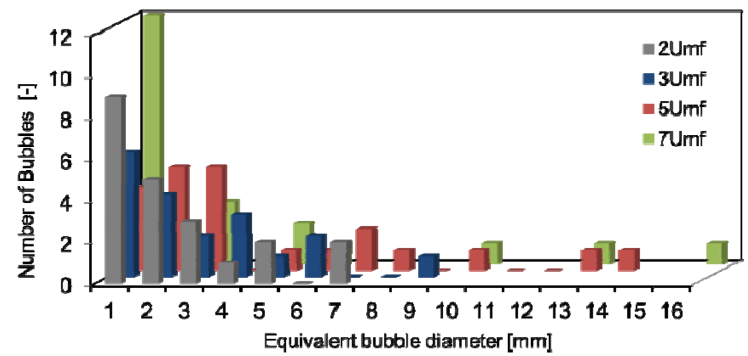
- **2-D bed being used for detailed measurements for validation data**



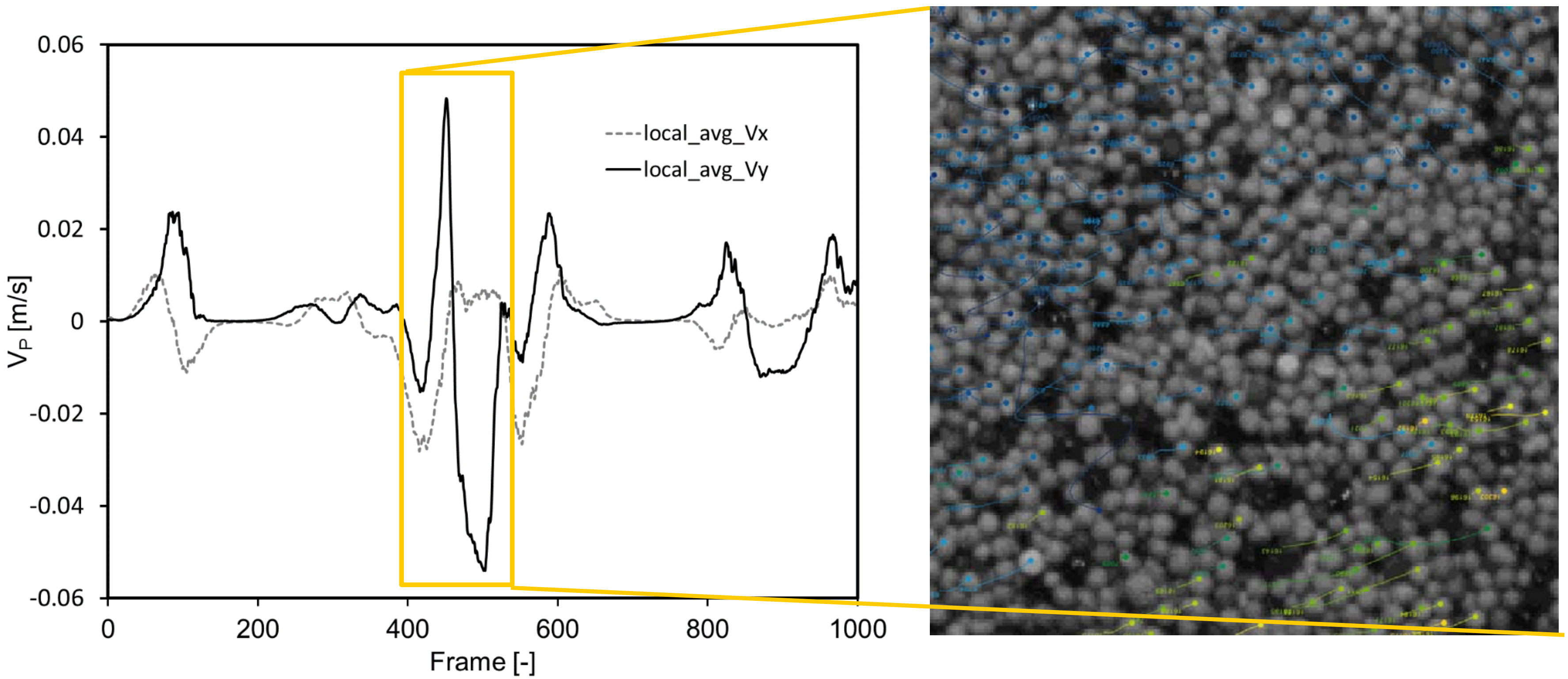








- **High Speed PIV for local particle velocity, solids concentration**



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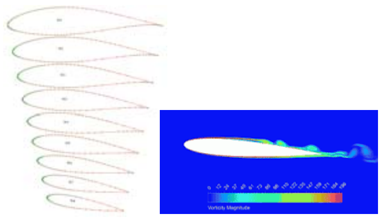
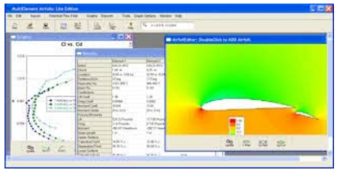
Radically Engineered Modular Systems (REMS)

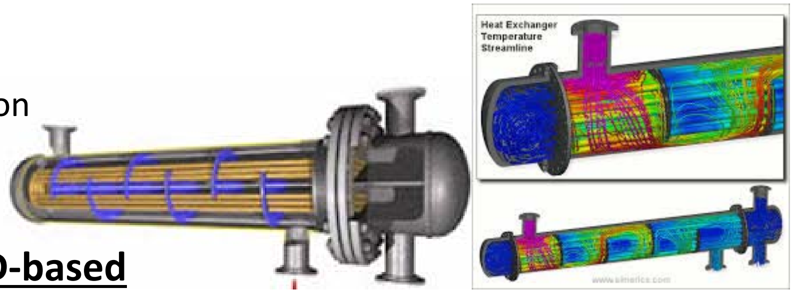
Use CFD Simulation-Based Optimization for Reactor Design

Build on Existing Techniques

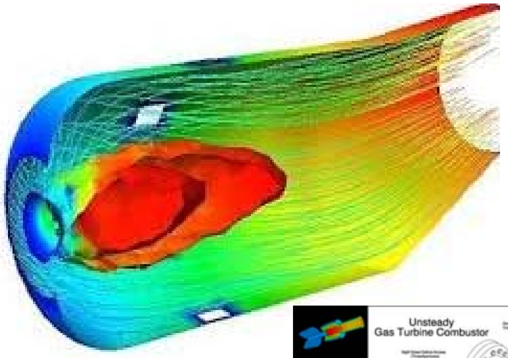
- **Use of CFD-Based Optimization is growing for single phase applications**
  - Proven technique in many engineering applications - chemical process, aerospace, turbomachinery, automotive
    - Optimization of airfoil shape for lift and drag
    - Optimization of heat exchanger tube shape, size, location
    - Optimal combustor design

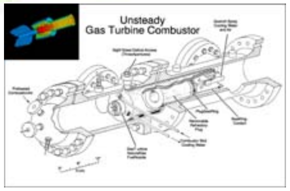






- **REMS will develop, validate, and apply a <u>Multiphase CFD-based Optimization Toolset</u>**
  - Multiphase CFD brings new challenges to the optimization process
    - Complex multiphase physics require accurate submodels for flow, heat transfer, chemical kinetics, coupling between phases
    - Very computationally intensive
    - Potential for huge datasets resulting from pilot and industrial scale applications
  - The new software capability will be based on the NETL **MFiX Suite** of multiphase flow CFD software

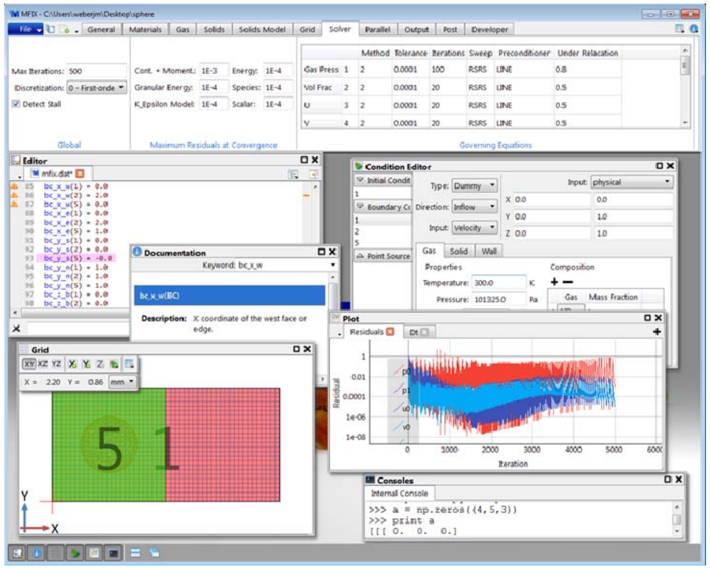


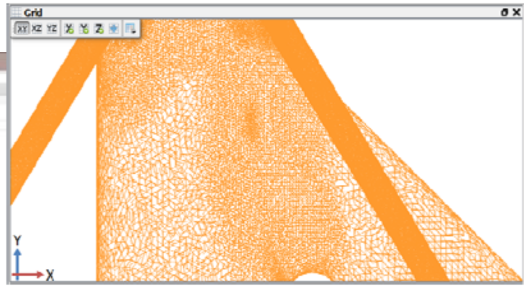


Radically Engineered Modular Systems (REMS)
Use CFD Simulation-Based Optimization for Reactor Design

User Interface and Toolset to Manage the Optimization Process

- **Design and develop GUI-based, Multi-objective Optimization software framework**
  - Code infrastructure for managing the optimization process
  - methodologies and code to create and manage reactor models created using MFIX Suite of multiphase flow software
- **The modeling tools will become part of the publicly available, Open Source MFIX Suite of codes (https://mfix.netl.doe.gov)**



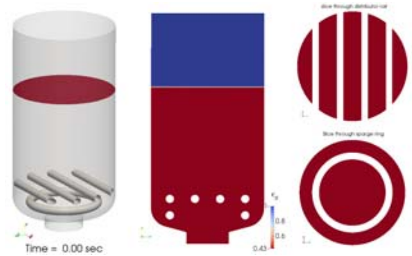


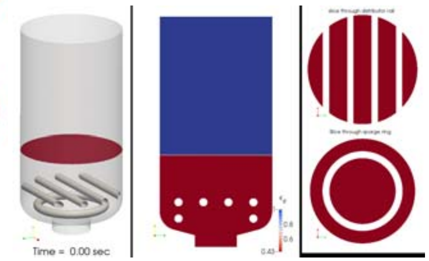
Radically Engineered Modular Systems (REMS)

Use CFD Simulation-Based Optimization for Reactor Design

Use CFD Simulation-Based Optimization for Reactor Design

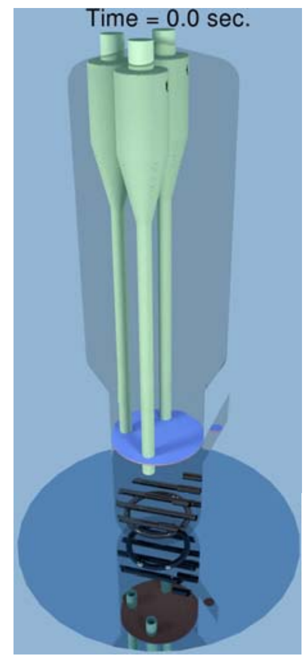
- **Optimization process will investigate radically different reactor geometries**
  - Allow for precise manipulation of different coal and biomass particles
    - segregation of low ash melting particles in a lower temperature part of the reactor
    - continuous removal of ash or volatiles as they are created,
    - segregation of char to a higher temperature part of the reactor
    - segregation of catalysts and reactive particles types for more efficient conversion
    - use of neutral/reactive particle addition and removal
  - Optimize reactant and product gas flow
    - improve particle-gas contacting to better control carbon conversion and product composition
    - Control heat addition/removal, etc.





Effect of Operating Conditions

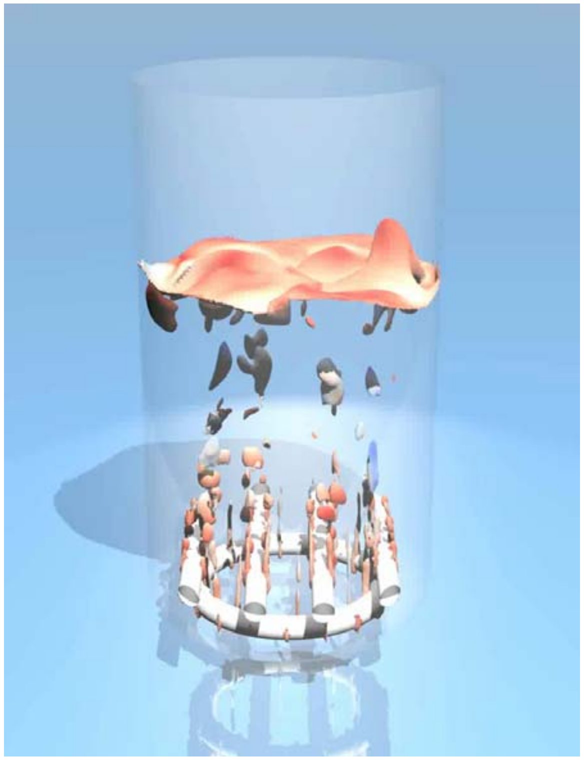
Geometry Changes



Scale Up Performance

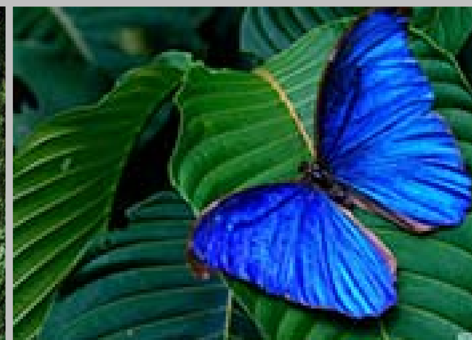
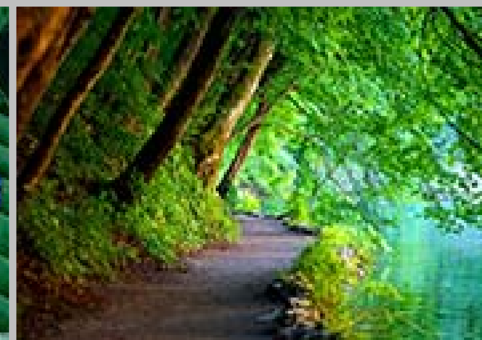
Summary

- **Multiphase Flow Science at NETL has a long and successful history of R&D**
- **Our emphasis is on Multiphase CFD for dense, reacting flow**
  - MFiX Suite of open source, multiphase CFD software
    - Development, VV&UQ, Application and Support
- **Experiments designed for model validation are critical to our program**
- **Gasification is a key focus for code capability development**
- **The goal is a practical and useful toolset for industry**



It's All About a Clean, Affordable Energy Future



For More Information, Contact NETL

the ENERGY lab

Delivering Yesterday and Preparing for Tomorrow