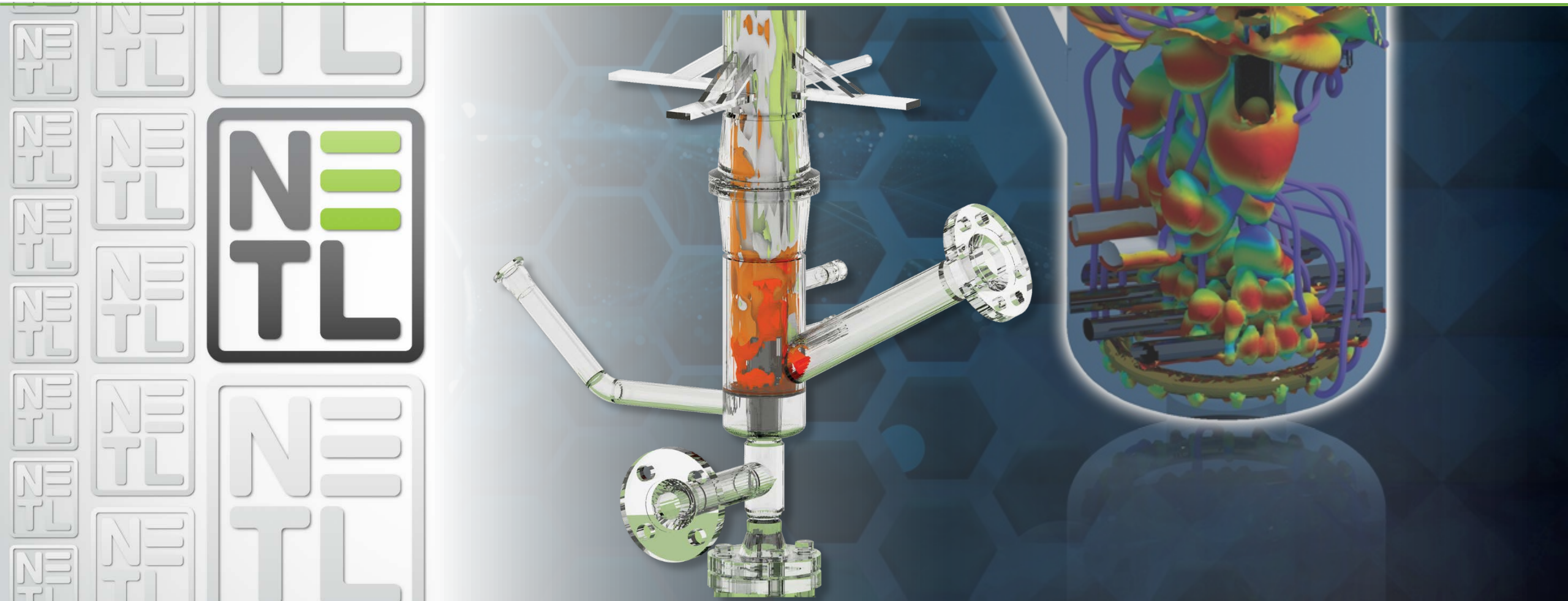
Multiphase Flow Science & the MFiX Suite

Software tools and expertise to address multiphase flow challenges in research, design, and optimization

NATIONAL ENERGY TECHNOLOGY LABORATORY

Mehrdad Shahnam

Research Engineer, RIC



Presentation Outline

- Multiphase Flow Science at NETL and its mission
- The MFS Team
- MFiX Suite of Multiphase CFD Software
- Status Today: Applications to FE Technologies
- Challenging new research: Reactor Optimization using MFiX
- Summary

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Significance of Multiphase Flow Science (MFS)

What is Multiphase Flow?

- Fluid flow consisting of 2+ phases or components (e.g., solid & gas)

Multiphase Flow in Industry

- **Sectors:** Power, chemical, petrochemical, metallurgical, environmental
- **Devices:** boilers, gasifiers, fluidized beds, cyclones, emissions controls

Multiphase Flow in FE

- Oxygen carriers
- Modular gasification
- Solvent/sorbent-based CO_2 capture
- Foamed cement
- Coal pulverizer

NETL has developed world class capabilities for FE and industry to address multiphase flow problems

- **Industrial processes across all sectors are challenged (design & operating) whenever solids are involved**
- **Scale-up of devices handling multiphase with solids: daunting task**
- **Problem not going away: ~40% U.S. chemical industry (worth significant piece of national GDP) involves particle/solids**

MFiX Critical to FE Priorities

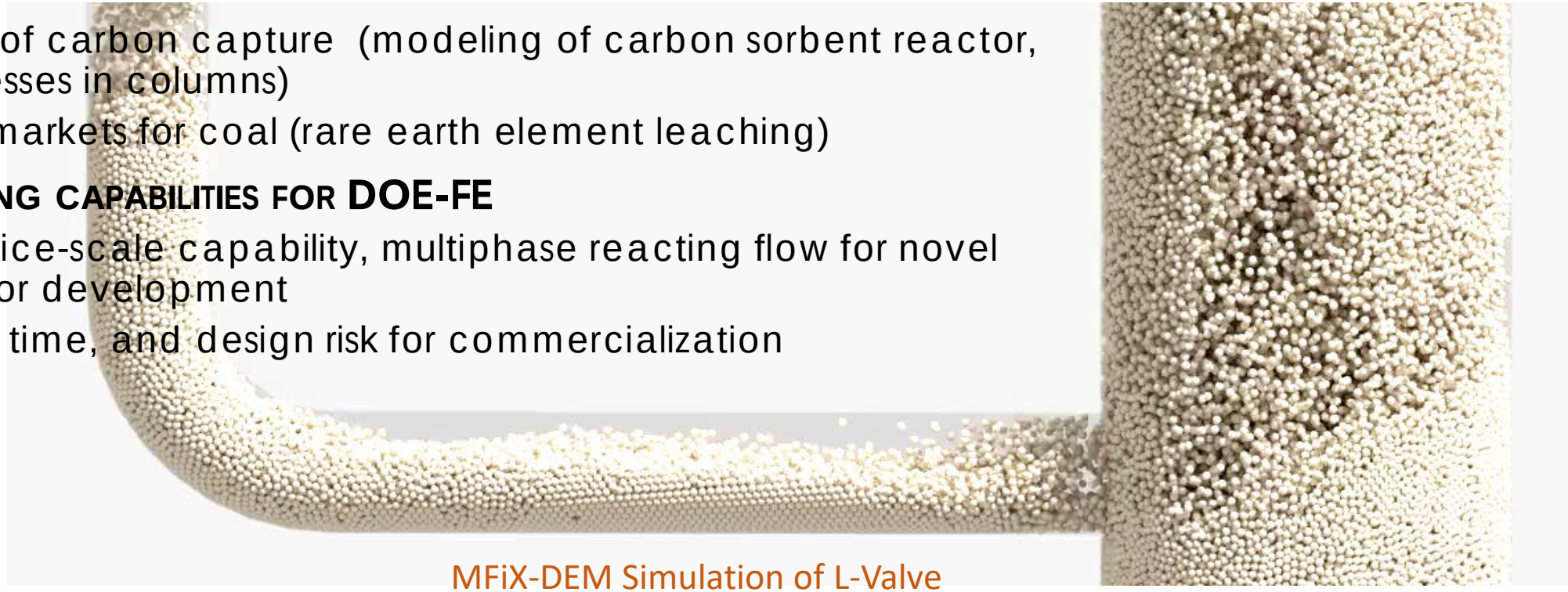
Addressing Key Priorities and Developing Capabilities

DOE-FE Coal Program support—addressing key priorities

- Improve performance of existing plants (circulating fluidized bed boilers at pilot and commercial scales)
- Advance small scale modular (reactor optimization, coal gasifier modeling)
- Reduce cost of carbon capture (modeling of carbon sorbent reactor, solvent processes in columns)
- Create new markets for coal (rare earth element leaching)

Developing modeling capabilities for DOE-FE

- Focus on device-scale capability, multiphase reacting flow for novel energy reactor development
- Reduce cost, time, and design risk for commercialization



MFiX-DEM Simulation of L-Valve

MFS and MFiX by Numbers

Legacy and Impact

30+
Researchers
In modeling and laboratory testing

3 Decades
of development history

5–10x speed increase
MFiX 18.2 (released December 2018)

300+
citations per year

5,000+
registered users

175+
downloads per month

MFS Mission at NETL

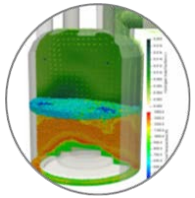
Goals, Capabilities, Application, and Impact

Goals of MFS

- **Solve critical national energy problems**
- **Support the mission of DOE**
- **Provide multiphase flow expertise cross-cutting many offices under the Department**

NETL MFS Capabilities

- Physics-based Modeling Tools
- Experimental Activities
- High-performance Computing



Office of Fossil Energy Application/Impact

- Coal Program Support/Modeling Capabilities for FE
- Modeling of energy systems, carbon capture, modular reactors

Department of Energy Application/Impact

- Support for Offices DOE-wide
- Exascale Computing, Environmental Management, EERE, others

MFiX Suite of Multiphase CFD Software

Capabilities and Benefits

MFiX is NETL flagship computational fluid dynamic (CFD) code

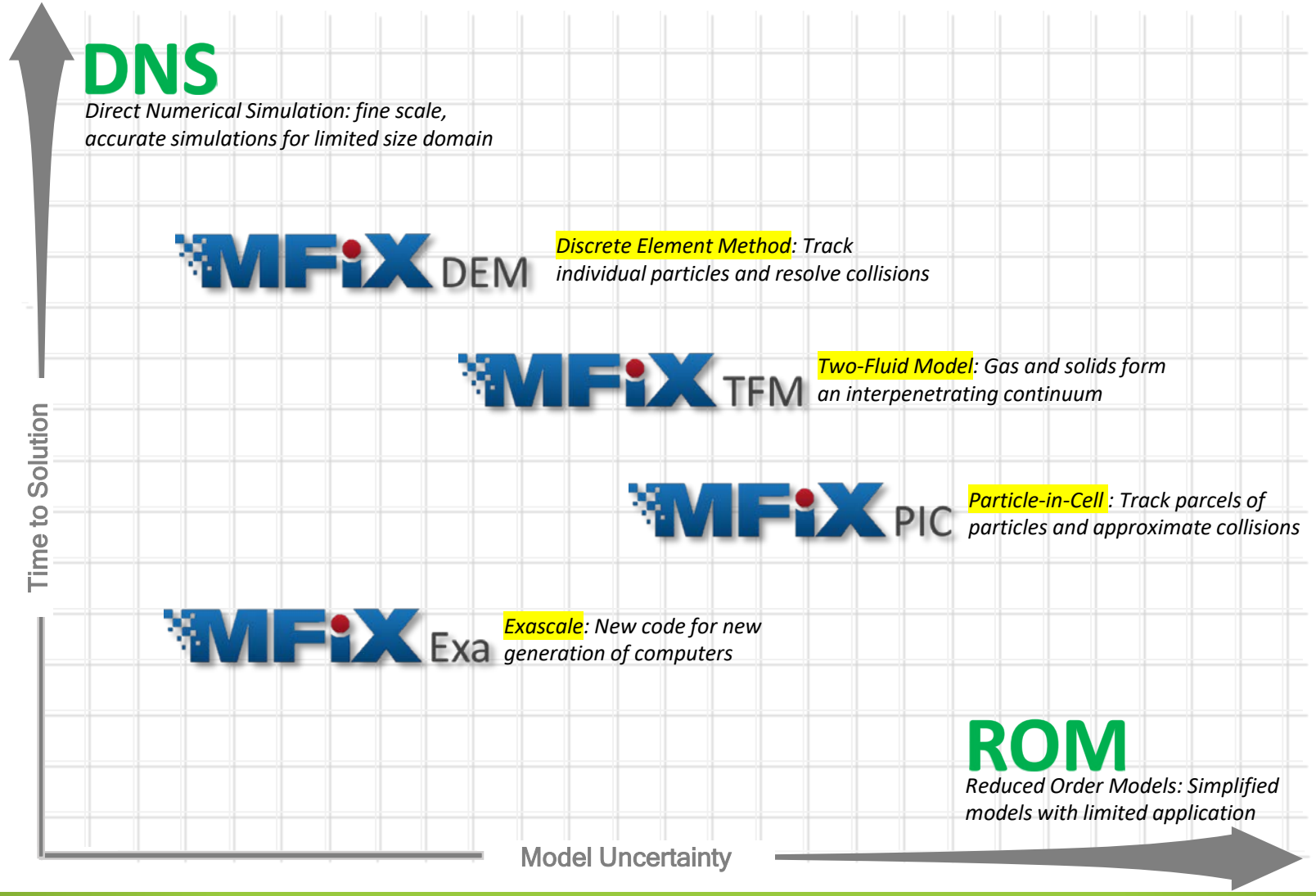
- **Versatile toolset** for understanding the behavior and characterizing the performance of energy conversion processes
- **Accelerate reactor development and reduce cost** by using multiphase flow reactor modeling and simulation tools
- **Optimizes performance** for equipment and unit operations, enabling more throughput and less process downtime
- **Reduces design risks** when validated by predictive science-based calculations, lowering risk in obtaining return on investment

- MFiX-TFM (Two-Fluid Model)
- MFiX-DEM (Discrete Element Model)
- MFiX-PIC (Multiphase Particle-In-Cell)
- MFiX Exa (Exascale) – under development
- C3M multiphase chemistry management software
- Nodeworks: Optimization and UQ Toolsets

MFS Software Portfolio

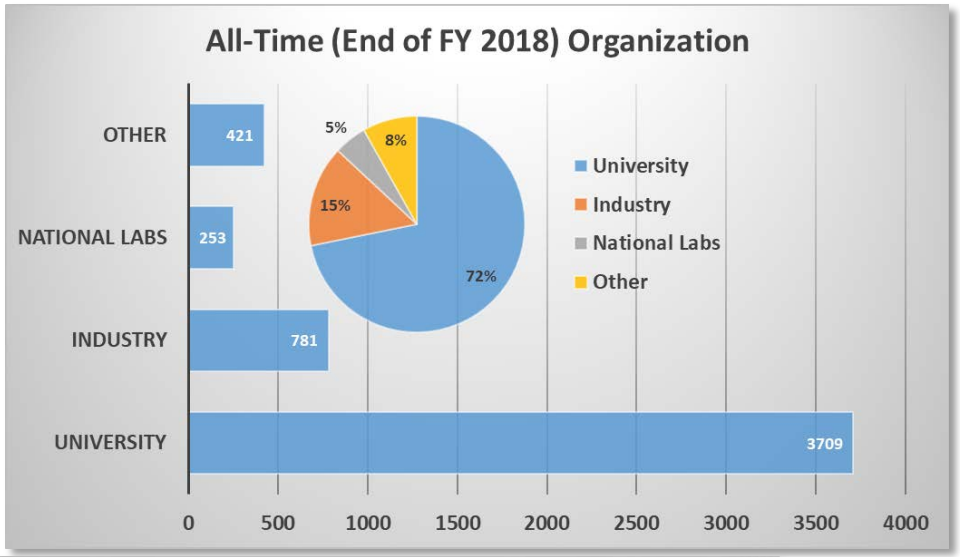
MFiX Suite of Multiphase CFD Software

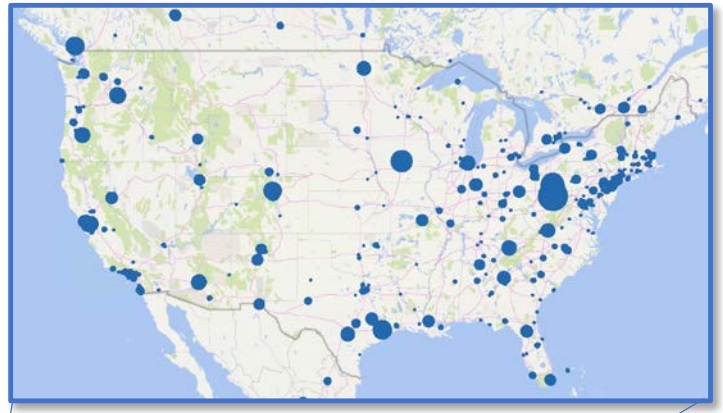
Managing the tradeoff between accuracy and time to solution



All-time MFiX Stats (as of Sept 2018)

- All-time MFiX registrations = **5,164**
  - University = 3,709
  - Industry = 781
  - National Labs = 253
  - Other = 421





- **84 countries, Top 5:**

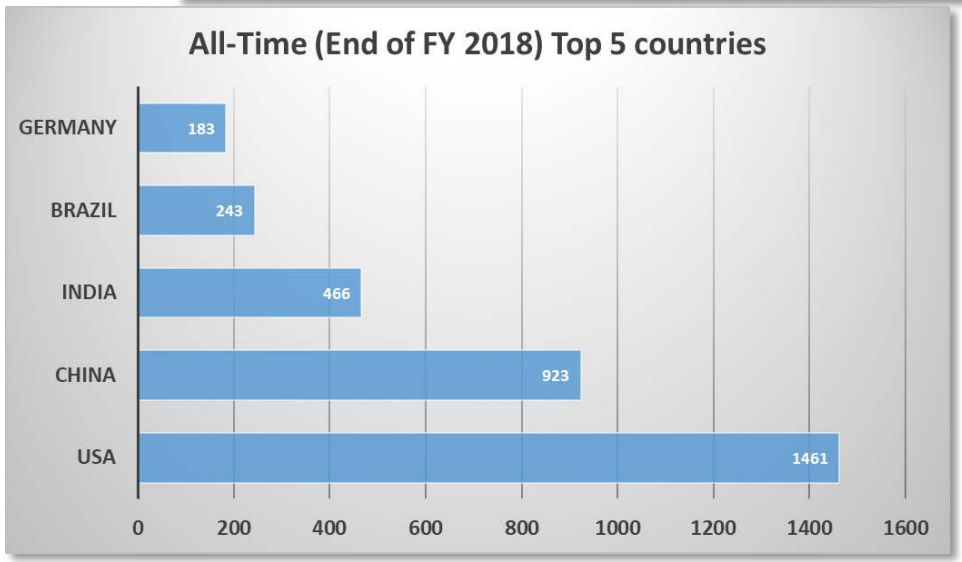

USA : 1,461

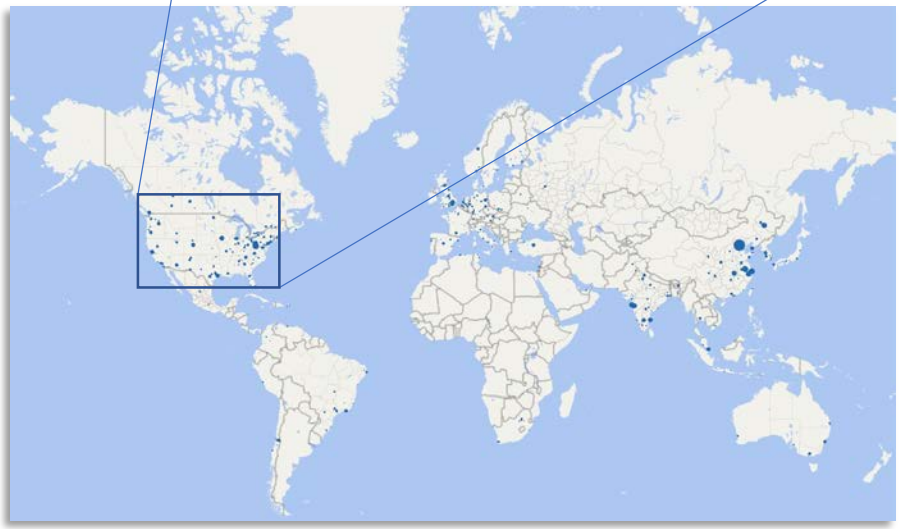

China : 923


India : 466


Brazil : 243


Germany : 183

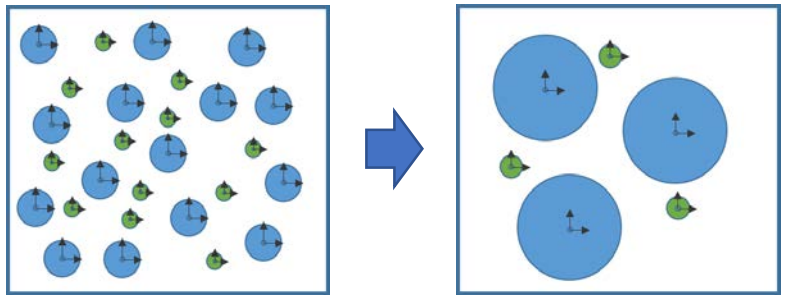




MFiX 19.1 Release

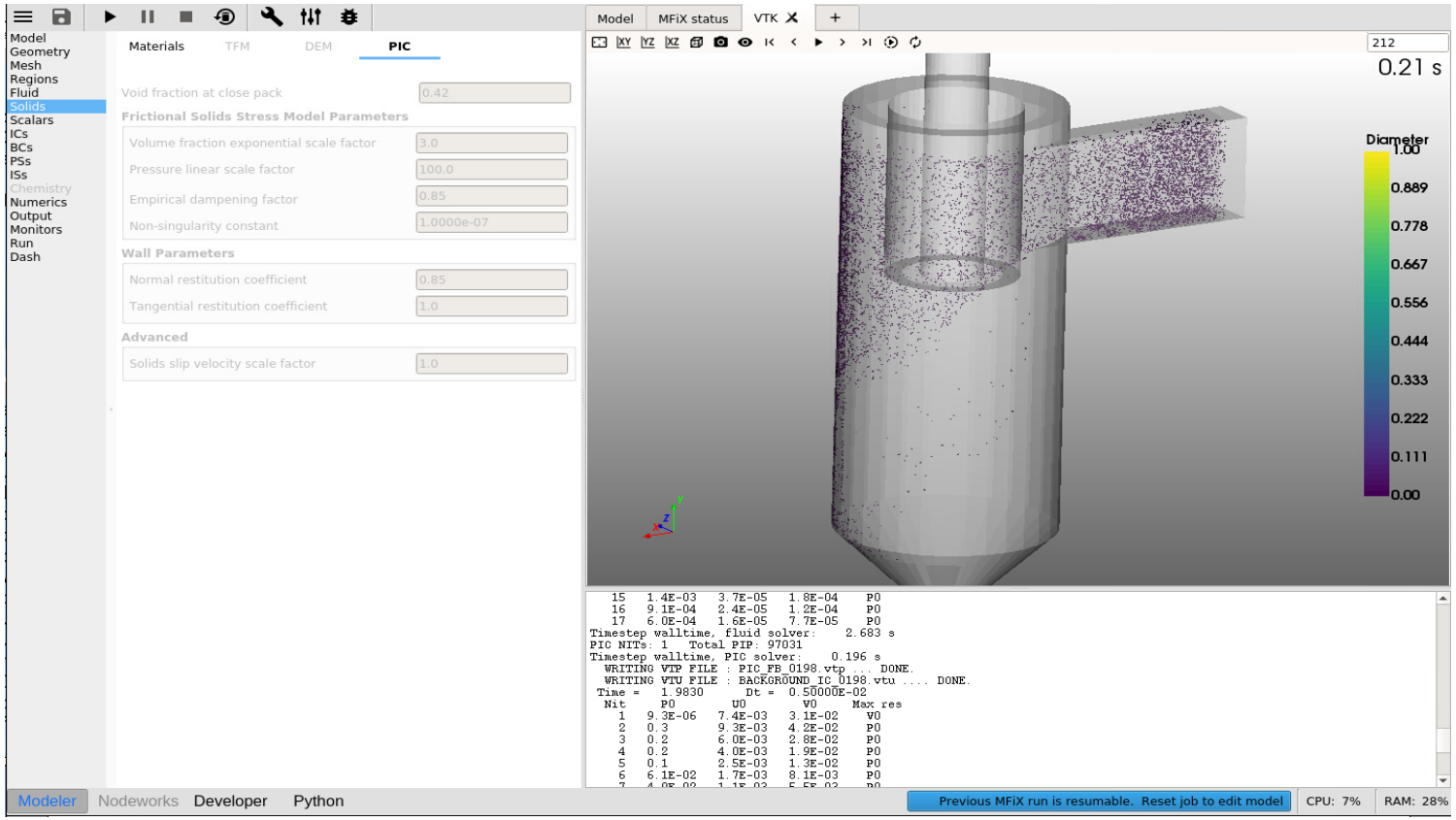
Released April 4, 2019

- Rewrite of MFiX PIC
  - Hydrodynamics
  - Heat transfer
  - Chemistry
  - Serial and parallel run



Identical physical particles are grouped into larger computational parcels. Multiple particle types can be managed as separate parcel distributions.

MFiX 19.1



The objective of MP-PIC is to maintain an averaged accuracy for larger scale problems while increasing computational speed.

A Long History of Partnerships

Active Portfolio of Collaboration

Driving partnerships across DOE's National Laboratories, industry, and university organizations

Annual Multiphase Flow Science Workshop

- Brings together international research leaders
- Encourages multiphase flow research and promotes the exchange of ideas

GOVERNMENT PARTNERSHIPS

Berkeley Lab · SRNL Savannah River National Laboratory · NREL National Renewable Energy Laboratory · CCPC Consortium for Computational Physics and Chemistry Bioenergy Energy Technology Office · U.S. Department of Energy Office of Environmental Management · INL Idaho National Laboratory · Oak Ridge National Laboratory · Argonne National Laboratory · U.S. Department of Energy Office of Science · Pacific Northwest National Laboratory · U.S. Department of Energy Energy Efficiency & Renewable Energy

INDUSTRY PARTNERSHIPS

Natural Resources Canada · intel · B&W · ANSYS Fluent · Bechtel · NVIDIA · CPFD Computational Particle Fluid Dynamics · Southern Company · SOTACARBO Sustainable Energy Research Centre · FLUOR · KBR

UNIVERSITY PARTNERSHIPS

UTSA The University of Texas at San Antonio™ · UND University of North Dakota · Iowa State University · MIT · Chinese Academy of Sciences · FIU Florida International University · University of Idaho · Illinois Institute of Technology · UCI · Princeton University · University of Colorado Boulder · West Virginia University

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Coal gasification simulations at industrial scale

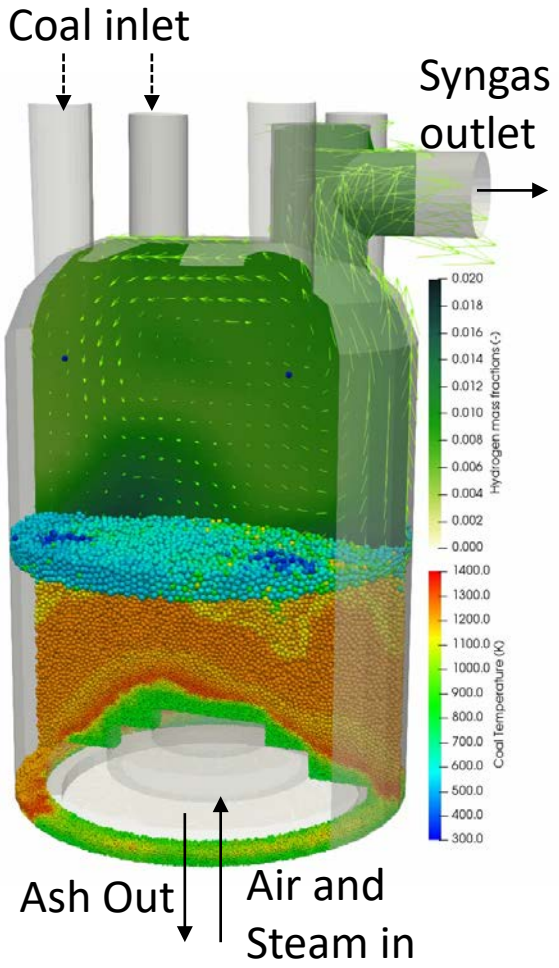
NETL is demonstrating newly developed software capabilities to accurately model industrial scale FE reactors to aid design and optimization

Accomplishments:

- Novel use of 1-D validation of complex coal gasification kinetics and also used to to accelerate reactor startup simulations
- Full 3-dimensional, transient simulations of 1MW-scale gasifier operating at CRADA partner site (Sotacarbo Research Center, Italy)

Impact:

- Simulations will be compared to data generated by CRADA partner for code validation
- Demonstration of unique capability to model industrial-scale systems using advanced NETL software running on high performance computing systems
- Demonstrate the ability to optimize design and operation of industrial-scale FE devices using simulation-based tools which will save money and reduce risk for optimizing existing plants and developing new designs



3-D full scale simulation

Coal gasification simulations at industrial scale

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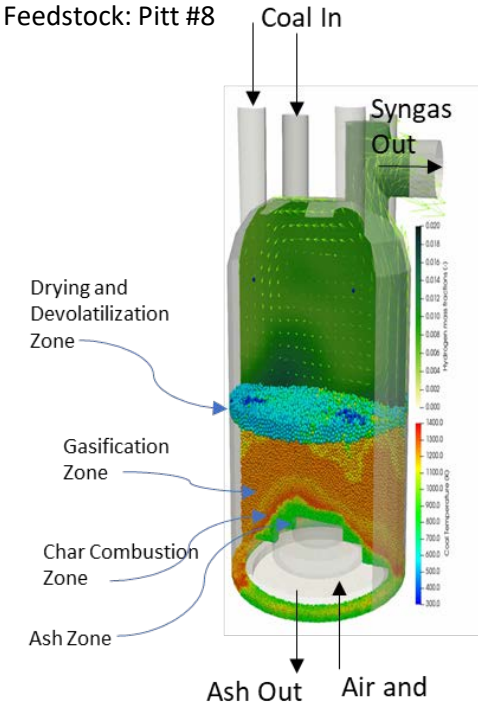
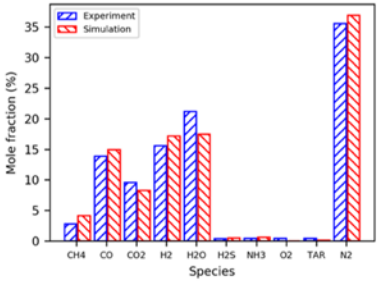
Gasifier Vessel:
ID =0.78 m, H=1.8 m
Feedstock: Pitt #8

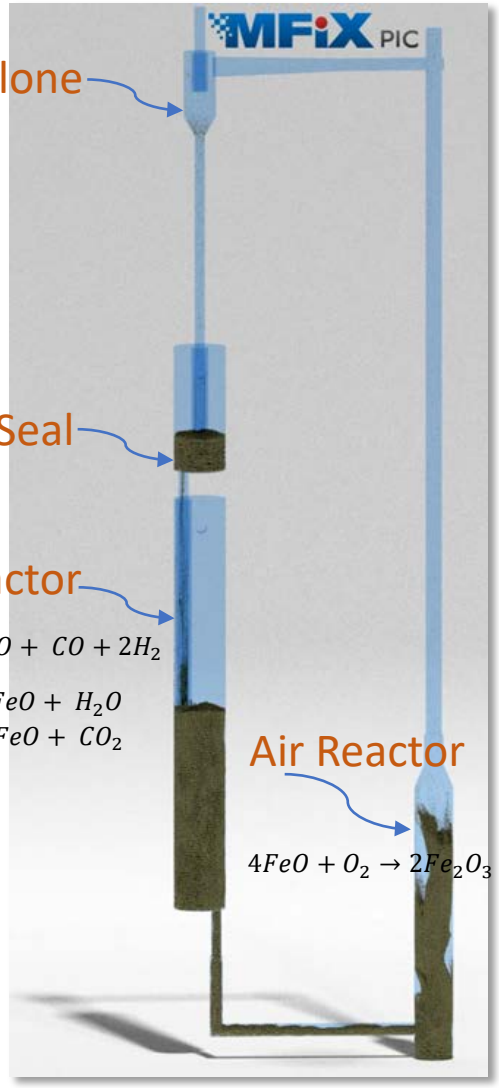




NETL Chemical Looping Reactor

Pilot scale simulations with new MFiX-PIC code

NETL 50 kWth Chemical Looping Combustor



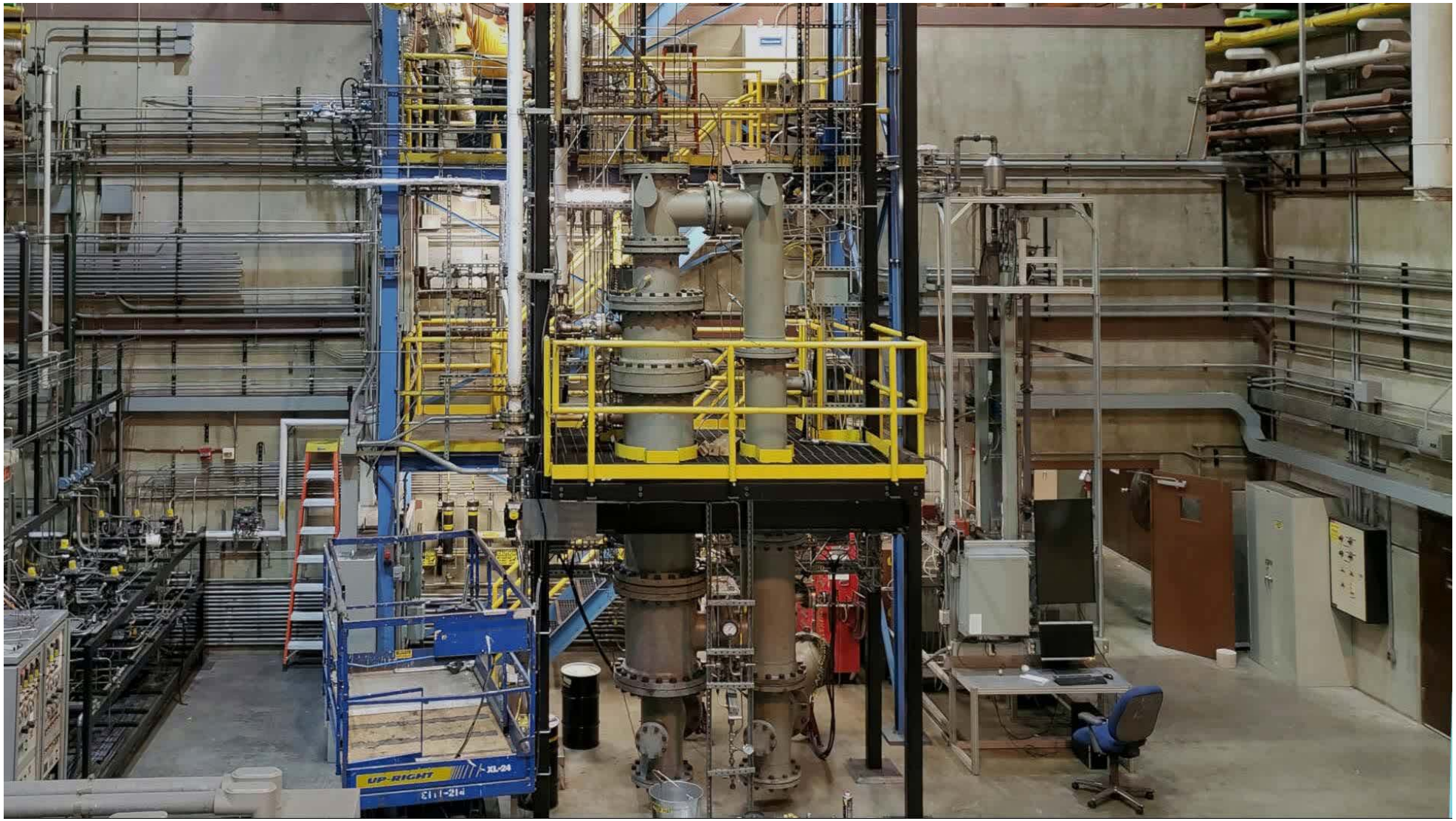
Accomplishments:

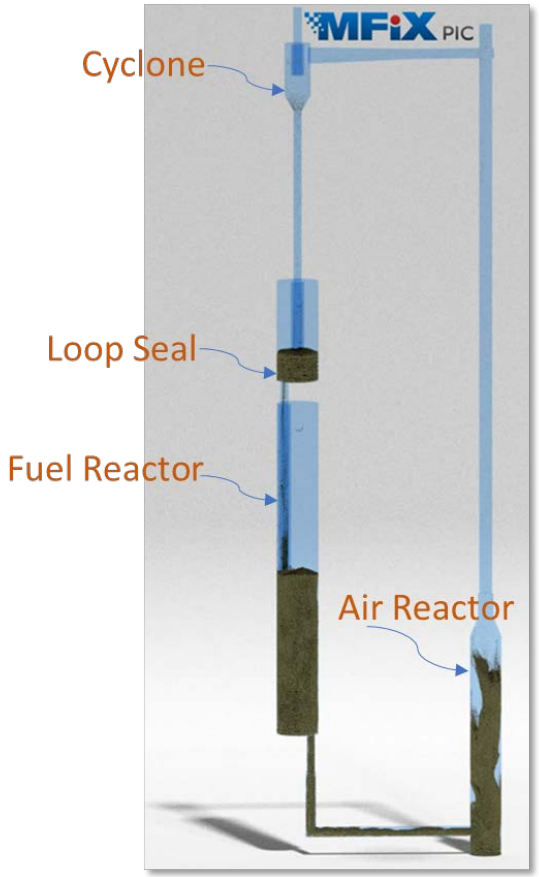
- Simulations of full pilot scale unit (~4m tall)
- Operating temp (500-980◦C)
- Metal oxide carriers – Ilmenite, hematite
- Methane fuel - Reaction rates based on Abad (2011)
- Basic Run Information:
  - ~13,000,000 PIC parcels
  - Representing ~650,000,000 carrier particles
  - ~1 cm3 mesh size
- Running ~15 s/day on 200 cores !

Impact:

- Simulations will be compared to data generated by NETL CLR Facility for code validation
- Demonstration of unique capability to model pilot and industrial-scale reacting systems on high performance computing systems

NETL Chemical Looping Reactor





Sorbent-based Carbon Capture

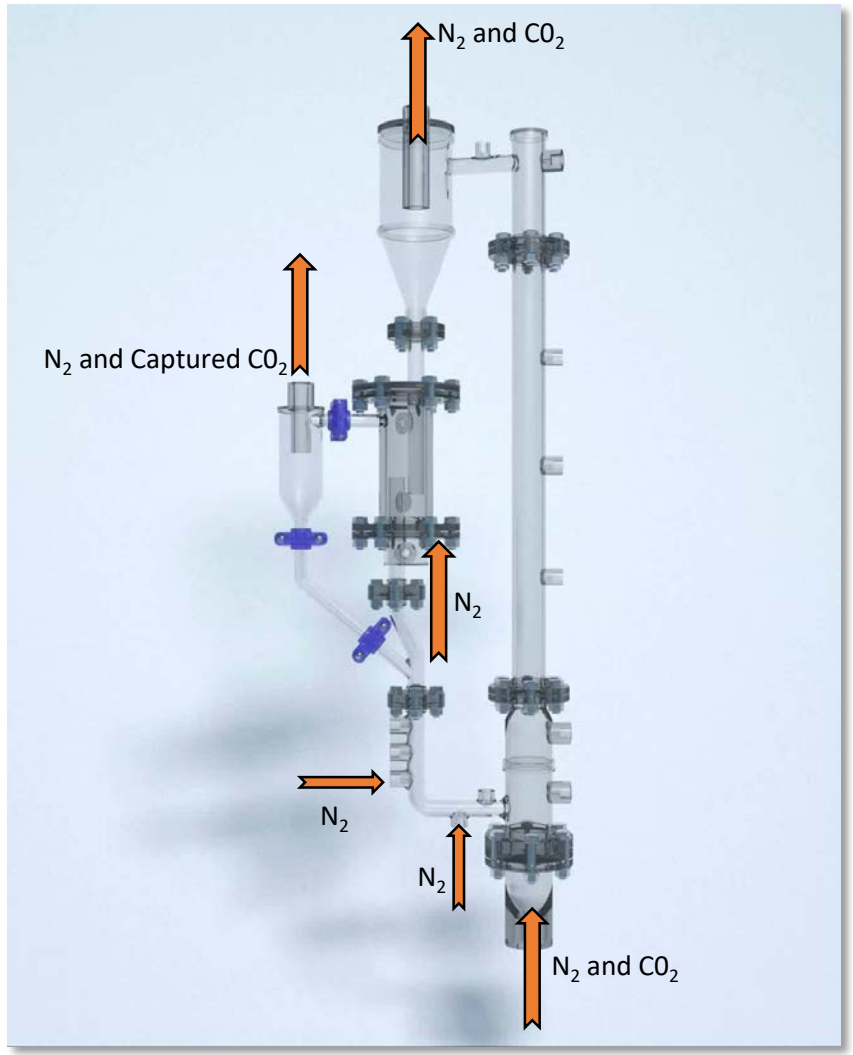
Compare Simulations to Small-Scale, Reacting Flow Measurements

Accomplishments:

- Experiments and simulations of small-scale unit (~0.6m tall)
- Operating temp (20-35◦C)
- Commercial Zeolite adsorbent
  - 800 micron SMD
- Chemical Kinetics parameters optimized with fixed-bed tests
- Basic Run Information:
  - MFiX-DEM simulation
  - 600,000 Zeolite particles
  - Reacting flow with heat transfer

Impact:

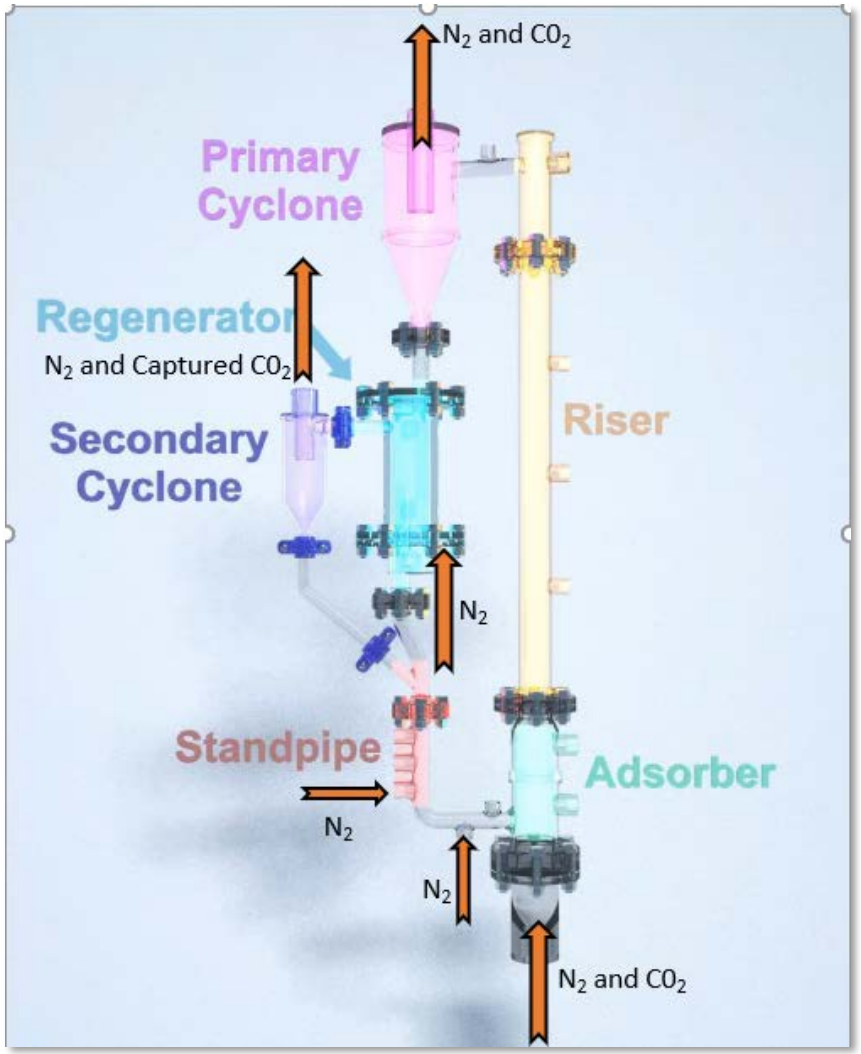
- Simulations are compared to data generated in the NETL Multiphase Flow Analysis Laboratory for code validation
- Demonstration of capability to model complex, reacting flow at high fidelity on high performance computing systems
- Future effort will demonstrate reactor optimization



Sorbent-based Carbon Capture

Compare Simulations to Small-Scale, Reacting Flow Measurements

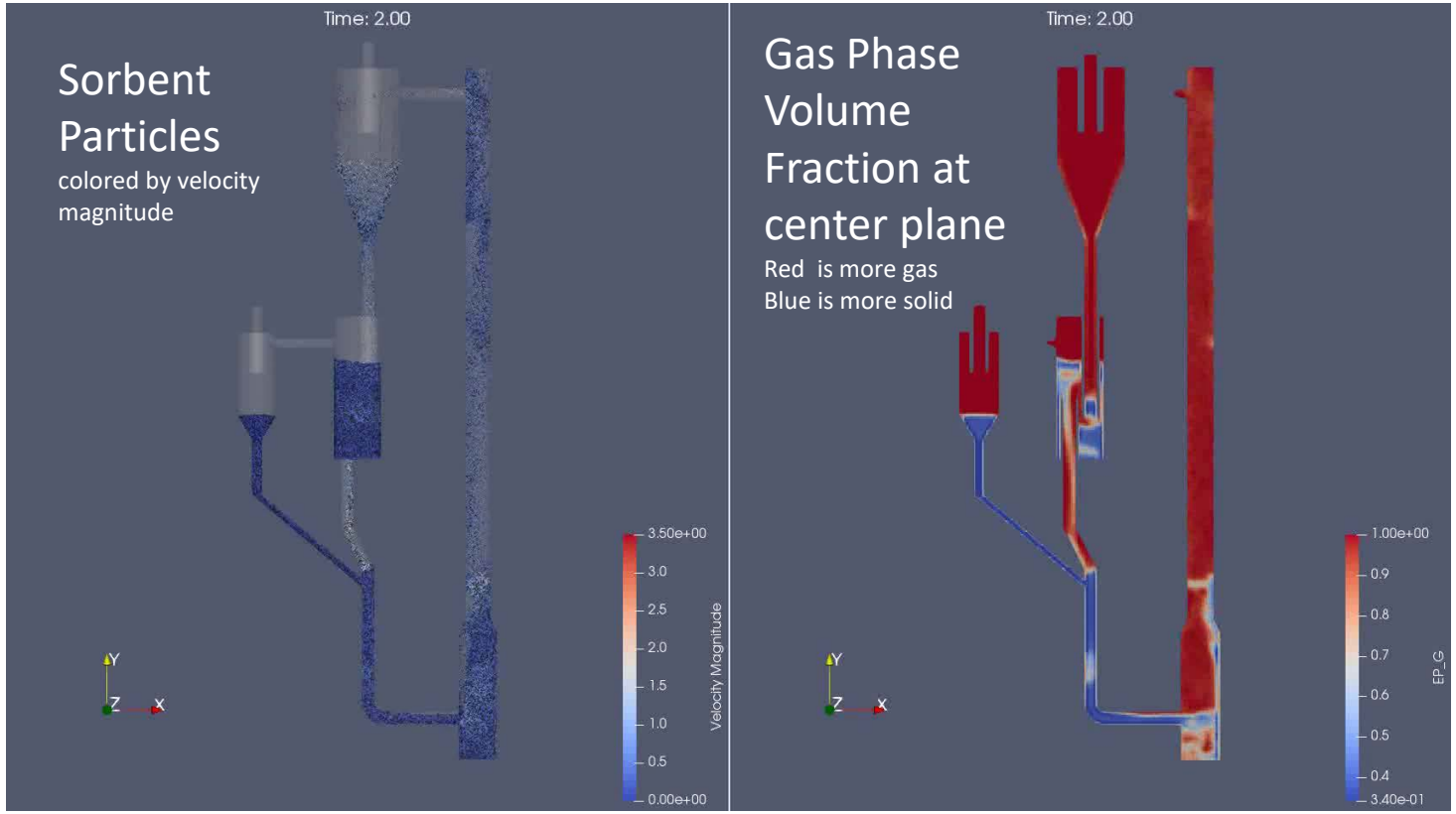
Simulation Results:
MFiX-DEM

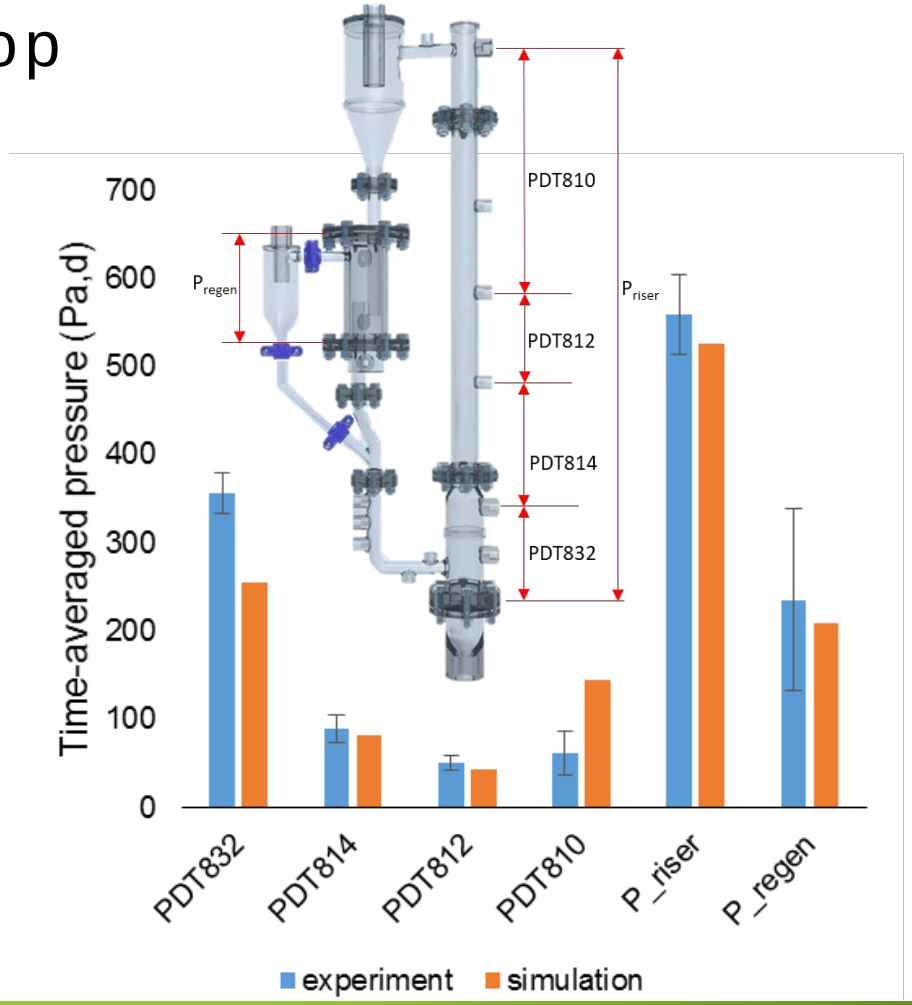


Sorbent-based Carbon Capture

Cold Flow Hydrodynamics

Excellent comparison between modeled and measured solids holdup(pressure drop values) around the flow loop





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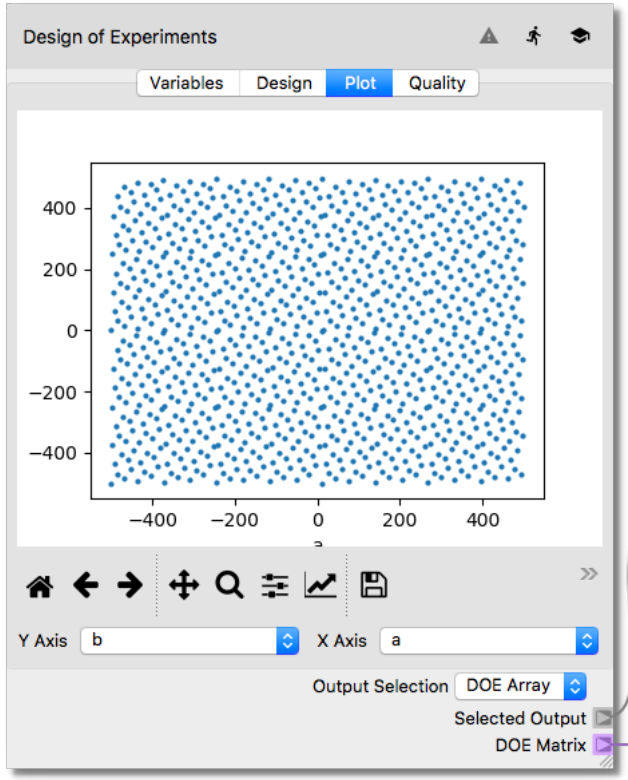
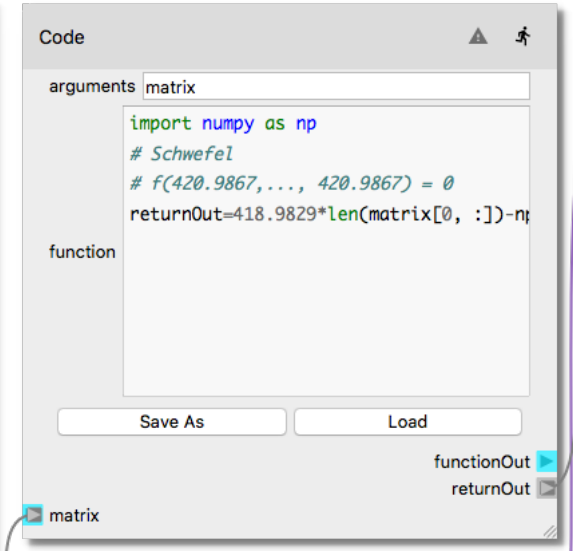
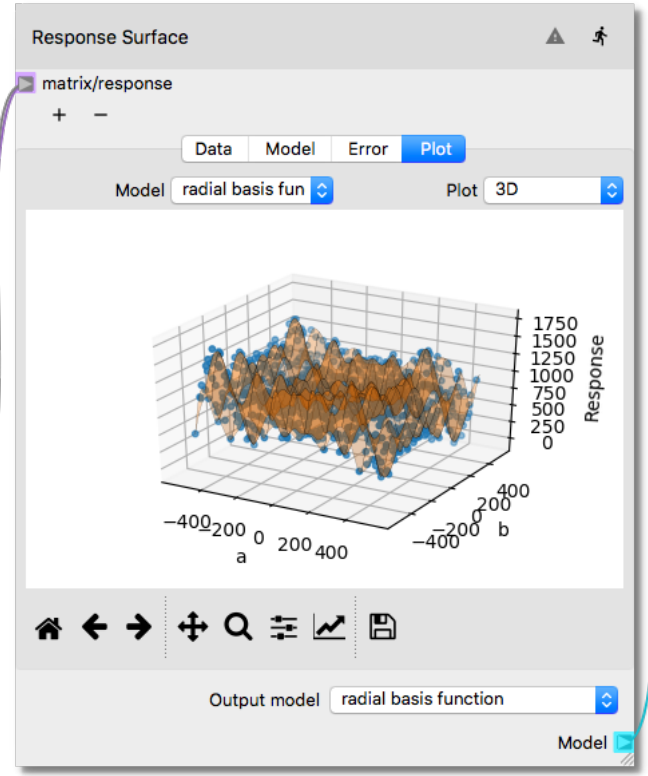
MFiX Suite with Optimization Toolset

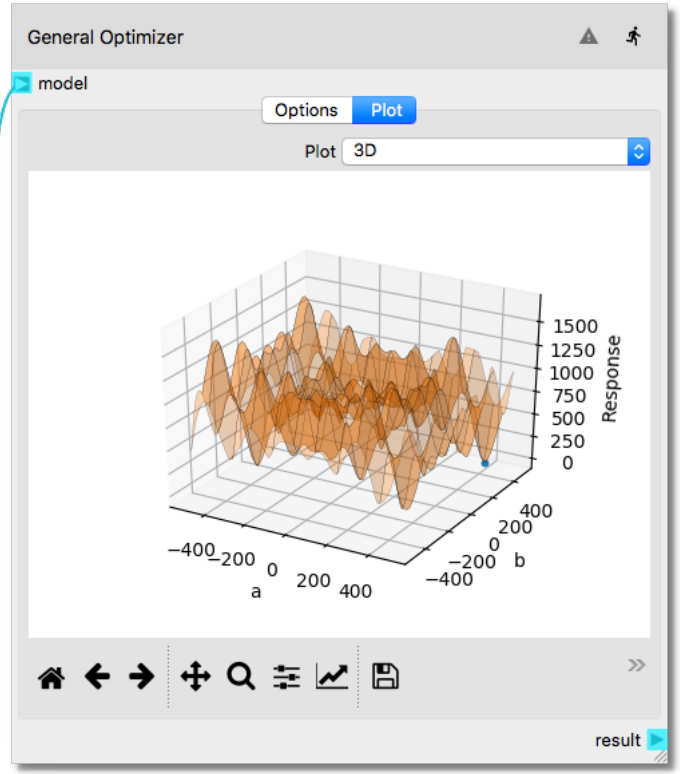
Use Multiphase CFD to optimize reactor performance

Design of Experiments for planning MFiX Simulations → Model evaluation for reactor performance → Response Surface Construction for Reduced Order Model → Optimization of Reactor Performance





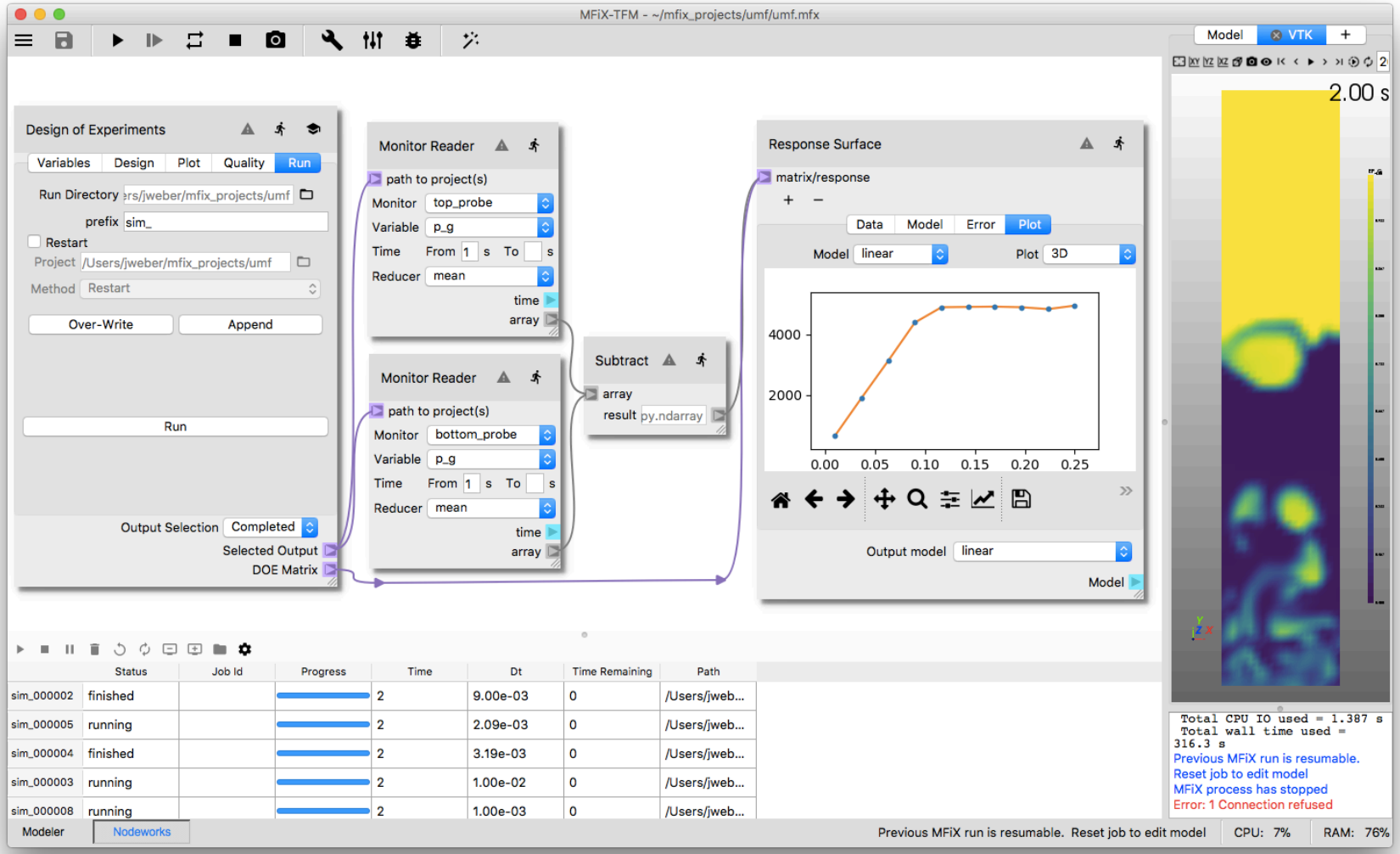




MFiX Plug-in for Optimization

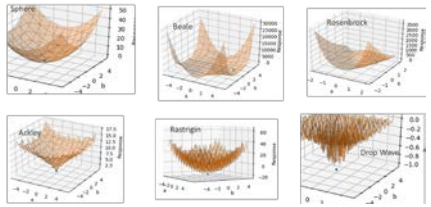
Leveraging the power of MFiX CFD

- Integrated in MFiX GUI
- "Inside" MFiX - click to switch the *Modeler* panel (where the problem is defined)
- MFiX "Wrapper" – select executables, launch jobs, monitor simulation progress, plot and post-process MFiX

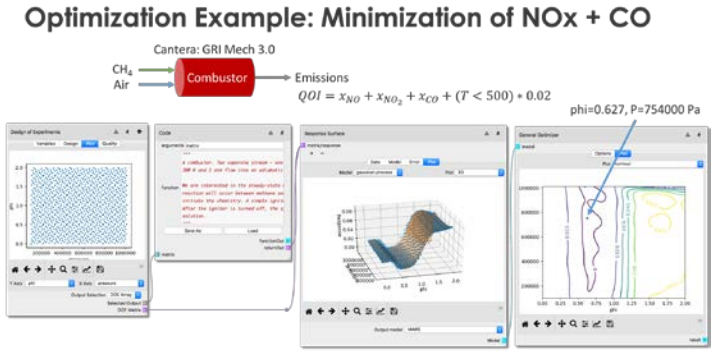


MFiX Suite with Optimization Toolset

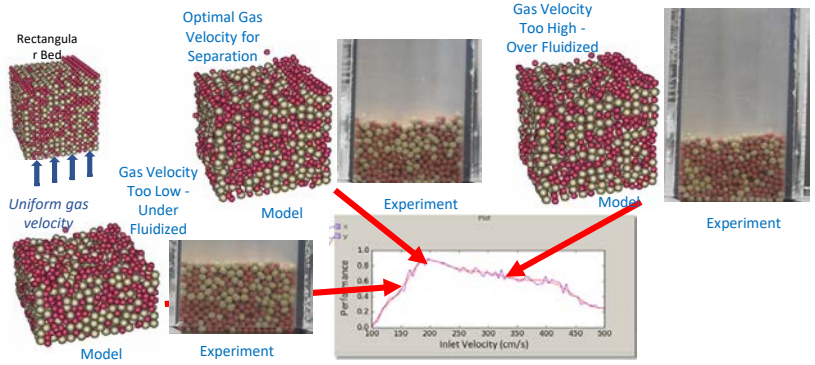
Extensive Validation Has Been Performed



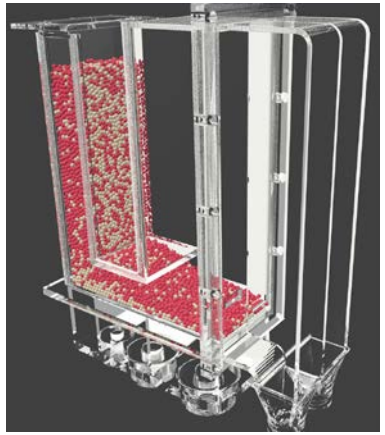
Standard Test Functions



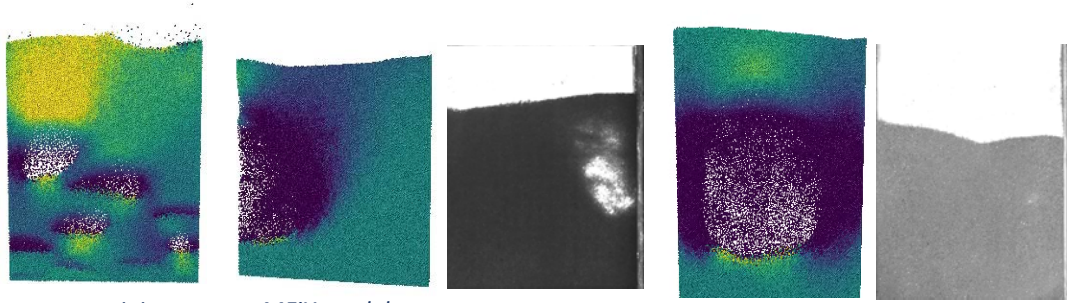
Complex Gas-Phase Chemistry



Batch Particle Separation in a Fluidized Bed



Continuous Particle Separation in a Fluidized Bed



MFiX model results random bubbling – base condition

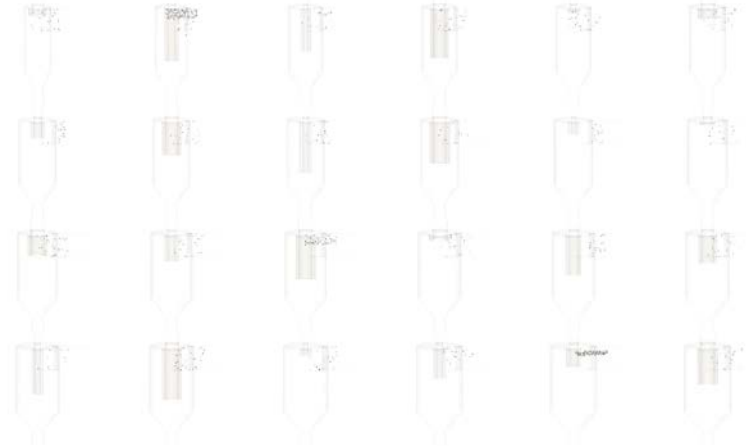
MFiX model results optimized for left-right bubble pattern

NETL Laboratory Bed at optimal conditions for left-right bubble pattern

MFiX model results optimized for slugging bubble pattern

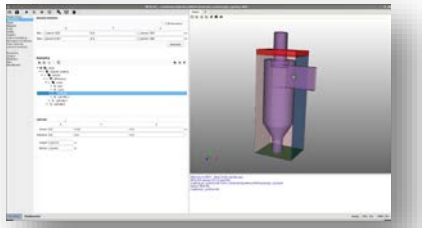
NETL Laboratory Bed at optimal conditions for slugging bubble pattern

Bubble Behavior in a Fluidized Bed

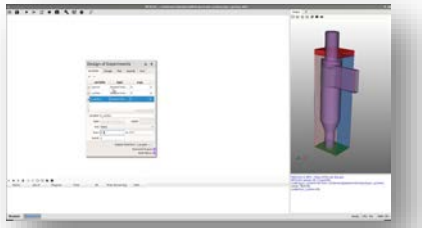


Cyclone Separator Geometry

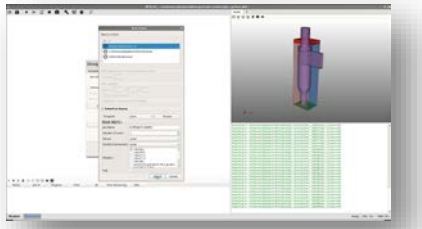
Application: Cyclone Optimization



Set up the base model with parameterized geometry

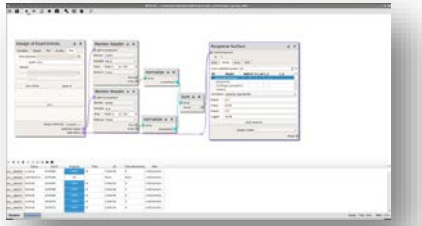


Add variables and create a design of experiments



Submit simulations to the supercomputer queue

Let the simulations run



Process the QoI, create a surrogate, and optimize

Original *vs* Optimal

MFiX Suite with Optimization Toolset

Applications underway and in the near future

Design and Optimization of Modular Gasification System Devices

- Novel gasifier designs

Pilot and Industrial Fluidized Bed Combustion Systems for Existing Power Plants

- Study fluidized bed combustion from lab-to-plant scales
- Study impact of varying operating conditions on combustor performance
- Collaboration with industrial partners

CO_2 Sorbent Tests

- Use data from fixed-bed lab scale tests optimize adsorption kinetic parameters
- Apply results to full-scale rig and validate
- Optimize rig performance for specific operating conditions and validate with Lab tests

CRADA with Sotacarbo

- Laboratory-scale gasifier data is available – biomass and coal – for kinetics
- Pilot-scale fluid bed gasifier is undergoing shakedown – data will be available to NETL

Summary

Simulation-based Reactor Design and Optimization

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The MFiX Suite of Multiphase Computational Fluid Dynamics Software for Predicting Reactor Performance continues to advance

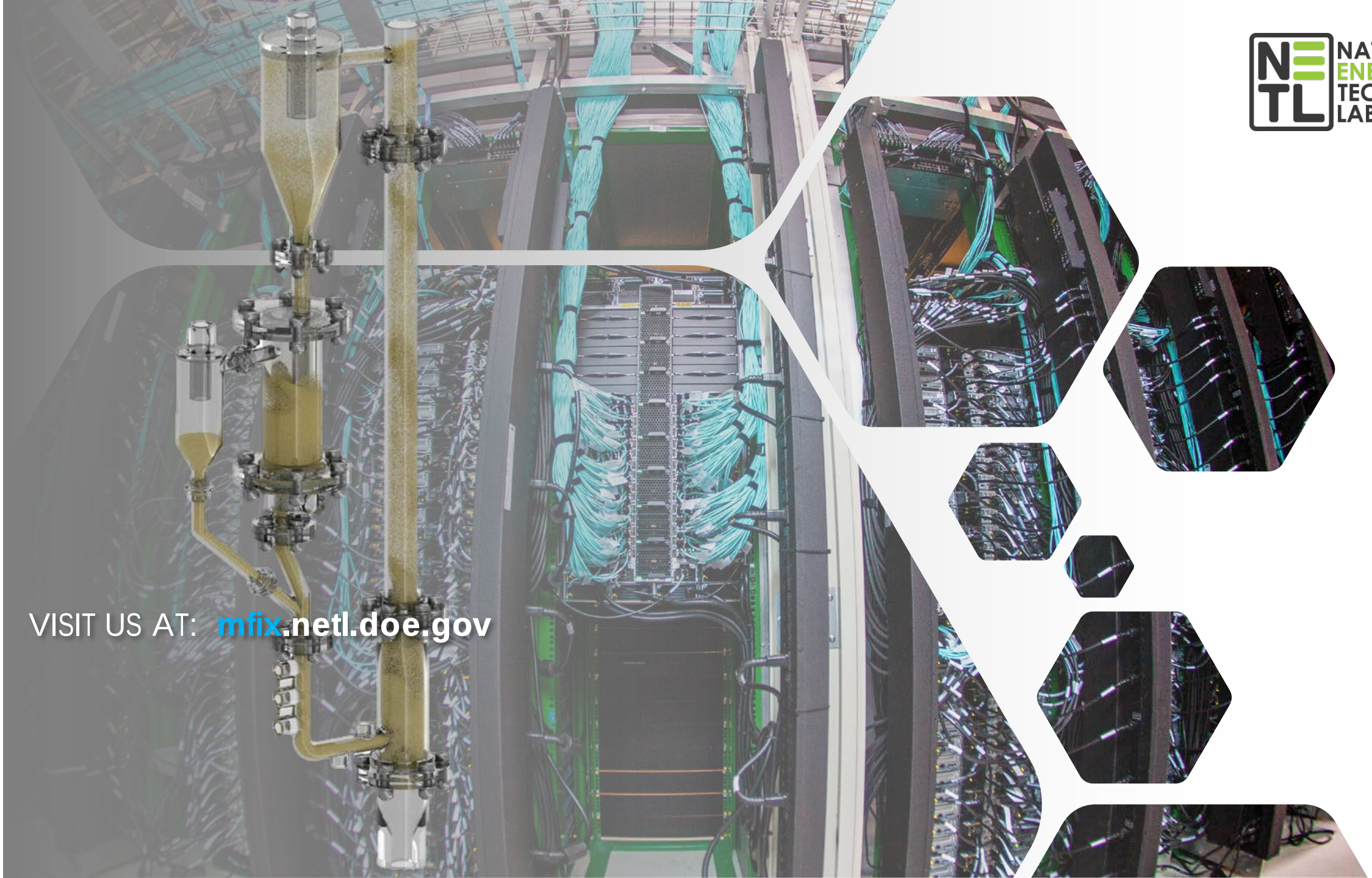
- Software for simulating reactor performance at various scales allowing optimal speed and accuracy

Simulation-based optimization tools have been developed for use with MFiX in a supercomputing environment

- Tools are designed for device-scale reactor optimization
- Fully integrated with MFiX and helps to guide and manage the process

Activities underway to validate and apply these tools to complex reactor configurations

- Gasifiers, pyrolyzers, chemical looping, carbon capture technologies



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