NETL Multiphase Flow Research Overview

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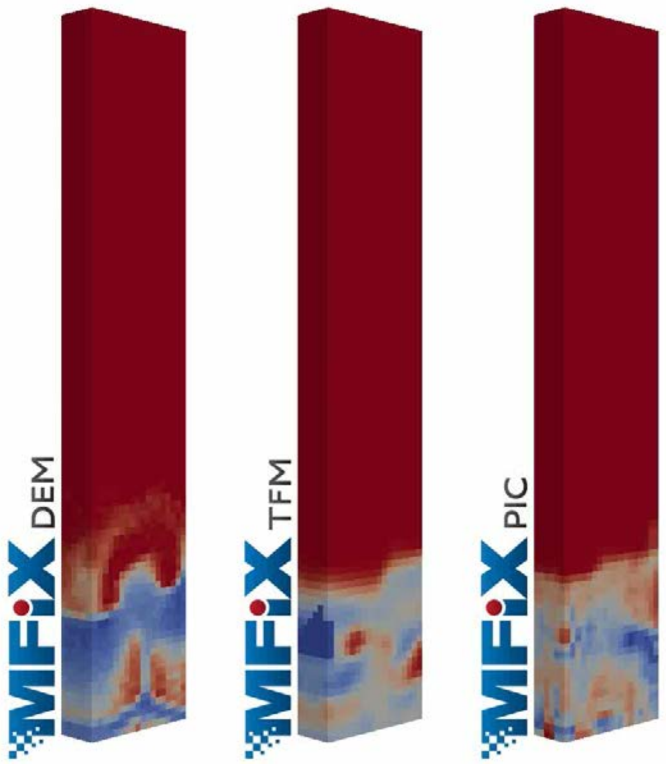
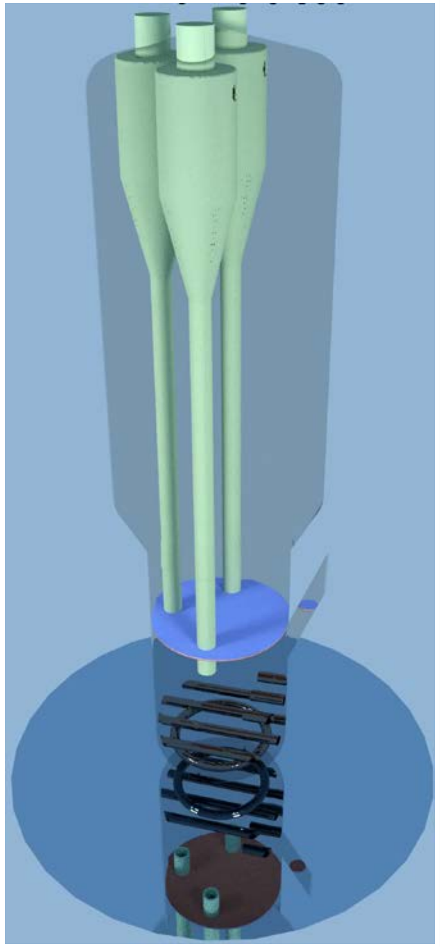
8 August 2017



MFS NETL Multiphase Flow Science
Home of the MFiX Software Suite.



Integrated Waste Treatment Unit

Simulations help to guide performance improvement of existing reactors

Idaho Cleanup Project

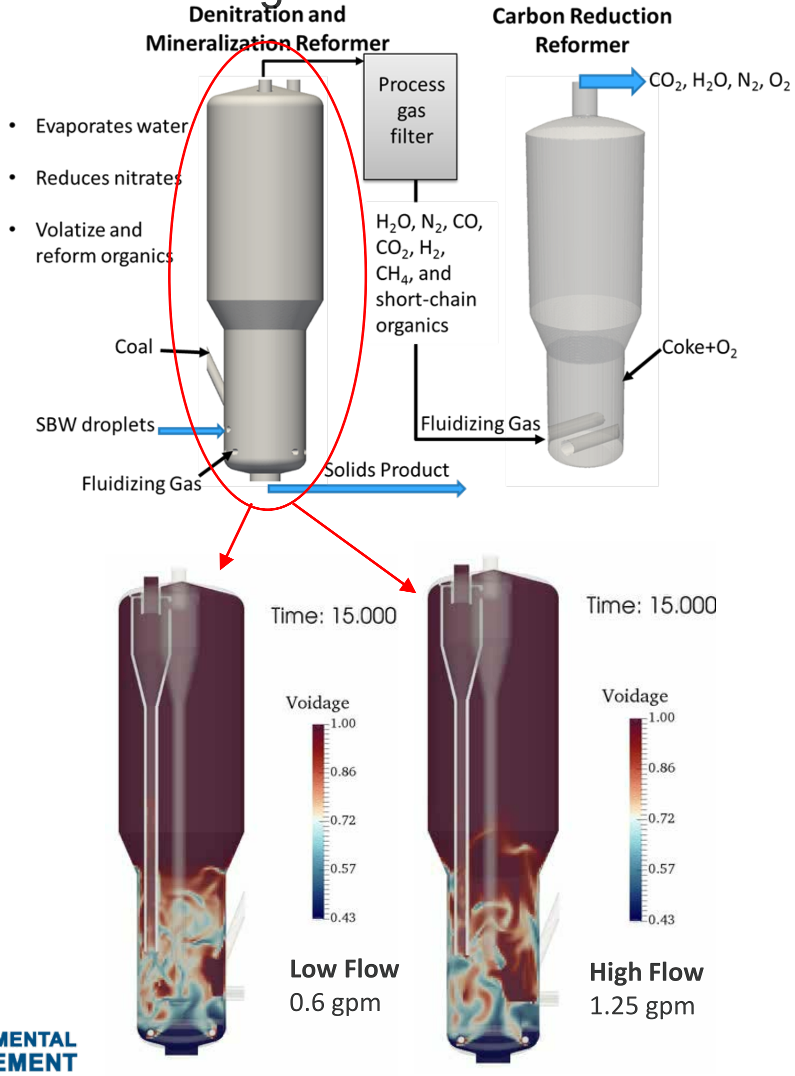
- Treat 900,000 gal of sodium bearing waste (SBW)
- "Lower" level nuclear waste from reprocessing spent nuclear fuel: ~5% Solids, ~95% Liquid
- Convert aqueous SBW to a solid granular product that can be transported and stored at long term facilities

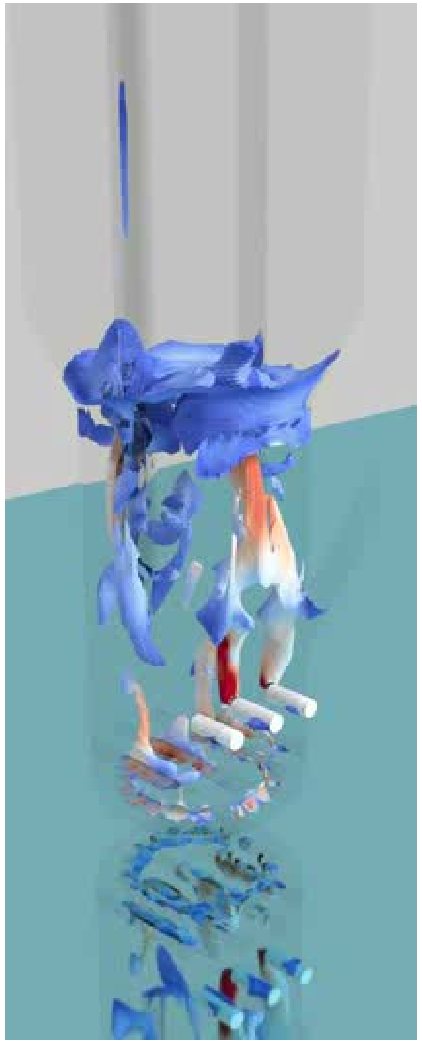
Challenge

Small-scale (1/10th) system successfully demonstrated; but challenges remain for large-scale system

Hydrodynamic Behavior of DMR

- Waste feed nozzles cause channels to form, causing gas bypassing and reduced residence time of SBW droplets
- Bed is not homogeneously mixed





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MECS based carbon capture

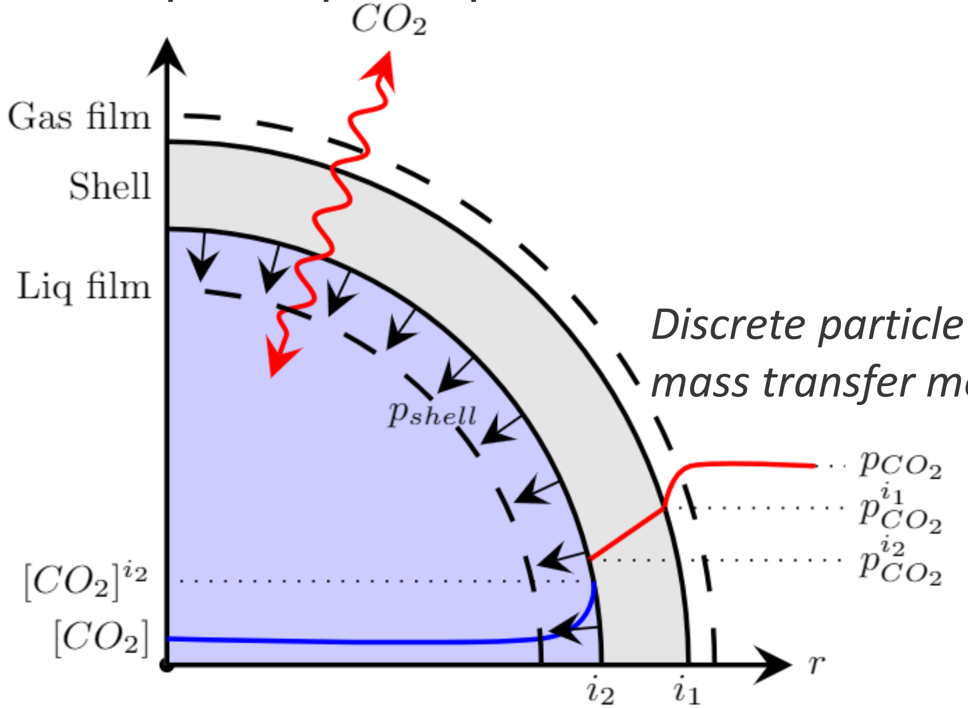
MECS capsules (Image: John Vericella, LLNL)

- New Micro-Encapsulated Carbon Sorbent (MECS) technology[1] **combines benefits** of solvent and sorbent based CO_2 capture.

[1]Vericella et al., Nature Comms, v. 6, 2015

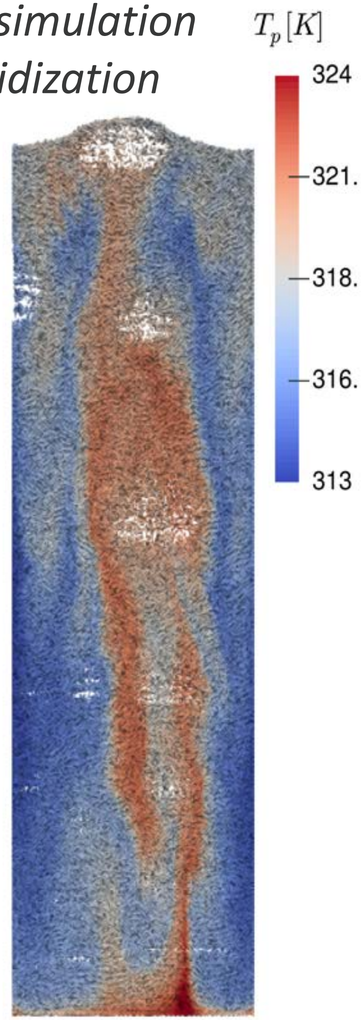
MECS Modeling considerations:

- Elastic, deformable shell
- Capsule size/density changes
- Precipitation of solids inside capsule
- Water loss/uptake during CO_2 capture
- Complex liquid equilibrium reactions



Discrete particle mass transfer model

MFIX-DEM simulation of MECS fluidization



Biofuels reactor

Develop upgrading reactor models to help pilot-scale testing and scale up

In FY17 NETL joined the Consortium for Computational Physics and Chemistry (CCPC), a research collaboration of national laboratories for the U.S. DOE Bioenergy Technologies Office.

CCPC's goal is to utilize core computational capabilities across the U.S. DOE national laboratory system to enable and accelerate the development of new materials and optimize process scale-up to advance the bioenergy economy.

http://cpcbiomass.org/

CCPC

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy
BIOENERGY TECHNOLOGIES OFFICE

Biomass Pyrolysis Vapor Upgrading

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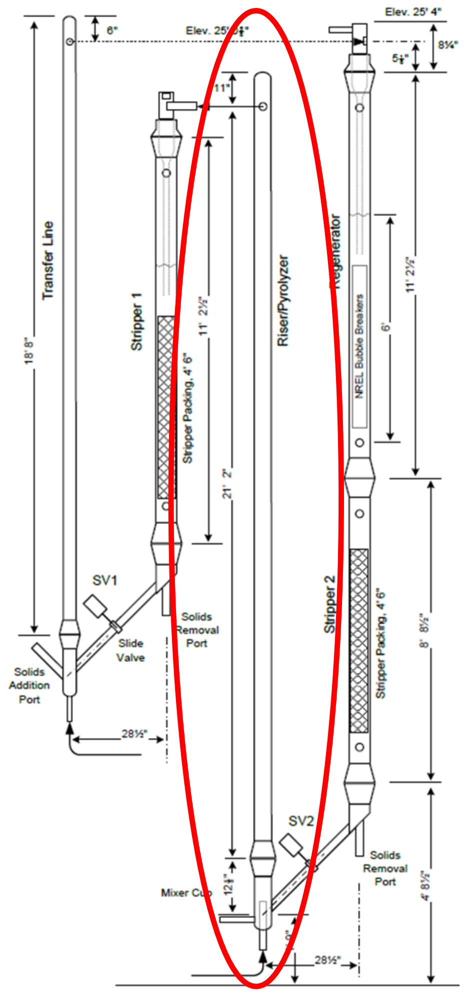
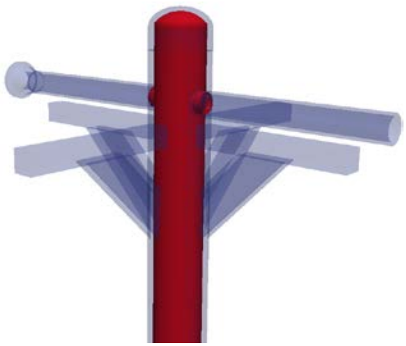
Model the NREL TCPDU Riser



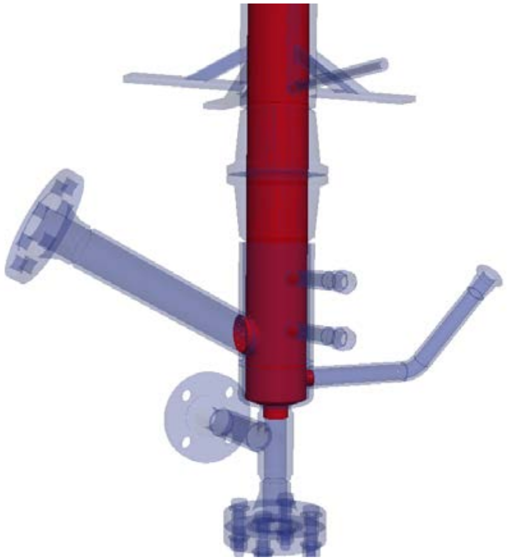
Upgrading Process

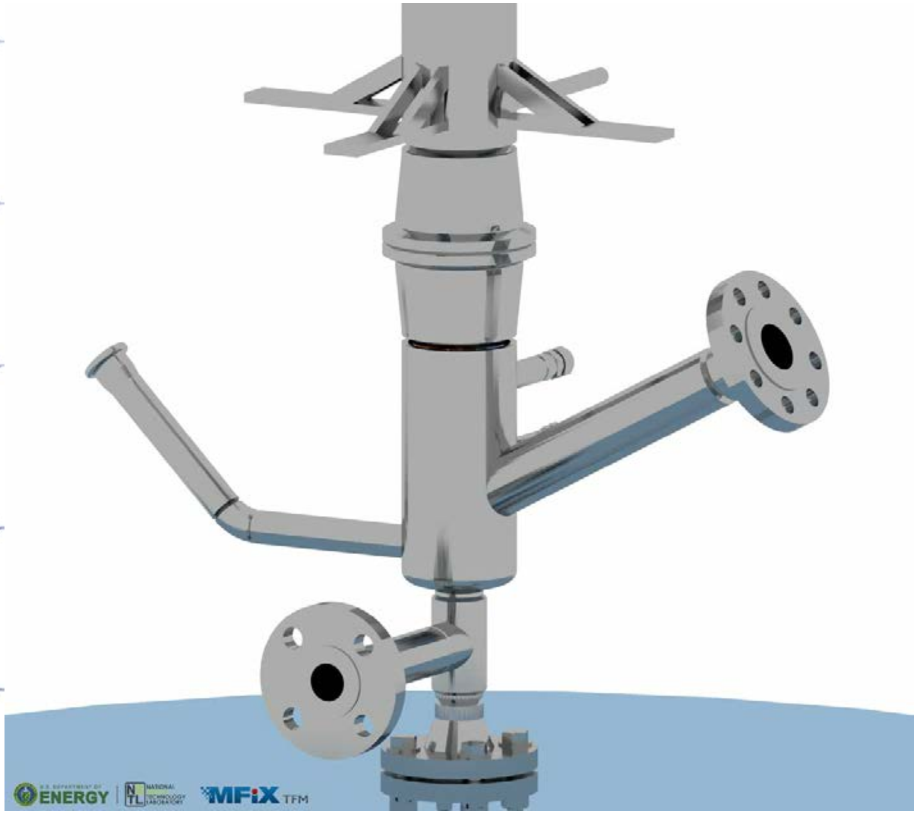
Riser Geometry

- Riser: Height: 7.05 m, diameter: 0.092 m
- Outlet diameter: 0.038 m
- Solids inlet diameter: 0.049 m
- Pyrolysis vapor inlet diameter: 0.047 m
- Distributor: 16 holes with diameter of 0.00625 m



Computational Domain

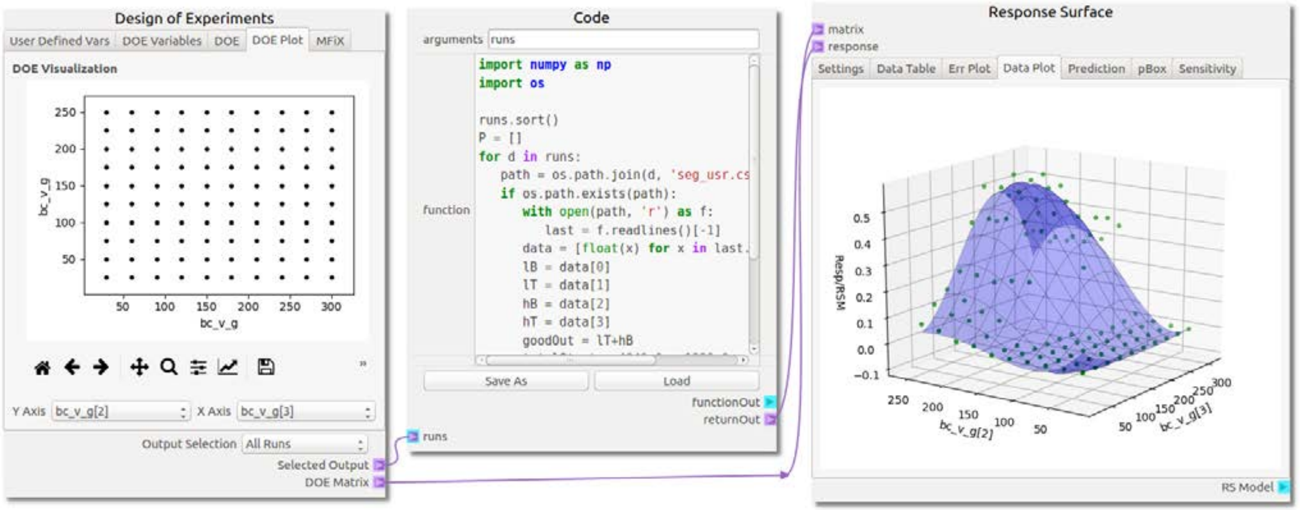




Reactor Design and Optimization

Multiphase CFD simulation-based tools for optimization

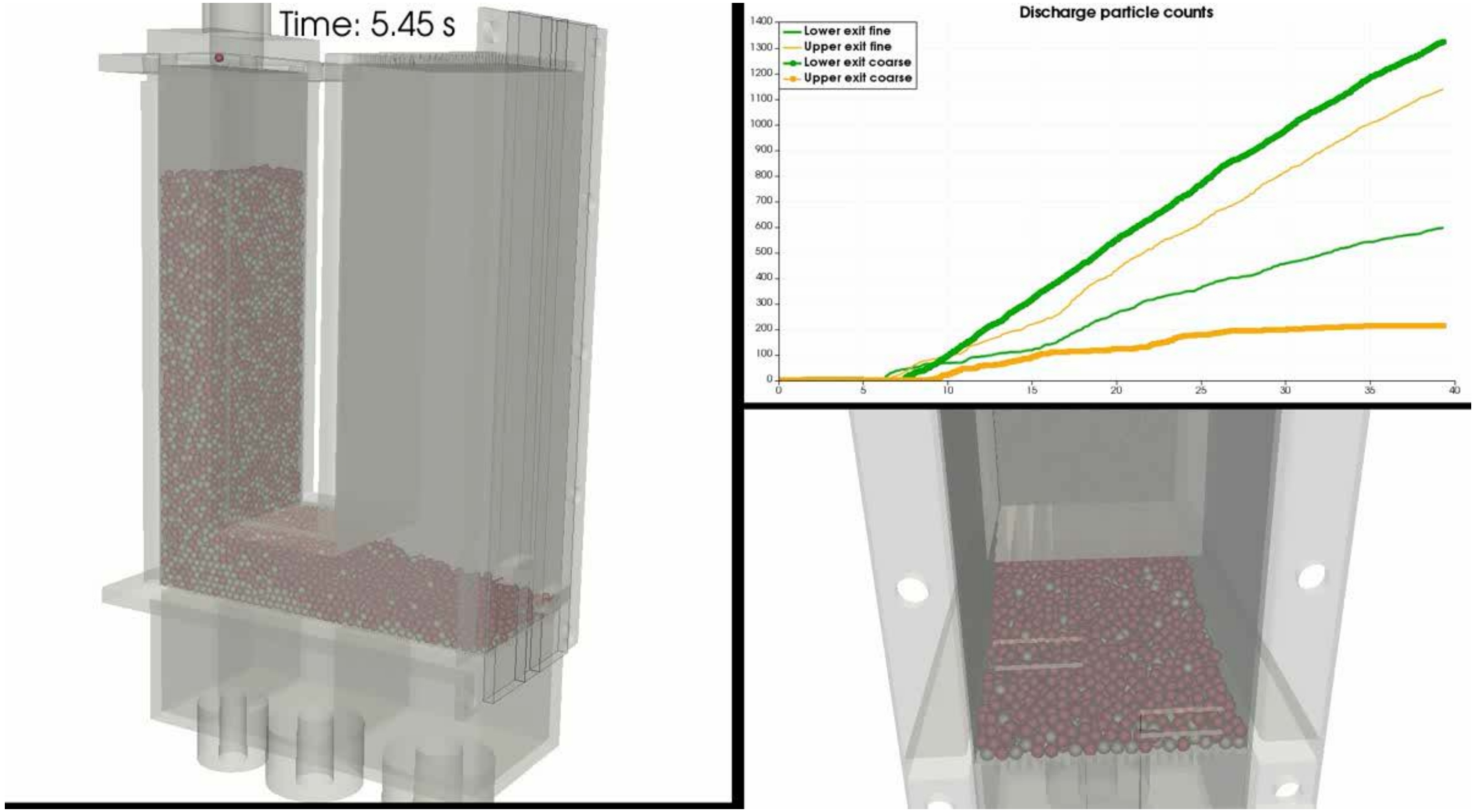
- Novel reactor designs will require understanding and control of reacting multiphase flows
- The ability to accurately simulate reacting multiphase flow is needed for optimal design and operation
- We are developing an *Optimization Toolset* based on multiphase Computational Fluid Dynamics (CFD)
    - Uses the NETL MFiX Suite of multiphase CFD software for predicting reactor performance
    - Demonstrate and validate optimal designs



Build a Design Matrix → Run MFIX → Create response surface and Optimize

Optimization Toolset

Optimized Flow for Separation – Model and Experiment



MFiX 17.1Release

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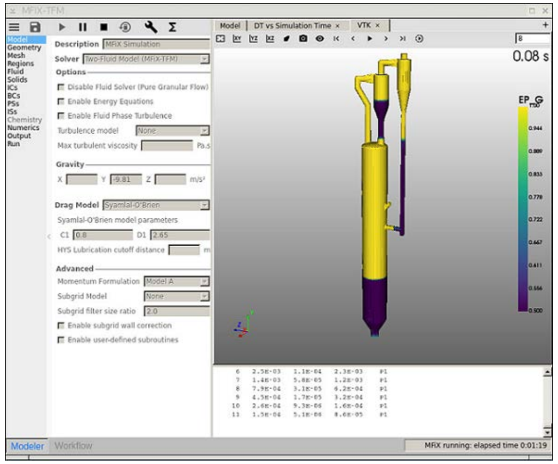
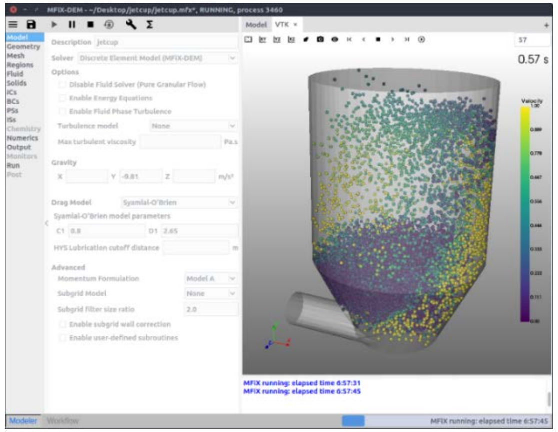
- 17.1 Release (July 2017), focus on usability
  - GUI completely redesigned
  - Works on Linux, macOS, Windows (same look and feel)
  - Setup, run, and visualize simulations
  - Build custom solver from GUI
  - Interact with solver (pause/modify setting/resume)
  - Submit jobs to queue system
- Special demo session on Thursday morning



TFM simulation



DEM simulation

What is the Exascale Computing Project (ECP)?

- As part of the National Strategic Computing Initiative, ECP was established to accelerate delivery of a capable exascale computing system that integrates hardware and software capability to deliver approximately 50 times more performance than today's 20-petaflops machines on mission critical applications.
  - DOE is a lead agency within NSCI, along with DoD and NSF
  - Deployment agencies: NASA, FBI, NIH, DHS, NOAA
- ECP's work encompasses
  - applications,
  - system software,
  - hardware technologies and architectures, and
  - workforce development to meet scientific and national security mission needs.

What is a capable exascale computing system?

- Delivers 50× the performance of today's 20 PF systems, supporting applications that deliver high-fidelity solutions in less time and address problems of greater complexity
- Operates in a power envelope of 20–30 MW
- Is sufficiently resilient (perceived fault rate: ≤1/week)
- Includes a software stack that supports a broad spectrum of applications and workloads

This ecosystem will be developed using a co-design approach to deliver new software, applications, platforms, and computational science capabilities at heretofore unseen scale

MFIX-Exa challenge problem

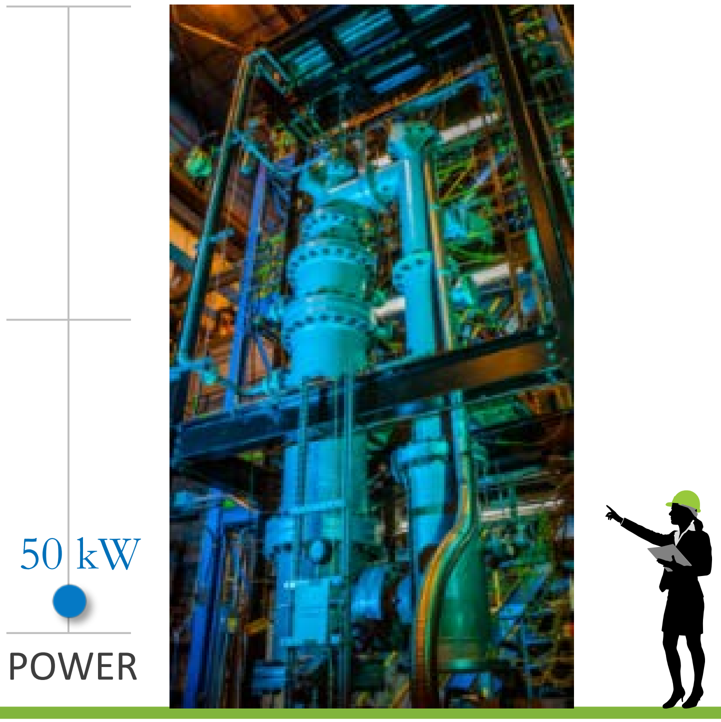
Simulate 1 MWe chemical looping reactor with CFD-DEM

2017

Particle Count: 60 x10^6

Time to Solution: 600 days

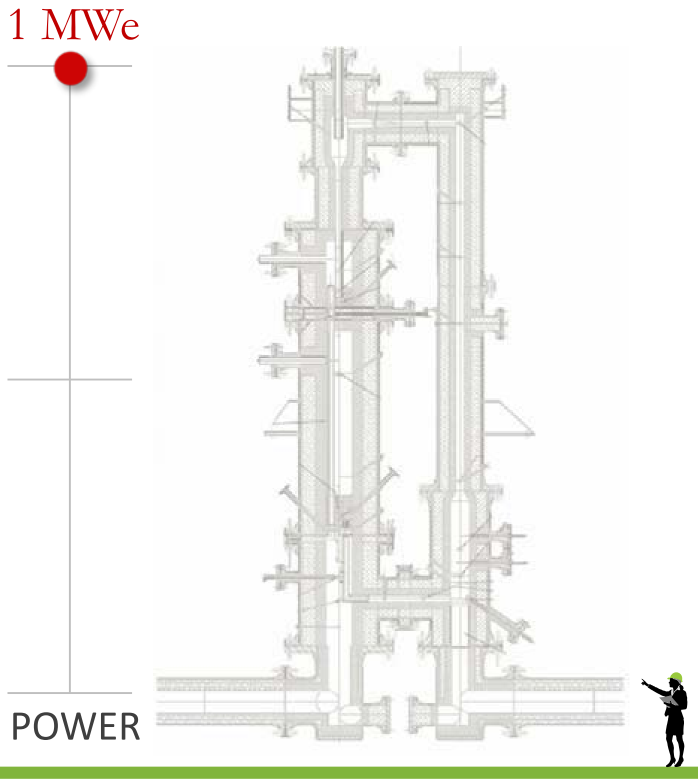
2023



Particle Count: 5 x10^9

Time to Solution: 0.5 days

2026



Particle Count: 100 x 10^9

Time to Solution: 2 days

Time-to-solution is estimated for 5 minutes of real time in all cases; the 2023/2026 values are guestimates.

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BERKELEY LAB

Boulder

MFiX Exa

ECP EXASCALE COMPUTING PROJECT

Thank You!


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Gas tracer
Solids tracer
X_{PV}
5.0e-02
2.0e-02
1.0e-02
2.0e-05
X_{CAT}
0.05
0.0200
0.0100
0.0050
0.0010
0.0005
ϵ_g
1.00
0.85
0.70
0.55
0.40
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