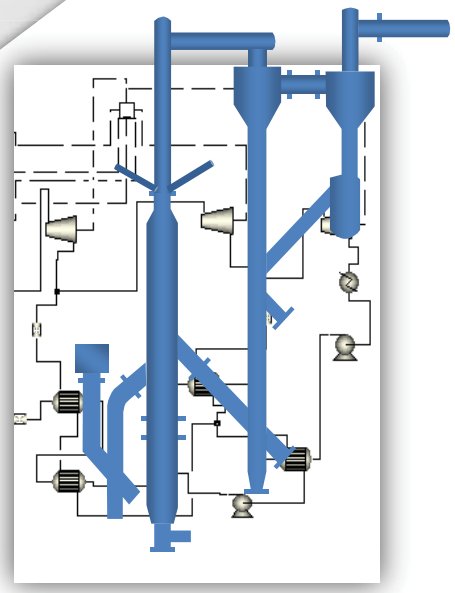
Welcome
to the
Simulation-Based Engineering Lab

Enable reaching larger scales, earlier

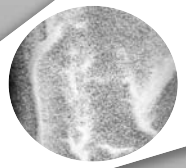


Reduce the time for design & troubleshooting

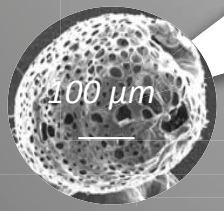
Designing 285 MW_e Commercial-Scale Gasifiers

13 MW_{th} gasifier at Power Systems Development Facility

Accelerate materials discovery



Gas-solids hydrodynamics

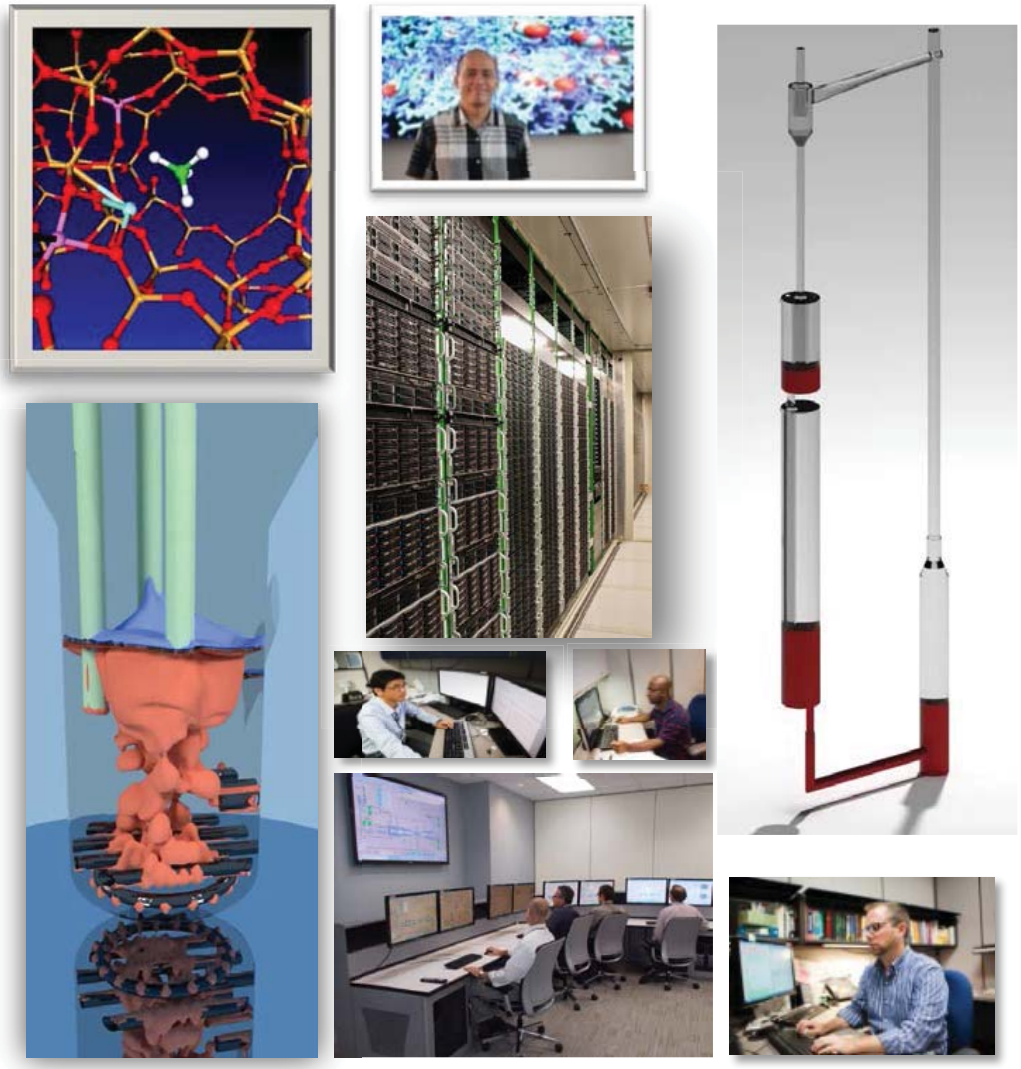


Coal gasification in syngas environment

Computational Science and Engineering

Science-based simulations for accelerating technology development

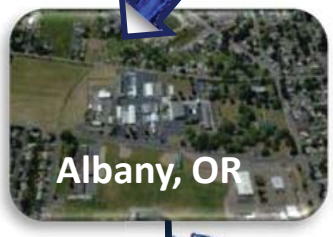
- **Atomistic Scale** develop and screen new materials; e.g., catalysts, sorbents, and high-entropy alloys.
- **Computational Multiphase Flow** design and troubleshoot devices; e.g., gasifiers, CO_2 capture devices, and chemical looping reactors.
- **Process Systems Engineering** develop innovative process systems through computational process synthesis and design, optimization, and process integration.
- **Multi-scale Simulation** link models across length and time scales, to conduct simulations of greater fidelity.

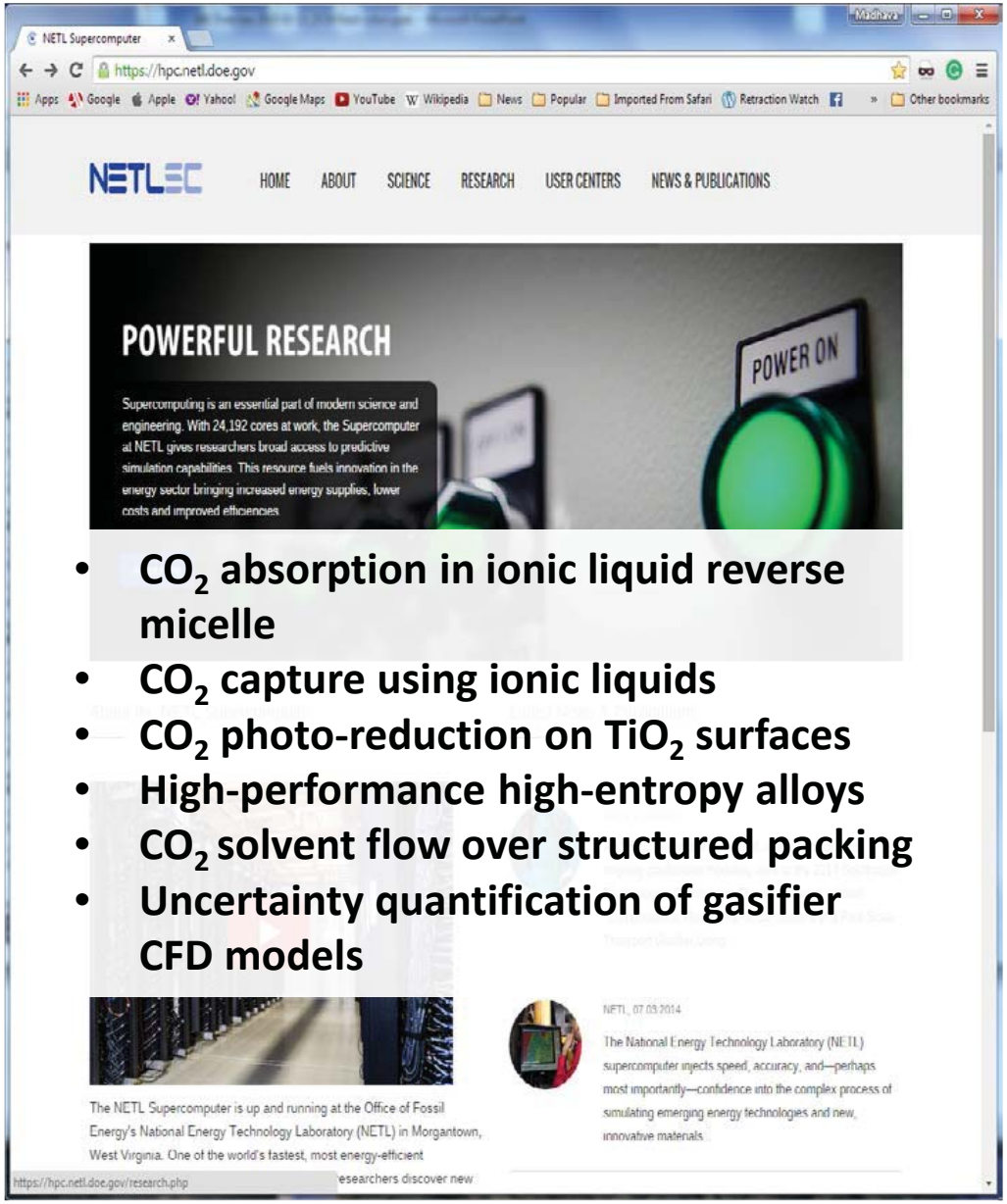


Science-based simulations powered by High Performance Computing

Supercomputer and visualization centers

503 Tflops; 26,000 Processor Cores
120th fastest supercomputer in the world





- CO_2 absorption in ionic liquid reverse micelle
- CO_2 capture using ionic liquids
- CO_2 photo-reduction on TiO_2 surfaces
- High-performance high-entropy alloys
- CO_2 solvent flow over structured packing
- Uncertainty quantification of gasifier CFD models

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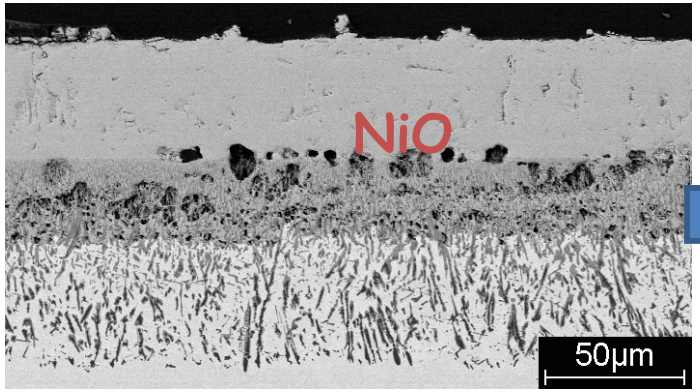
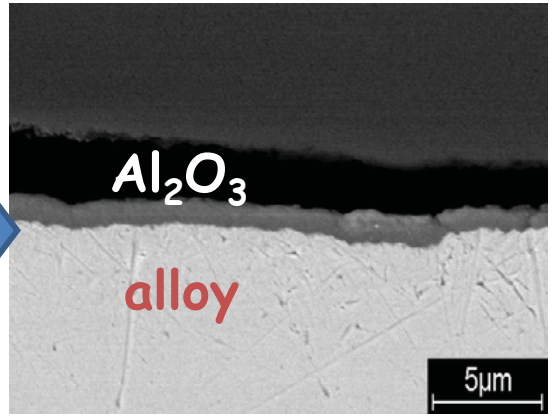
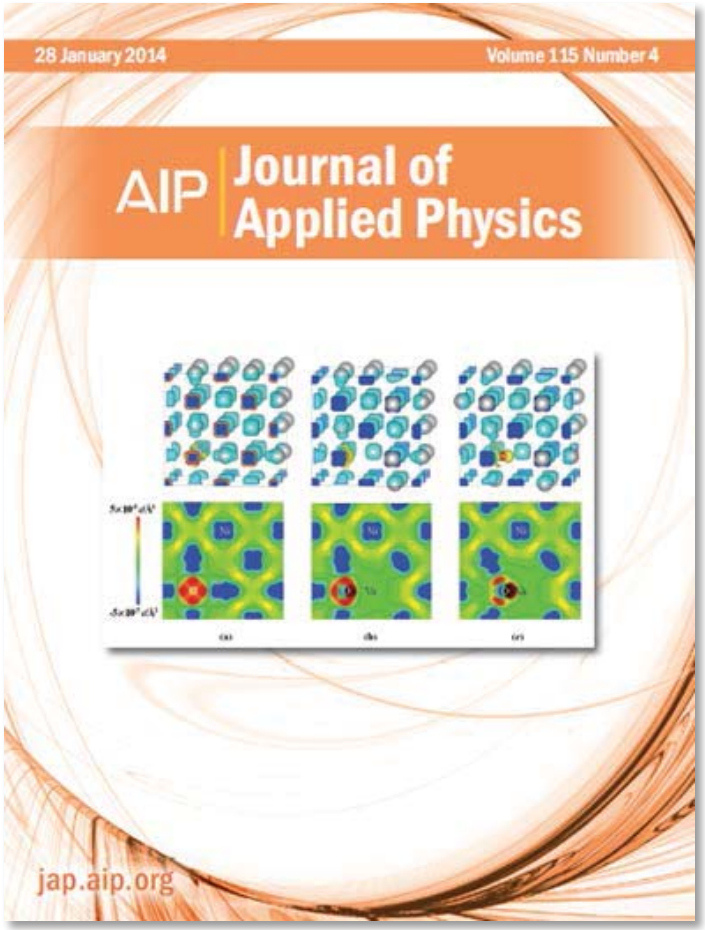
https://hpc.netl.doe.gov

New tool for predicting transport properties in alloys





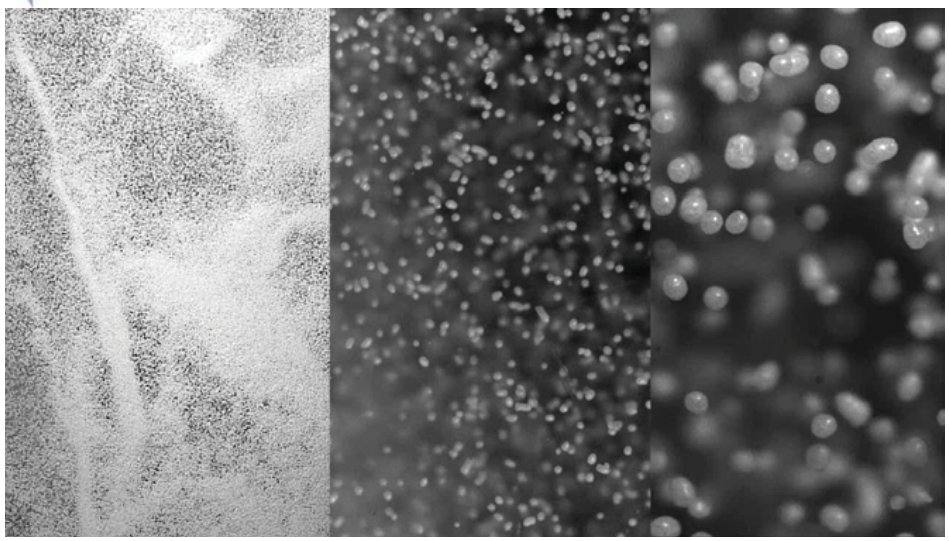


Developed a new multi-scale tool based on density functional theory and kinetic Monte Carlo

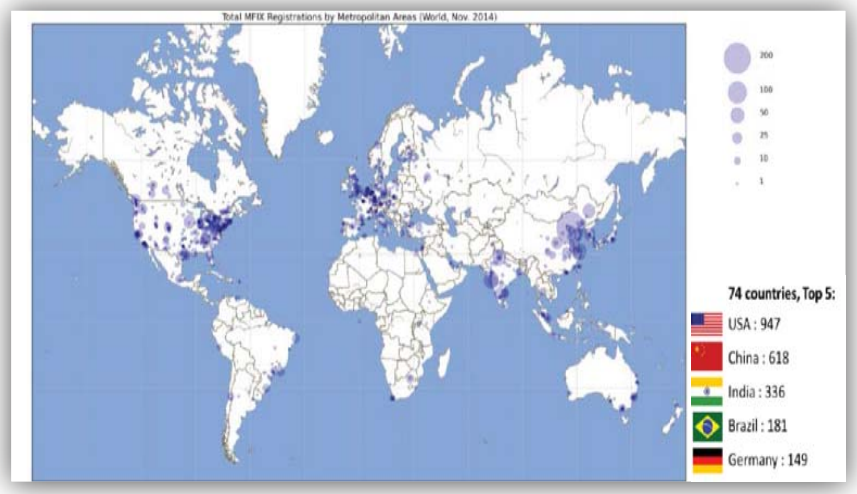
Predicted oxygen diffusivity in nickel used in Wagner model to design oxidation resistant alloys

Alfonso et al. *J. Appl. Phys.* 115, 043501 (2014)

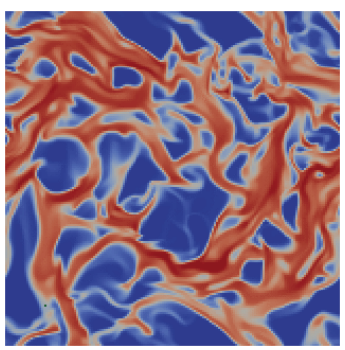
Impact on world-wide R&D in gas-solids flow

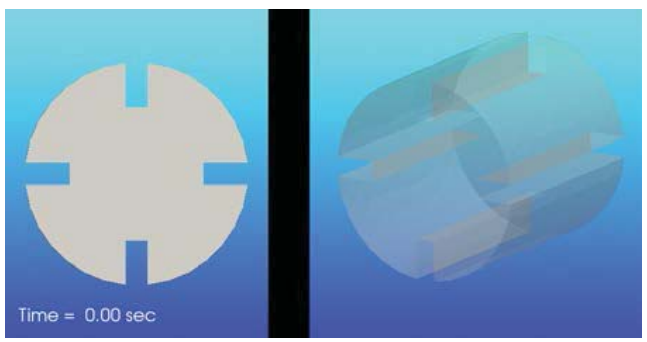


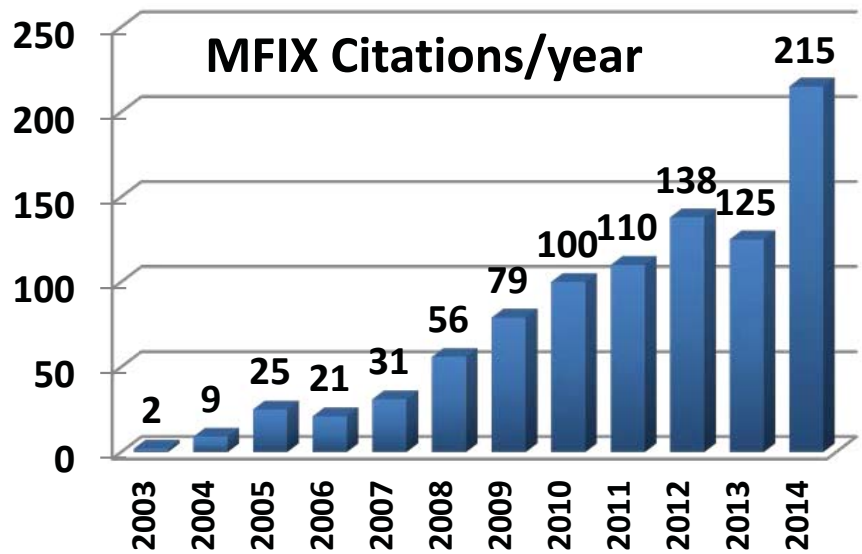
3500+ registered users world-wide



Open-source software

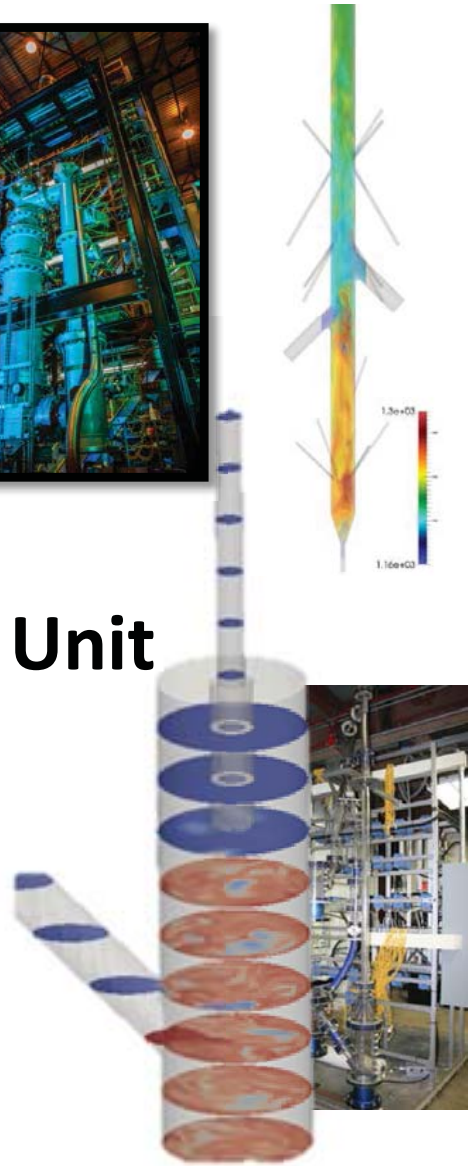


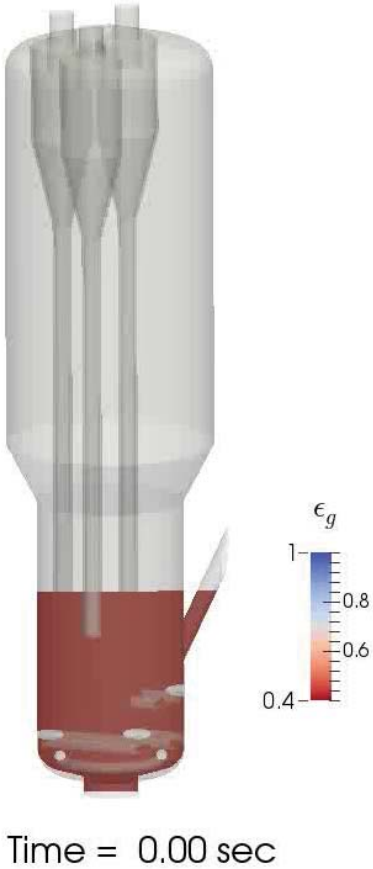




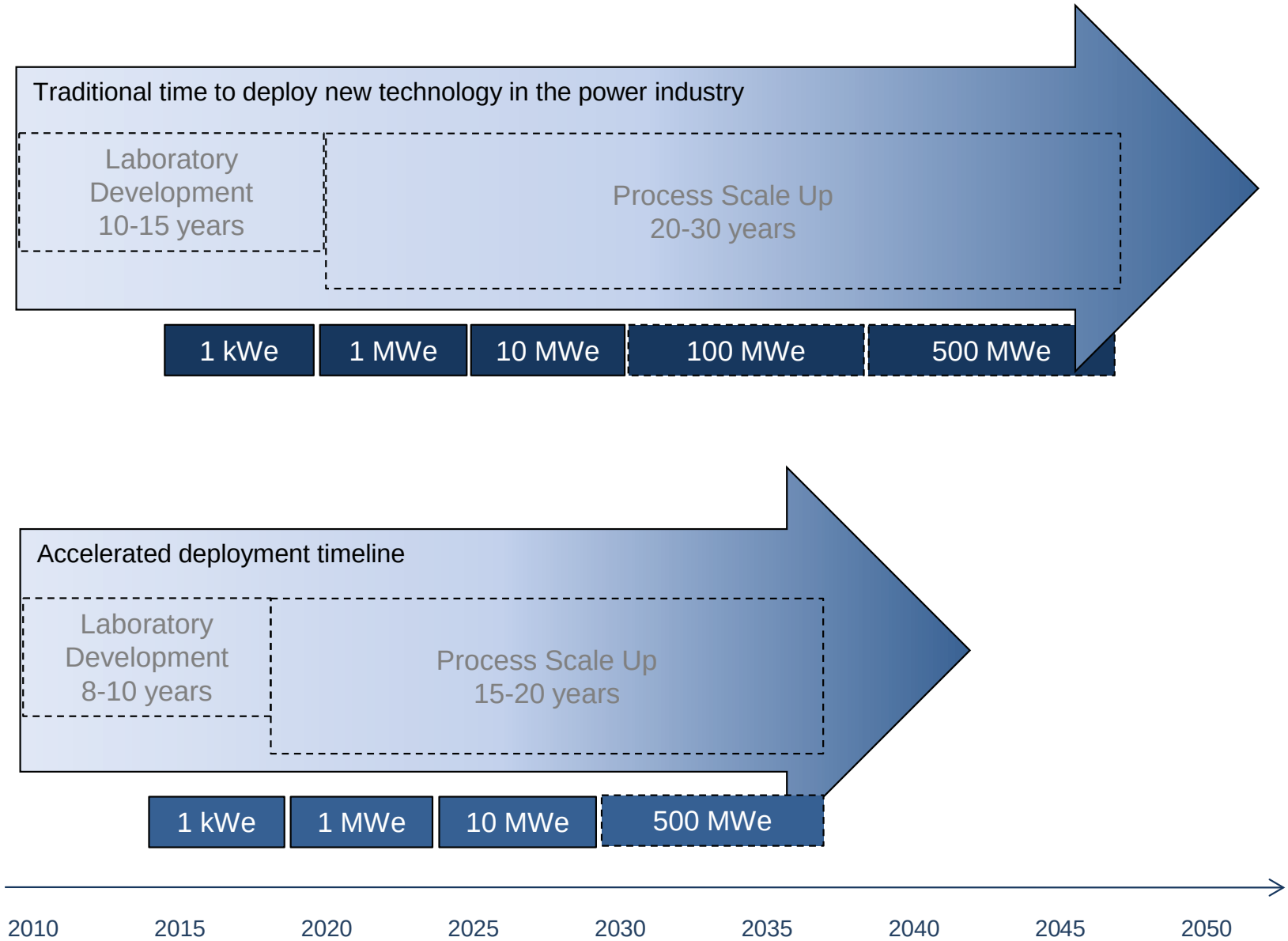
MFiX applications at NETL

- Gasifiers
- CO_2 capture reactors
- Chemical looping reactor
- Coal pulverization
- Integrated Waste Treatment Unit
- Foamed cement



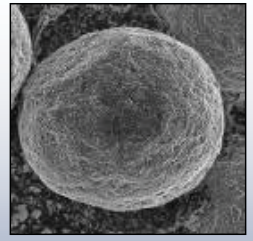
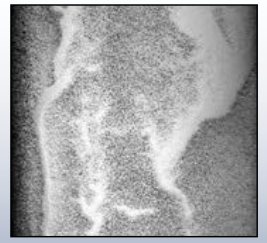
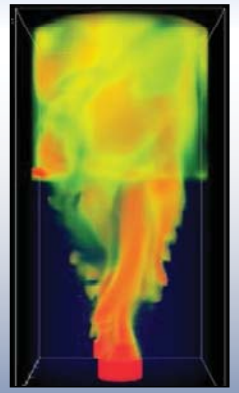


Challenge: Accelerate Development/Scale Up



CCSI A Partnership to Accelerate Technology Development

Carbon Capture Simulation Initiative

Rapidly synthesize optimized processes to identify promising concepts → Better understand internal behavior to reduce time for troubleshooting → Quantify sources and effects of uncertainty to guide testing & reach larger scales faster → Stabilize the cost during commercial deployment

Berkeley Lab · Pacific Northwest National Laboratory · NETL · Los Alamos National Laboratory EST. 1943 · Lawrence Livermore National Laboratory

Carnegie Mellon · West Virginia University · Princeton University · Boston University · The University of Texas at Austin

ADA · Alstom · B&W · GE · EPRI Electric Power Research Institute · PSE · Fluor · Phillips 66 · AEP American Electric Power · Southern California Edison · URS · aspentech · Chevron · ExxonMobil · ANSYS · Southern Company · Air Products · Eastman · Schneider Electric

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CCSI Impact

Carbon Capture Simulation Initiative

Statistics

3rd Generation Release Tools/Models: 30

Invited Keynotes: 7
Journal Papers: 42
Conference Papers: 78

PhD Students: 13
Postdocs:10
Undergrads: 3

10 MWe Projects

NDA

CRADA

CRADA

Current Licensees

CCSI Toolset Development

CCSI Toolset Deployment

2010 2015 2020 2025 2030 2035 2040 2045 2050

NETL at the forefront of research in simulation-based engineering

1995-2000	**Fluent, Inc. CRADA – transfer multiphase CFD methods to commercial code**
1999-2002	Multiphase Fluid Dynamics Research Consortium
2000-2003	**Linking FLUENT® and AspenPlus® for higher fidelity process simulations**
2001	MFIX released as open-source software
2002-2006	Transport gasifier modeling to support Southern Co. and KBR
2006-2015	**Modeling of the dynamic response of energetic materials to support DOD**
2009	Multiphase flow conference series started
2010, 2013	Multiphase challenge problems
2010	**Maximum oil leak rate estimation after BP Deepwater Horizon Incident**
2011-2012	Dynamic simulators and 3D immersive virtual plant – IGCC with CO_2 capture
2011	Carbon Capture Simulation Initiative (CCSI) launched
2012	Hanford nuclear waste clean up tank modeling to support DOE-EM
2013	**Non-Newtonian multiphase slurry workshop in support of DOE-EM**
2013	ADA-ES CRADA – CO_2 reactor modeling
2014	Integrated Waste Treatment Unit modeling to support DOE-EM