

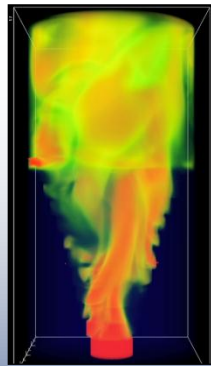
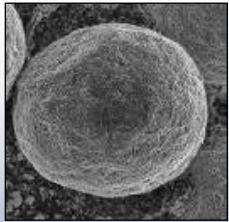
2ND ANNUAL **ENERGY** & **INNOVATION** CONFERENCE

Simulation-Based Engineering

David C. Miller, Ph.D.

Technical Team Lead, Carbon Capture Simulation Initiative
National Energy Technology Laboratory

Multi-Scale Simulation-Based Engineering



Kinetic and
Particle Scale
Models

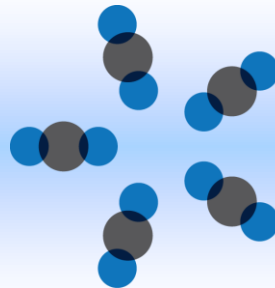
Detailed Device
Scale Simulation

Process Synthesis,
Design & Optimization

Dynamic Process
Simulation & Advanced
Control



mfix.netl.doe.gov



CCSI

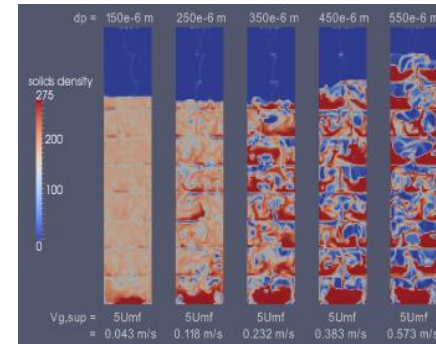
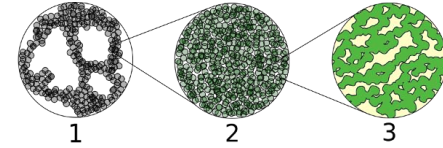
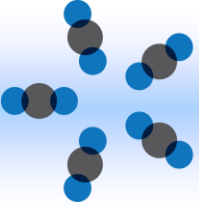
Carbon Capture Simulation Initiative

acceleratecarboncapture.org

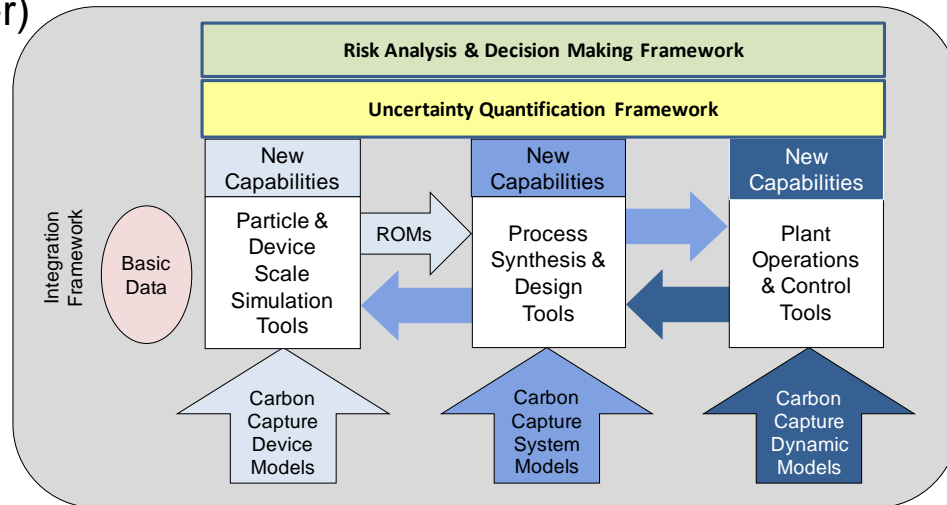
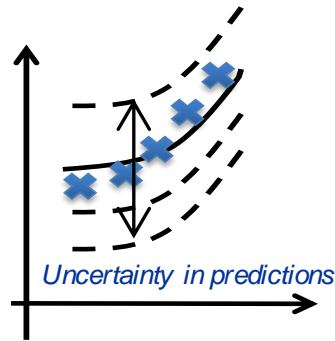
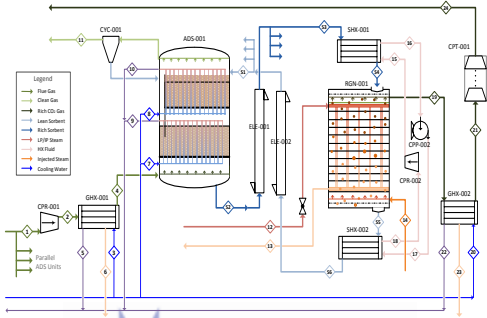


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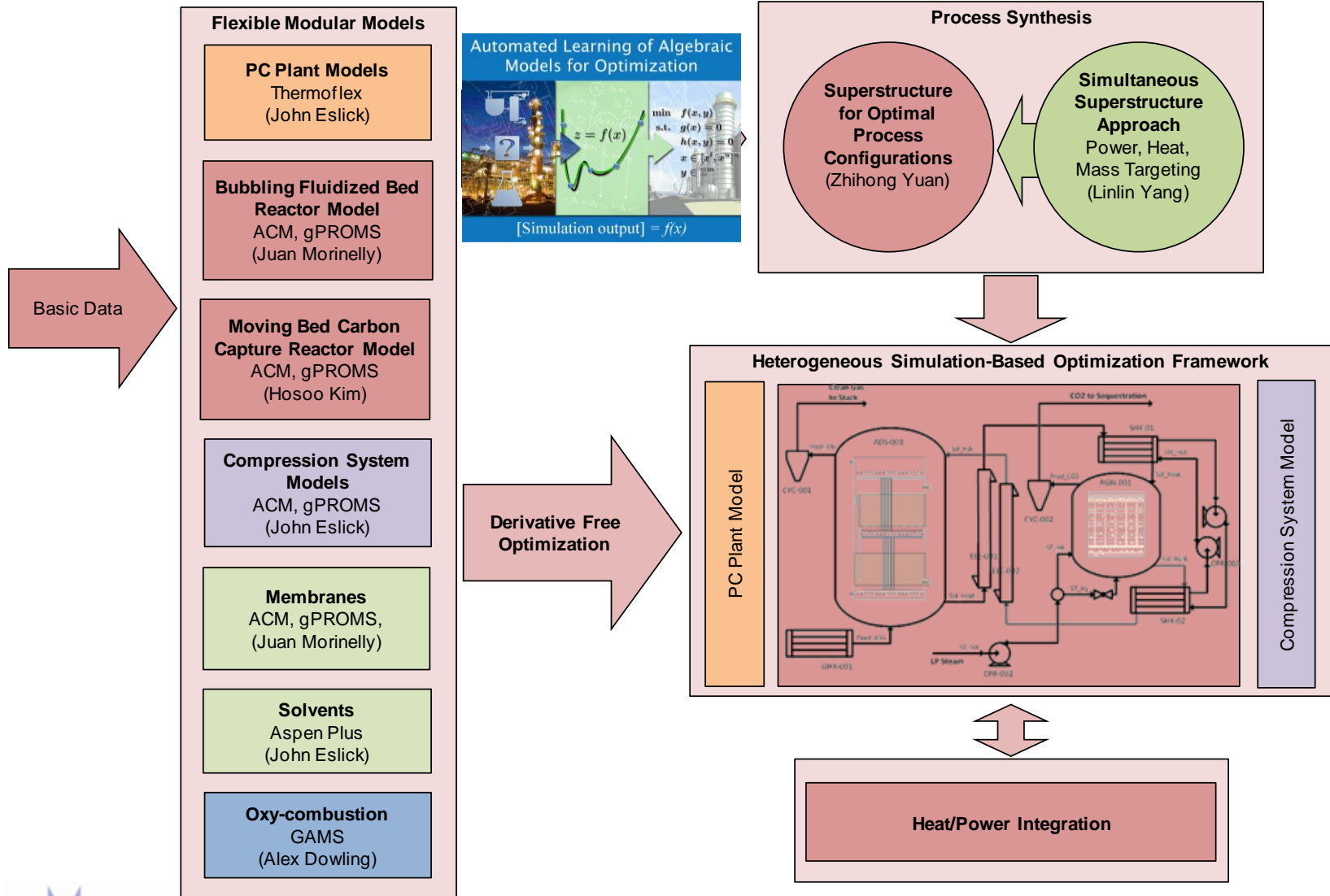
Demonstrated success in generating information beyond the reach of experiments alone, by integrating science-based models at particle, device and process scales, with verification, validation and uncertainty quantification.



- **Accelerating technology development and scale-up**
- **Initial release 1 year ahead of original schedule**
- **Over 21 Components of the CCSI Toolset available**
 - Kinetic model and fitting algorithm
 - 1 MW scale CFD adsorber & regenerator models
 - Detailed process models (solid sorbents, compression, membrane)
 - New optimization tools (ALAMO, superstructure, framework)
 - Advanced dynamic & control models (adsorber, compression)
 - Integration tools (REVEAL, Turbine, Sinter)
 - Uncertainty Quantification Framework
 - Financial Risk Tool



Process Synthesis, Design & Optimization



CFD Modeling for Gasifier Design Confirmation

Models

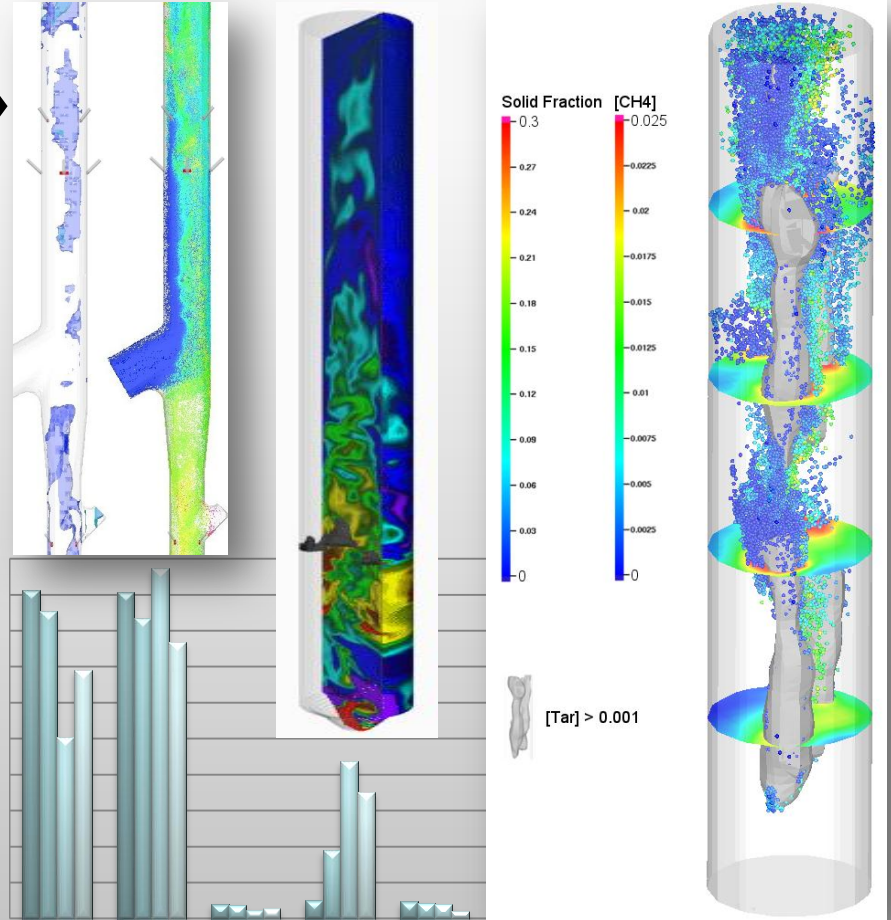


Open-source/licensed software used for creating gasifier models

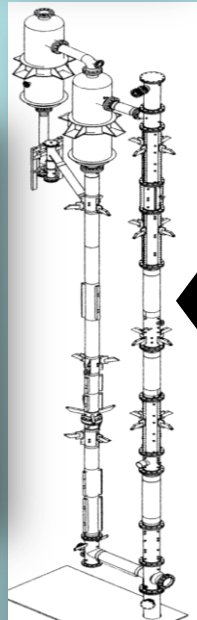
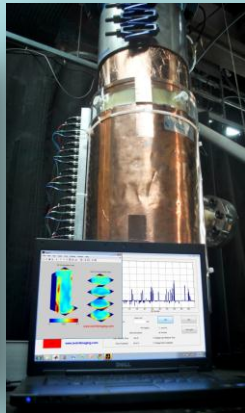
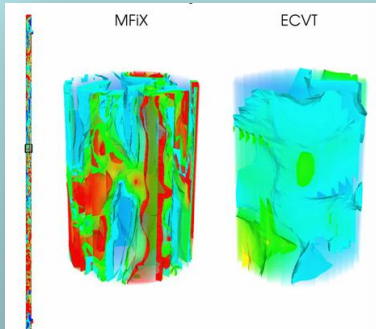
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Design Confirmation



Experiments



New physical phenomena revealed by modeling studies are investigated with experiments, yielding additional data

Validated models are being used to optimize commercial gasifier designs (e.g., KBR/Southern, APS)





Advanced Virtual Energy Simulation Training And Research

- **Key Objectives**

- **Simulation-based Technology and Tools Development**

- Develop portfolio of virtual energy plant test beds
 - High-fidelity real-time dynamic simulators
 - Full-scope operator training systems (OTSs)
 - 3D virtual immersive training systems (ITSs)

- **Collaborative Research**

- Bring together dynamic simulation/control technologies, state-of-the-art facilities, and leading energy experts
 - Conduct collaborative research on dynamics, automation, controls/sensors, real-time optimization, virtual plants, smart manufacturing, and modern grid

- **Training and Engineering**

- Train industry workforce and educate engineering students using hands-on, simulator-based experiential learning

Simulation Based Engineering User Center (SBEUC)

Starting operation in December 2012

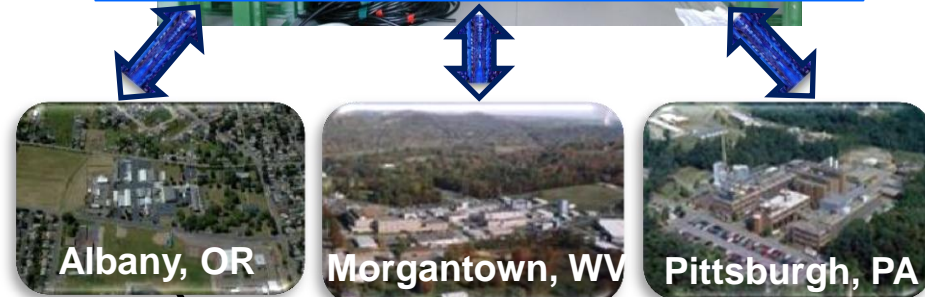


503 Tflops; 26,000 Processor Cores
22nd fastest supercomputer in the world



SBEUC interior: processor racks

Sites linked w/ high-speed connectivity & data visualization



Albany, OR



Morgantown, WV



Pittsburgh, PA



Industry Significance

- Screen alternatives faster
- Develop more optimal designs faster
- Explore design alternatives
- Understand system interactions and sensitivity
- Prioritize research and development resources
- Reduce the time for design & troubleshooting
- Quantify the uncertainty in predictions, technical risk

Partnership Opportunities

- CRADA opportunities
 - Apply computational tools to new problems of interest
 - Modify tools for application to new areas
 - Demonstrate capabilities
- CCSI Industry Advisory Board
 - Use tools and provide feedback to development team

Benefits to Partner

- Access to advanced simulation capabilities
 - Expertise to Solve Challenging Energy Problems
 - Detailed device scale modeling (internal flow and reaction)
 - Process systems engineering & optimization
 - Advanced control and dynamic simulation capabilities
 - Uncertainty quantification of simulation results
- Gain more in depth understanding of complex phenomena and systems
- Accelerate the development of new energy technologies

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