CCSI

Carbon Capture Simulation Initiative

NETL CO_2 Capture Technology Meeting

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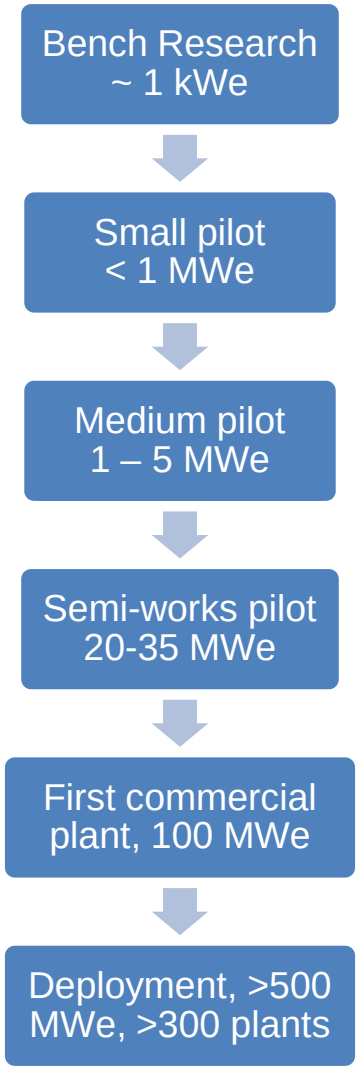
The U.S. DOE's Carbon Capture Simulation Initiative for Accelerating Commercialization of CCS Technology

- Motivation
- CCSI Toolset
- 5 Year Development Plan
- Technical Accomplishments

Carbon Capture Challenge

- The traditional pathway from discovery to commercialization of energy technologies is long, i.e., ~ 20-30 years.
- President's plan requires that barriers to the widespread, safe, and cost-effective deployment of CCS be overcome within 10 years.
- To help realize the President's objectives, new approaches are needed for taking concepts from lab to power plant, quickly, at low cost and with minimal risk.
- CCSI will accelerate the development of CCS technology, from discovery through deployment, with the help of science-based simulations .



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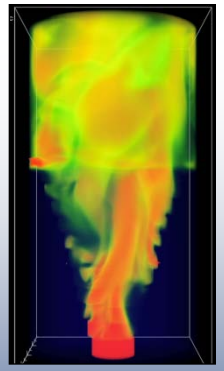
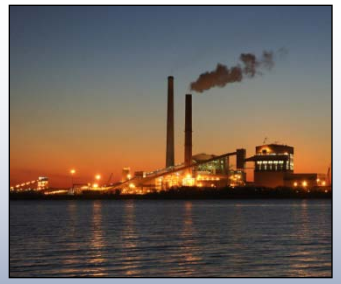




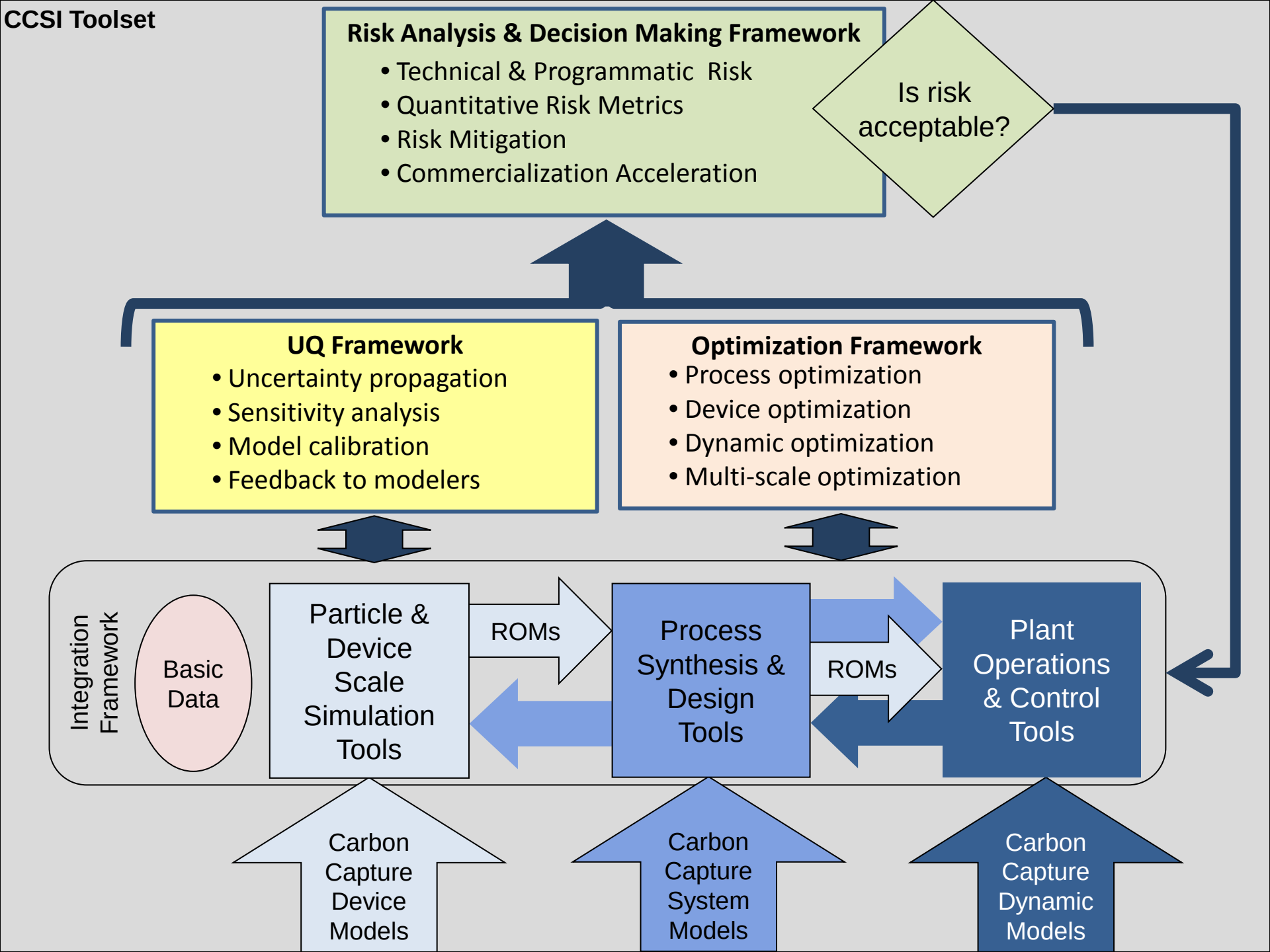
Identify promising concepts → Reduce the time for design & troubleshooting → Quantify the technical risk, to enable reaching larger scales, earlier → Stabilize the cost during commercial deployment

National Labs

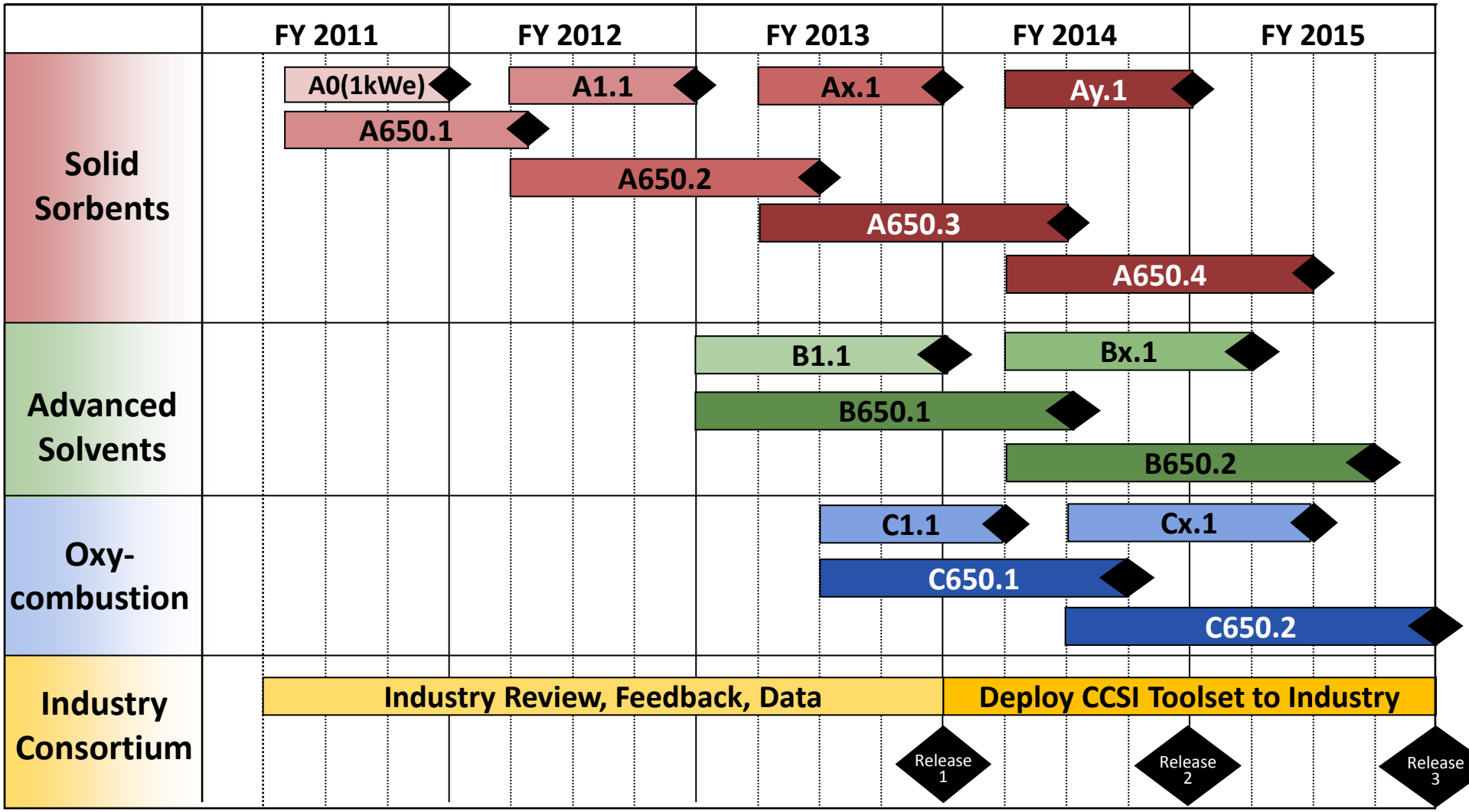
Academia

Industry

Essential for accelerating commercial deployment


CCSI Toolset
Risk Analysis & Decision Making Framework
• Technical & Programmatic Risk
• Quantitative Risk Metrics
• Risk Mitigation
• Commercialization Acceleration
Is risk acceptable?
UQ Framework
• Uncertainty propagation
• Sensitivity analysis
• Model calibration
• Feedback to modelers
Optimization Framework
• Process optimization
• Device optimization
• Dynamic optimization
• Multi-scale optimization
Integration Framework
Basic Data
Particle & Device Scale Simulation Tools
ROMs
Process Synthesis & Design Tools
ROMs
Plant Operations & Control Tools
Carbon Capture Device Models
Carbon Capture System Models
Carbon Capture Dynamic Models

5 Year Development Plan Overview



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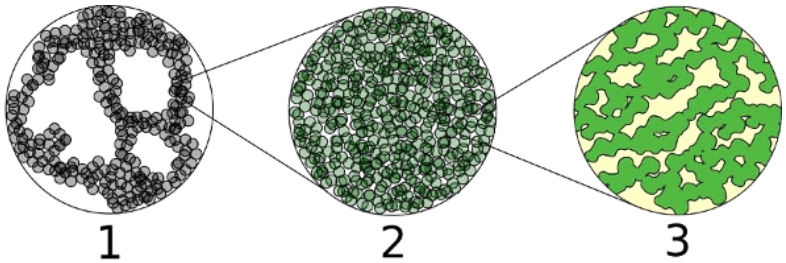
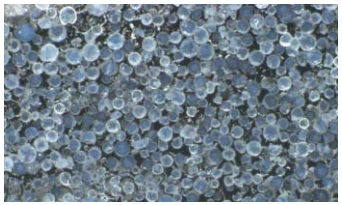
PEI-Silica Sorbent Reaction Model

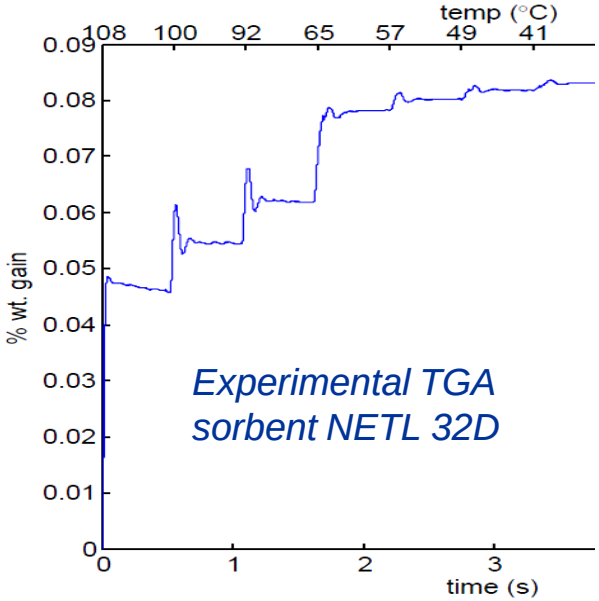
- Sorbent microstructure broken down into three length scales
- Consider gas and polymer-phase transport and surface reactions
- Accurately describes CO_2 uptake kinetics in device-scale models
- Use directly or in a reduced-order form in CFD or 1-D device models

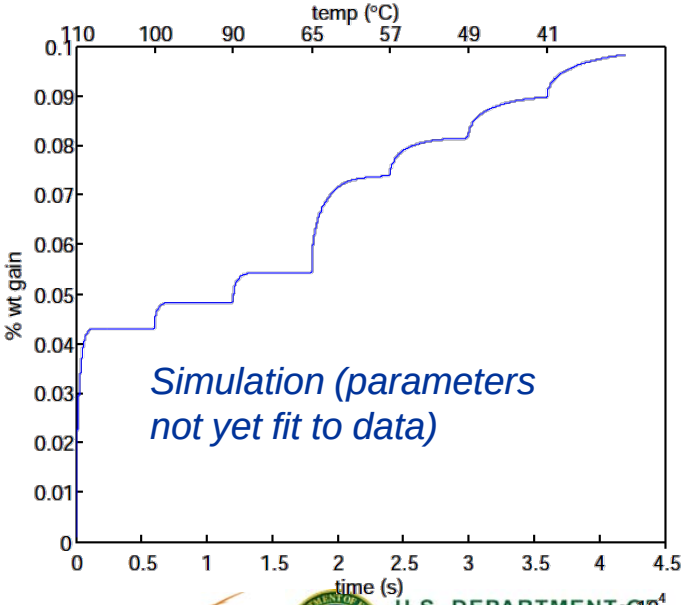




PEI on CARiACT Q10 (100 to 350 µm dia.)

D.S. Mebane, K.G. Bhat, L. Moore, J. Wendelberger, D. Fauth, M. Gray, 2011 International Pittsburgh Coal Conference, in preparation.

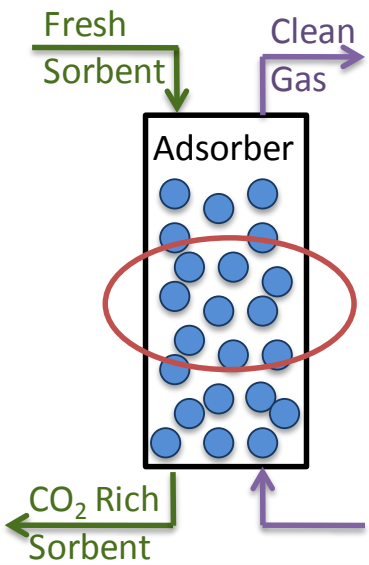


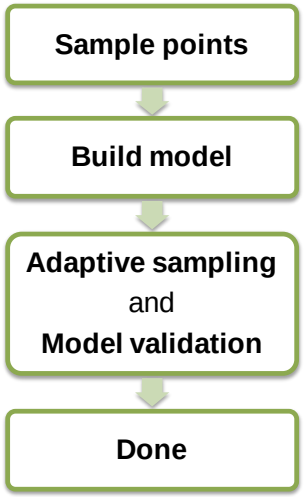


Methodology for Determining Optimal Process Configurations

- Surrogate models will be used to speed up process synthesis
- Method applied to develop surrogate model for CO_2 adsorber

Detailed adsorber model developed in Aspen Custom Modeler®

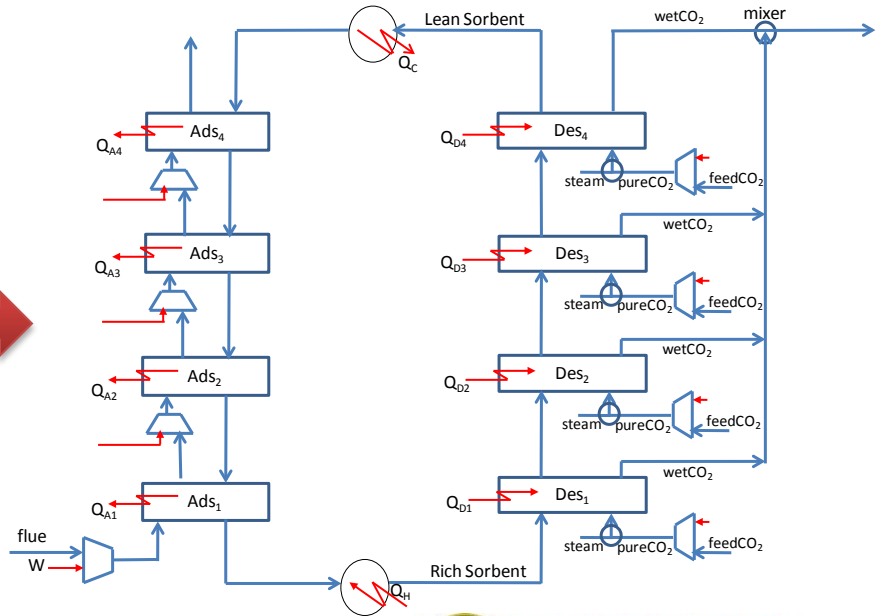




$$f(x)$$

Algebraic Surrogate Model

Superstructure to determine optimal process configuration



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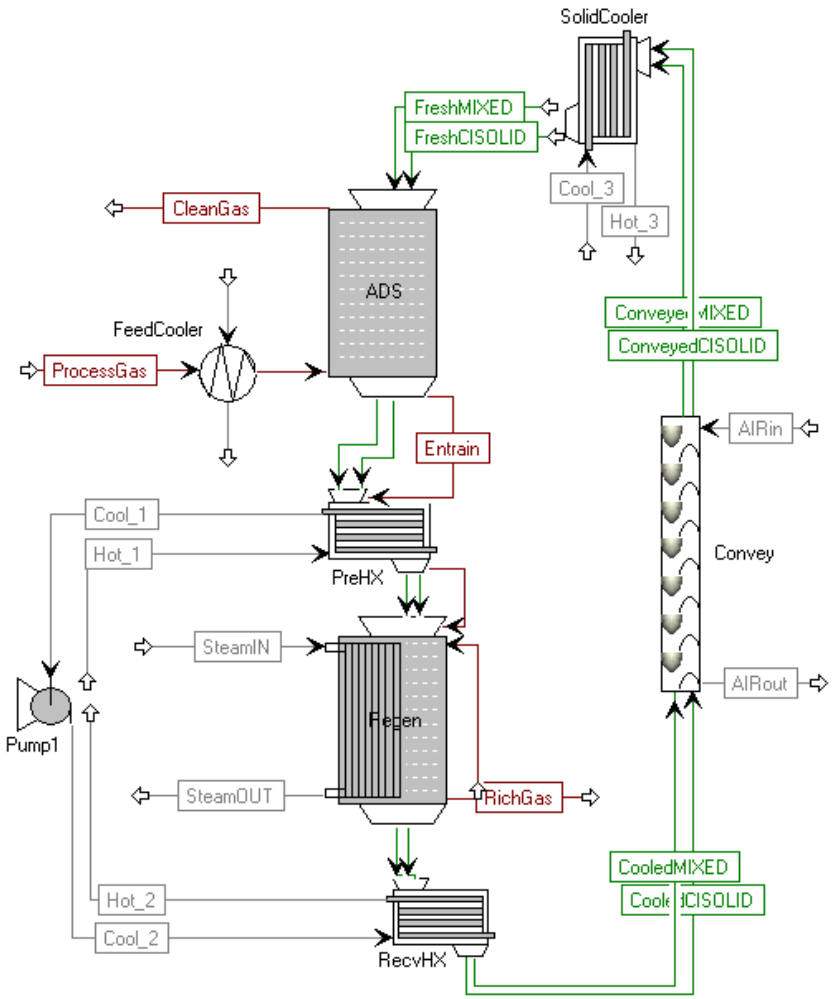
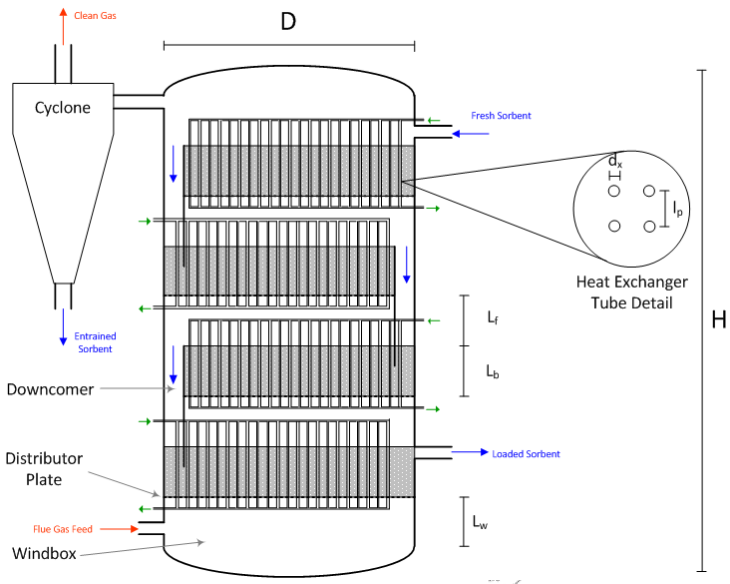
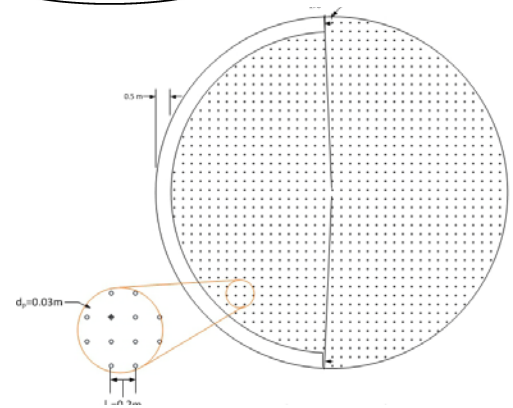
Preliminary Conceptual Process Simulations

Moving Bed-Based Solid Sorbent Capture Process Simulation



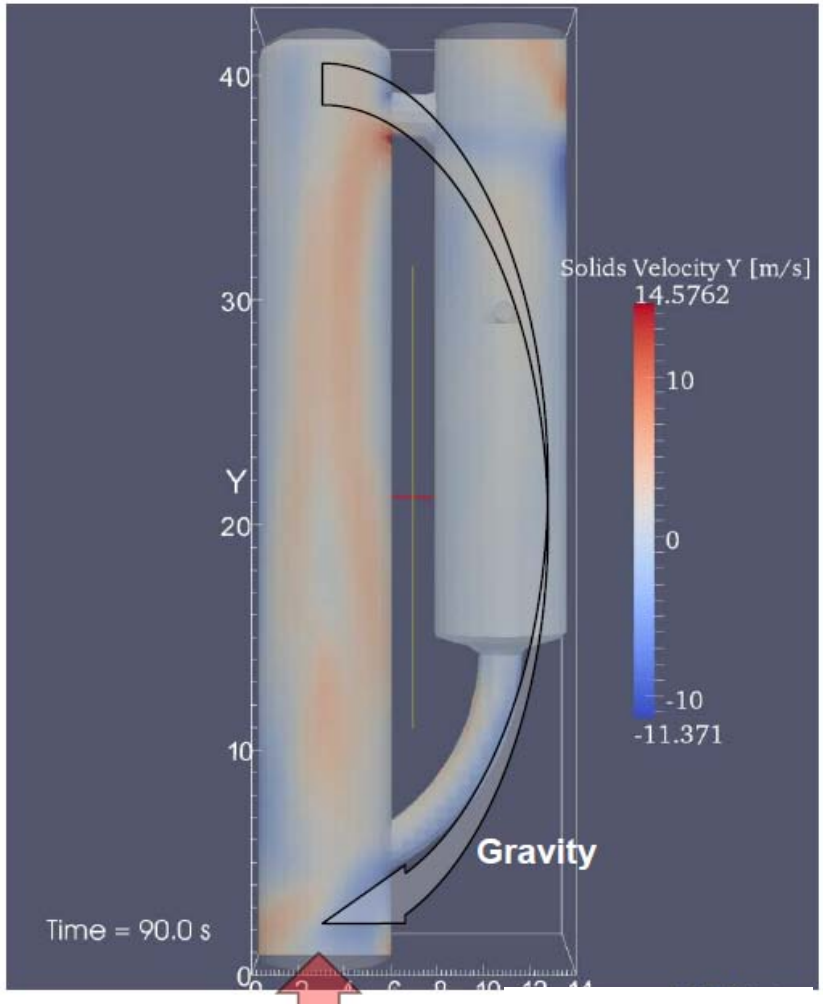
Multi-Stage Bubbling Bed Solid Sorbent Adsorber





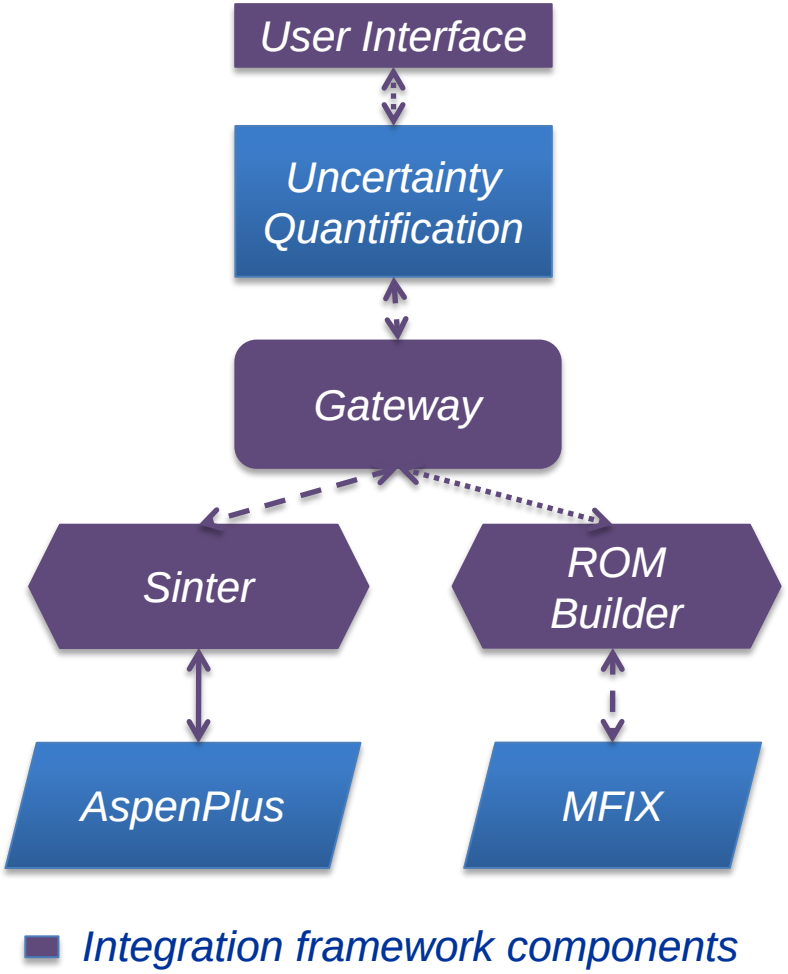
Device-Scale Models

- Validation of CFD codes for 1 kW pilot scale process
- Implemented a full-scale case in the open-source software MFIX
- Successfully ran initial simulations based on CFB
- Full scale case considering bubbling bed adsorber
  - Overall hydrodynamics
  - Interaction with cooling tubes



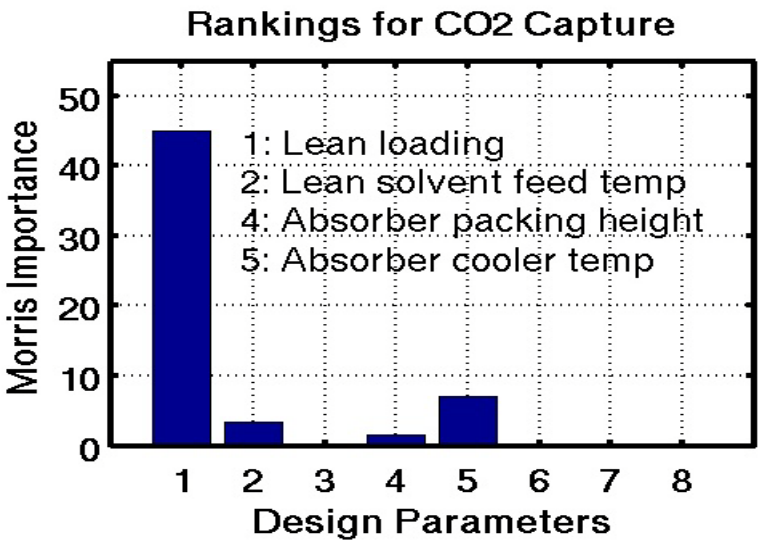
CCSI Integration Framework Developments

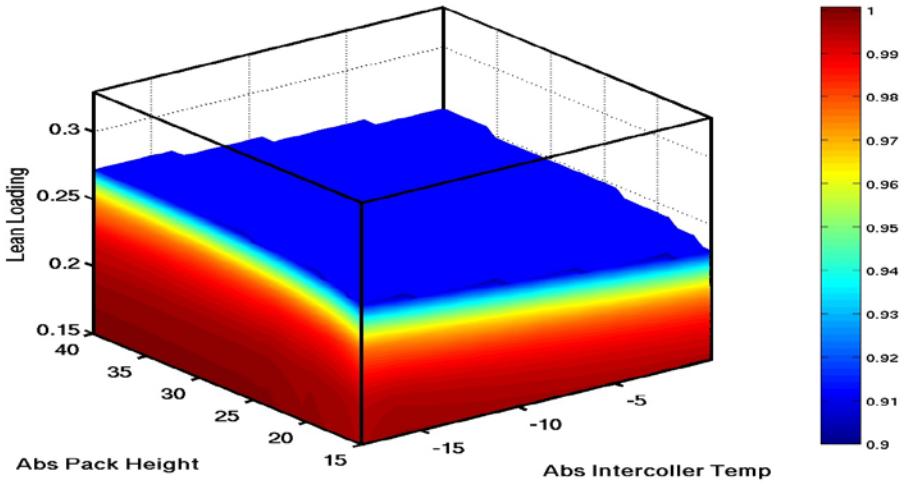
- Surveyed IAB to understand end user tool needs and deployment environment
- Added robustness and support for UQ and CCSI gateway to Sinter
- Performed 1000s of simulations of MEA process needed by UQ
- End-to-end connection of UQ through gateway and ROM development underway now
- Prototype UQ user interface designed – implementation underway



Uncertainty Quantification Demonstration

- Used an MEA capture model in Aspen Plus to start the development of CCSI UQ framework
- Equilibrium constants and mass transfer coefficients identified as major sources of uncertainties
- Parameter ranking study conducted for design parameters with known ranges



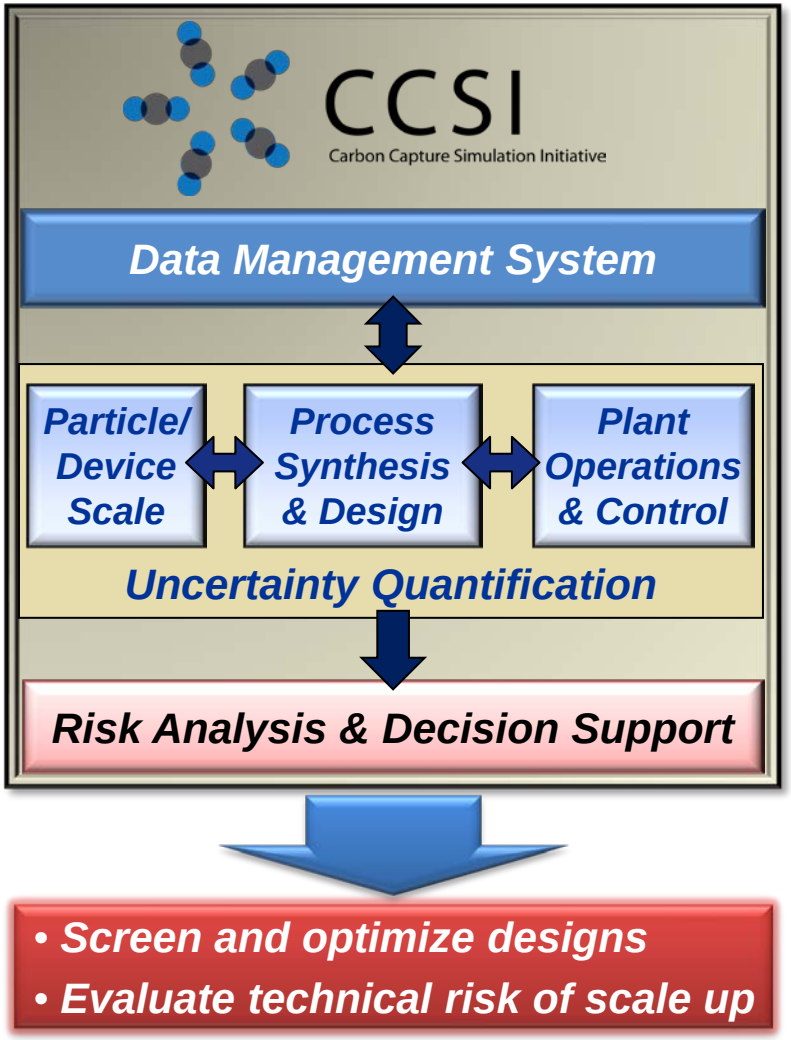


Colored region satisfies >= 90% CO_2 capture

1. J. Eslick and D. Miller , Computers & Chemical Engineering, 2011

Integrated M&S with UQ & Risk Analysis for Accelerating CC Technology Development

- Complements experimental projects in DOE's CCS RD&D roadmap
- Three industrial challenge problems: Solid-sorbents, Solvents, Oxy-combustion
- Embodies innovations in Model Integration, UQ, Optimization, and Technical Risk Analysis
- Promotes early adoption by integrating existing tools into the CCSI Toolset
- Leverages core strengths of industry, academia, and national labs
- Primary users of CCSI Toolset
  - Technology providers: screening and optimizing designs
  - Power generators: evaluating technical risk of scale-up



Acknowledgements

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Executive Committee: Juan Meza, Madhava Syamlal, Melissa Fox, David Brown, Mohammad Khaleel, Ed Rubin, S. Sundaresan

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4: Plant Operations & Control, Lead: Steve Zitney, Richard Turton, Debangsu Bhattachaaryya, Priyam Mahapatra, Eric Liese
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6: Uncertainty Quantification (UQ), Lead: Charles Tong, Co-lead: Guang Lin, Joanne Wendelberger, David Engel, Gardar Johannesson, Brenda Ng, K. Sham Bhat, Lisa Moore
7: Risk Analysis & Decision Making, Lead: Bruce Letellier, Co-lead: David Engel, Rene Leclaire, Ed Jones, Mary Ewers, Brian Edwards, Julie Thompson
8: Software Development Support, Lead: Paolo Calafiura, Bora Akyol, Greg Pope, Tim Carlson, Keith Beattie
9: Industrial Challenge Problems, Lead: Geo Richards, Charlie Freeman, Mark Williams, Carl Richardson, Bill Hoskins
10: Industry Collaboration, Lead: John Shinn

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