CCSI

Carbon Capture Simulation Initiative

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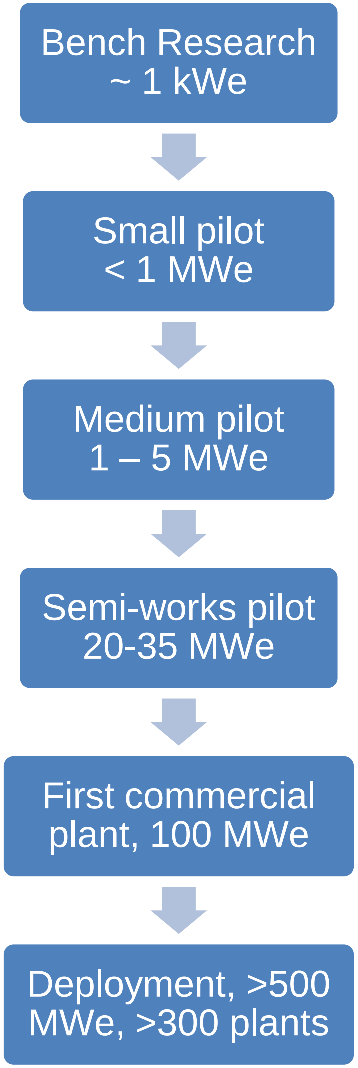
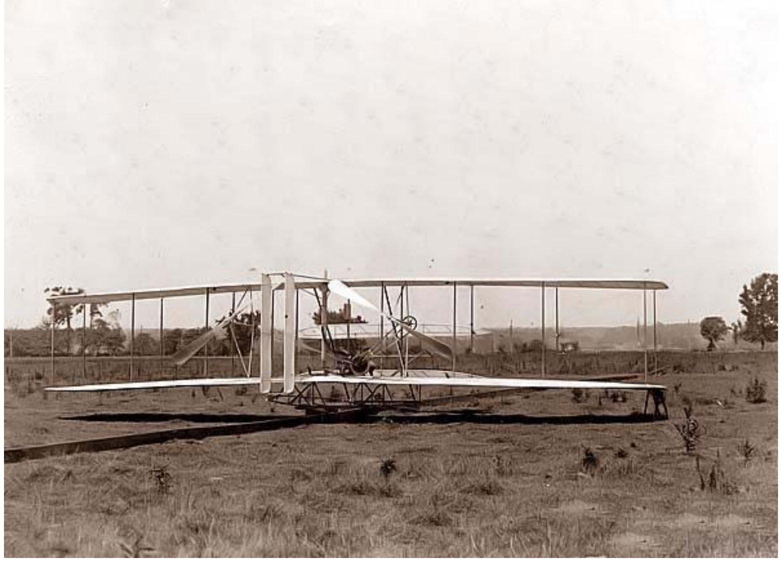
Carbon capture challenge

- **The traditional pathway from discovery to commercialization of energy technologies can be quite long, i.e., ~ 2-3 decades**
- **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 CCS concepts from lab to power plant, <u>quickly</u>, and at low cost and risk**
- **CCSI will accelerate the development of CCS technology, from discovery through deployment, with the help of science-based simulations**



How can we accelerate technology development for carbon capture and storage?

Key differences in the design process used to create these two machines:
better science, more engineers…..and also large-scale simulations



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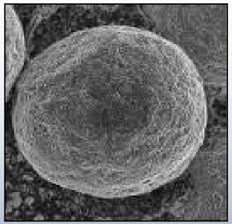
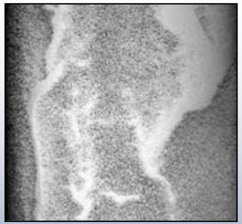
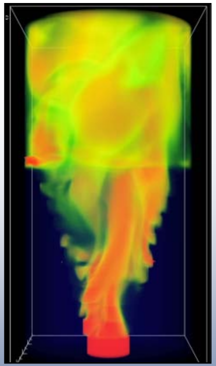
Goal is to develop M&S tools to accelerate the commercialization of CCS


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

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

Academia

Carnegie Mellon
VirginiaTech
PennState 1855
Princeton University
West Virginia University
University of Pittsburgh

Industry

ADA Environmental Solutions
Ameren
B&W the babcock & wilcox company
Babcock Power Inc.
Air Products
ALSTOM
FLUOR
RAMGEN Power Systems USA
AEP American Electric Power
Duke Energy
GE
PG&E
Southern California Edison An EDISON INTERNATIONAL Company San Onofre Nuclear Generating Station
Southern Company
Chevron
Eastman
EPRI Electric Power Research Institute
WorleyParsons resources & energy
URS

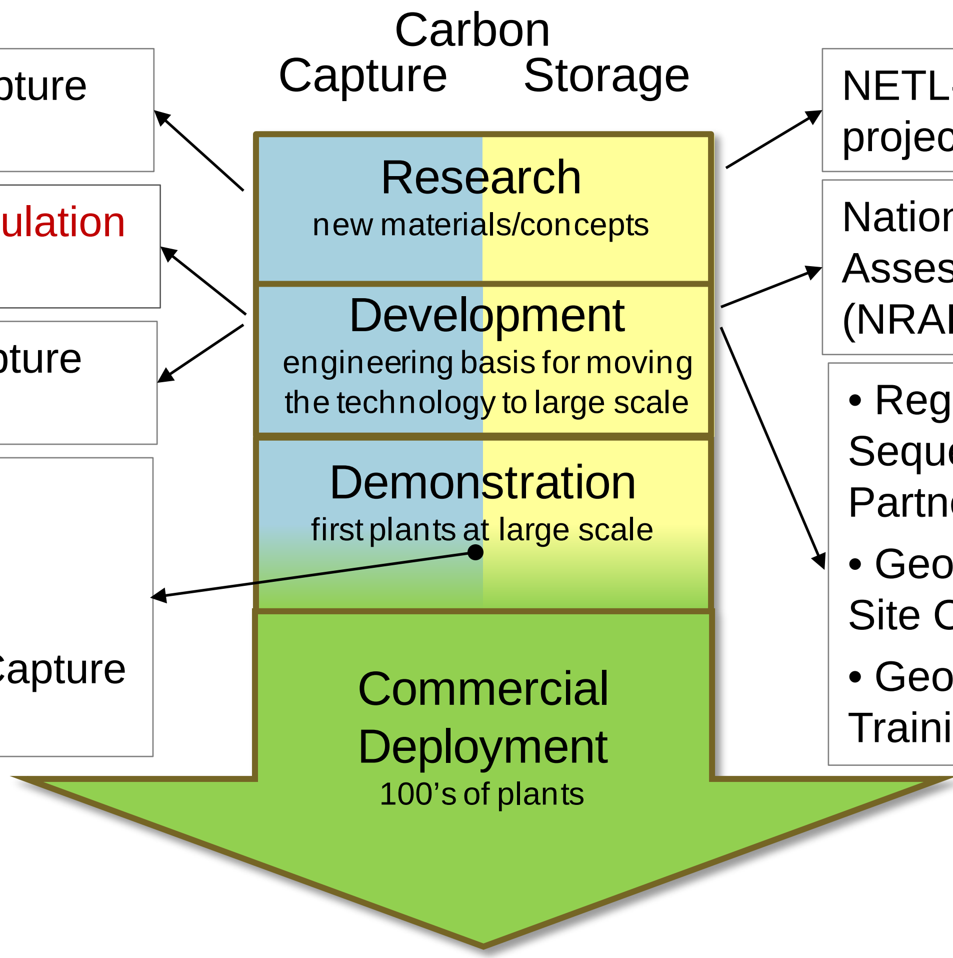
CCSI is a pathway on DOE CCS RD&D roadmap

NETL-sponsored capture projects

Carbon Capture Simulation Initiative (CCSI)

National Carbon Capture Center (NCCC)

- Clean Coal Power Initiative (CCPI)-III
- FutureGen 2.0
- Industrial Carbon Capture & Storage



NETL-sponsored storage projects

National Risk Assessment Partnership (NRAP)

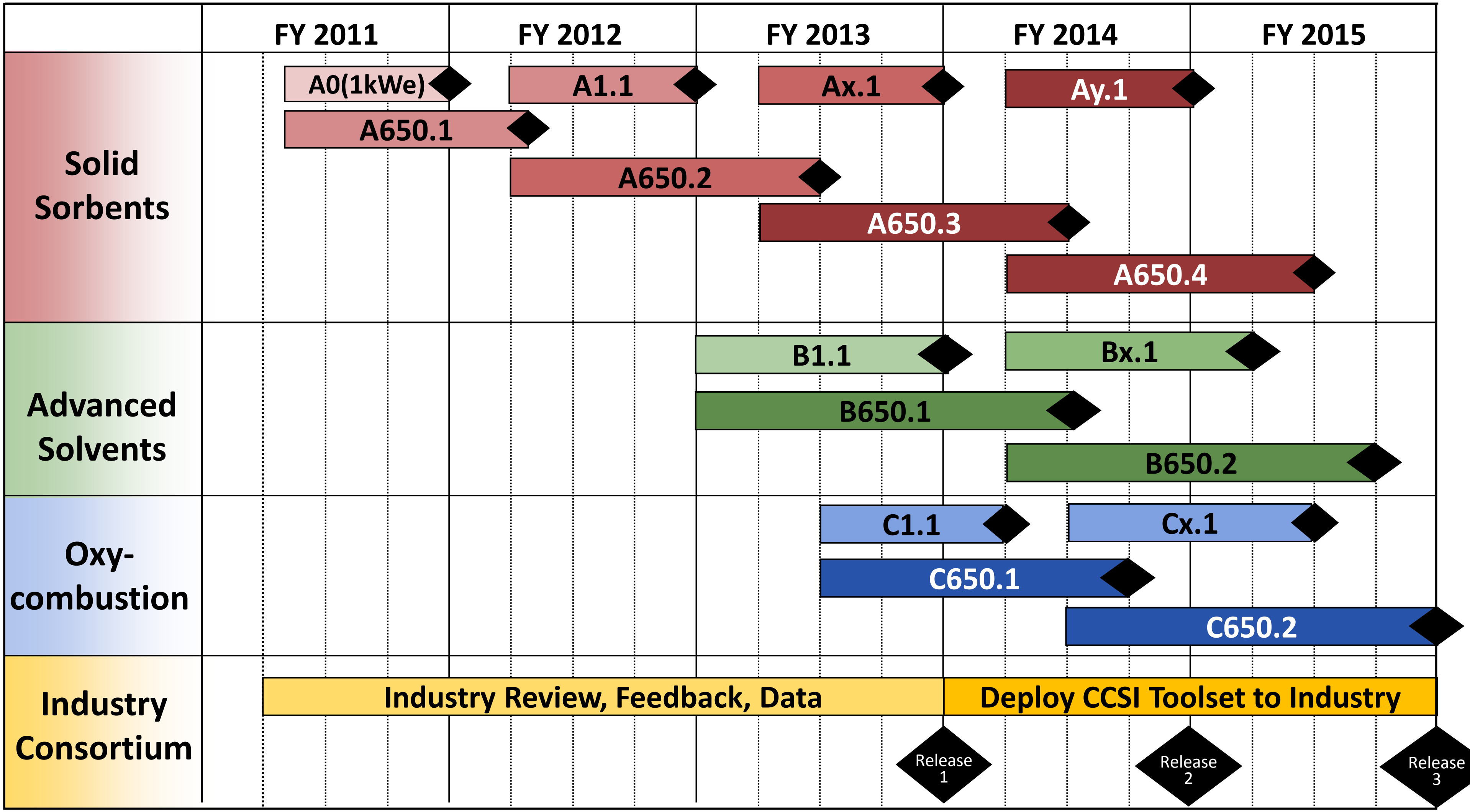
- Regional Carbon Sequestration Partnerships
- Geologic Sequestration Site Characterization
- Geologic Sequestration Training & Research

http://www.netl.doe.gov/publications/press/2011/110106-DOE-NETL_CO2_Capture_and_Storage_RDD_Roadmap.html

Industrial challenge problems (ICP) will underpin CCSI Toolset development

- **Desirable ICP Attributes**
  - Validation data are available
  - Provides relevant results to problems of current interest
  - Extendable for a wide range of applications later (e.g., IGCC, NG)
- **ICP priority: Pulverized coal plants**
  - Two coal IGCC now, more to come
  - Approximately 280 U.S. PC plants are CCS candidates
- **ICPs will focus on near-term applications**
  A. Sorbents – significant impact on reactor/process design and optimization
  B. Advanced Solvents – Directly extend sorbents approach
  C. Oxy-combustion adds the complexity of full plant

5 Year development plan overview



CCSI product and its applications

Category	Description	Benefits for industrial users
Data	Data management system and hierarchy of V&V data sets for different scales	• Manage data and access data provenance info • Verify the basis for UQ • Reuse V&V hierarchy for other sorbents/reactors
Models	Physicochemical models of particles, devices, or processes developed for the ICPs	• Evaluate process concepts • Determine optimal device and process configurations • Analyze controllability and operability
Software	Software encoding custom models or ROMs, the integration framework, and UQ and risk analysis tools.	• Speed up model integration and execution • Quantify the confidence in simulation results • Conduct technical risk analysis based on simulation results
API Standards	Specs external developers can follow to access CCSI data management system and integration framework	• Integrate new tools and proprietary models into the framework
Best Prac tices	Specific modeling practices most suitable for the ICPs	• Use as templates or examples that users can adapt for their problems

Leadership structure

Board of Directors
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Doug Ray, PNNL
Don DePaolo, LBNL
Paul Dotson, LANL
Cindy Powell, NETL

Executive Committee Chair
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Mohammad Khaleel, PNNL
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S. Sundaresan, Princeton U.

Industry Advisory Board
John Shinn, Chevron

Director
Madhava Syamlal, NETL
Deputy Director
Juan Meza, LBNL

Technical Team Lead
David Miller, NETL

Project Coordinator
Roger Cottrell, NETL

Communications and Media Relations Lead

Education/Outreach Lead

Intellectual Property/ Commercialization Lead
Susan Sprake, LANL

Physicochemical Models and Data

Task Set 1: Basic Data and Models
J. Kress, LANL
Task Set 2: Particle & Device Scale Models
X. Sun, PNNL
Co-Lead: S. Sundaresan, Princeton
Task Set 3: Process Synthesis & Design
D. Miller, NETL
Co-Lead: N. Sahinidis, CMU-NETL
Task Set 4: Plant Operations & Control
S. Zitney, NETL

Analysis & Software

Task Set 5: Integration Framework
D. Agarwal, LBNL
Task Set 6: Uncertainty Quantification
C. Tong, LLNL
Co-Lead: G. Lin, PNNL
Task Set 7: Risk Analysis & Decision Making
B. Letellier, LANL
Co-Lead: D. Engel, PNNL
Task Set 8: Software Development Support
P. Calafiura, LBNL

Industrial Applications

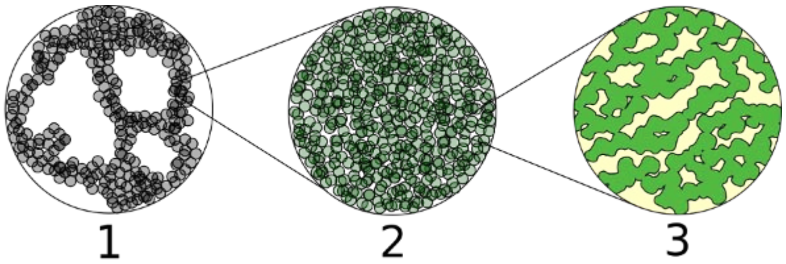
Task Set 9: Industrial Challenge Problems
G. Richards, NETL
Task Set 10: Industry Collaboration
J. Shinn, Chevron/LBNL

Focus of year-1 effort

- **Identify promising solid-sorbent capture processes and support the scale-up from small-scale to full-scale**
- **Physicochemical Models**
  - Develop reaction model for silica-supported amine sorbent materials
  - Develop CFD model of ADA-ES 1 kW system and a full scale system
  - Demonstrate a process synthesis approach and develop a detailed process design
  - Develop dynamic simulation and conduct controllability study
- **Analysis & Software**
  - Develop prototype data model for data management
  - Develop CCSI integration framework
  - Demonstrate UQ methodology for process and CFD simulations
  - Demonstrate an initial risk analysis framework and methodology
- **Industrial Applications**
  - Establish Industry Advisory Board
  - Review the development of earlier coal power systems, to understand how simulations could have impacted the development cycle

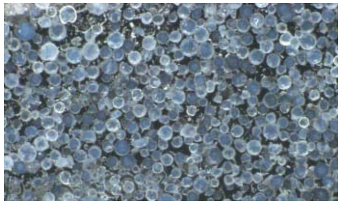
PEI-Silica sorbent reaction model

- 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



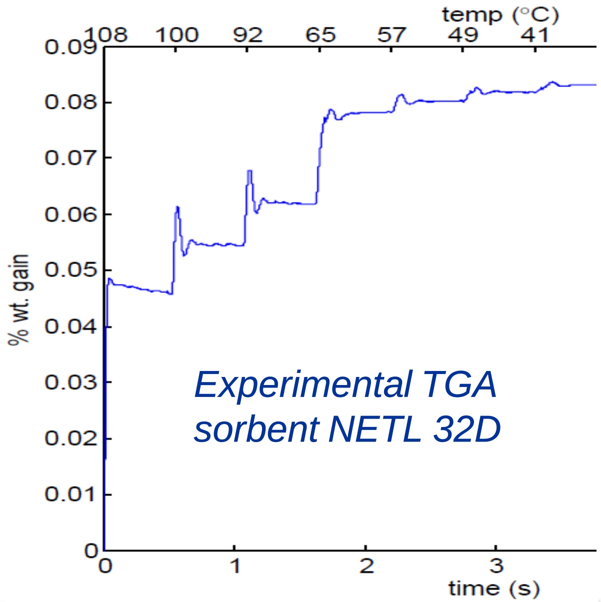
$$R_2NH + CO_2 \rightleftharpoons R_2NH^+ : CO_2^-$$
$$R_2NH^+ : CO_2^- + R_2NH \rightleftharpoons R_2NH_2^+ + R_2NCO_2^-$$

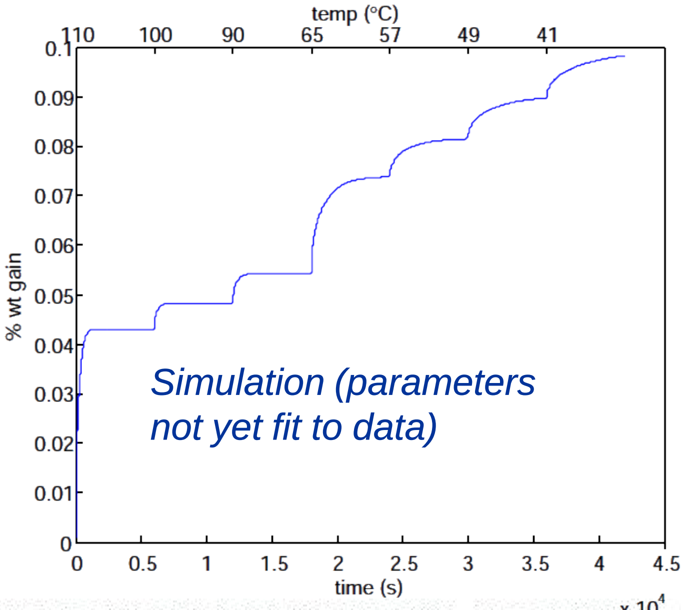
zwitterion mechanism (anhydrous)



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

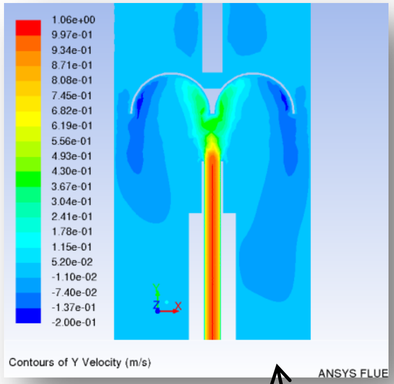
D.S. Mebane, K.G. Bhat, L. Moore, J. Wendelberger, D. Fauth, M. Gray, 2011 International Pittsburgh Coal Conference, in preparation.

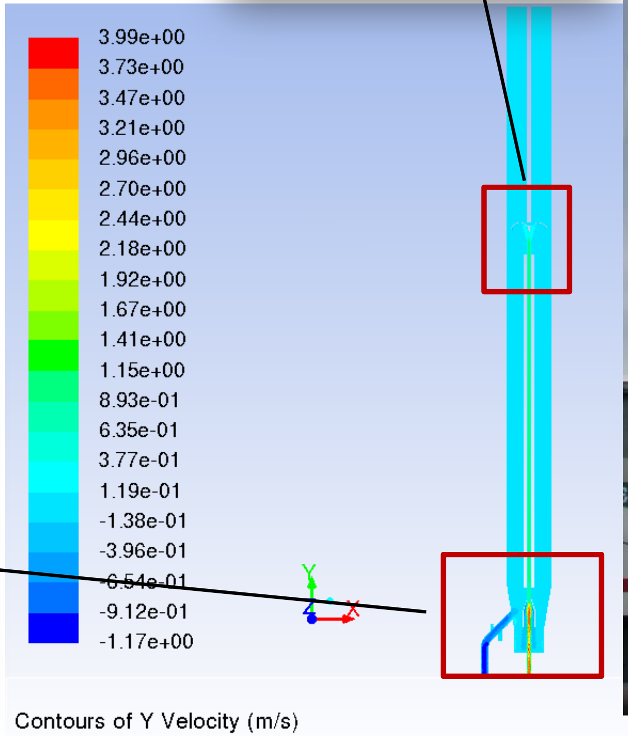


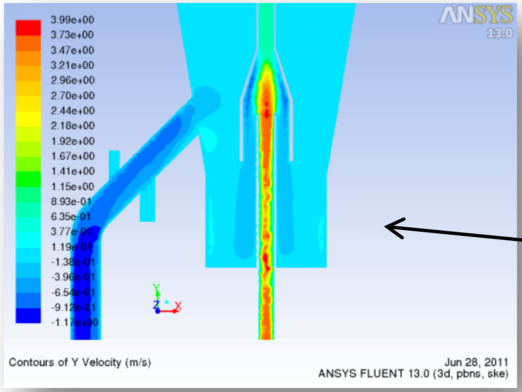


1 kW-scale device model being built

- Collected ADA-ES experimental data and geometry for case A0
- Divided the system into 3 reactors: riser, internally circulating fluidized bed (ICFB), and regenerator
- Built models of riser and ICFB with the commercial software FLUENT

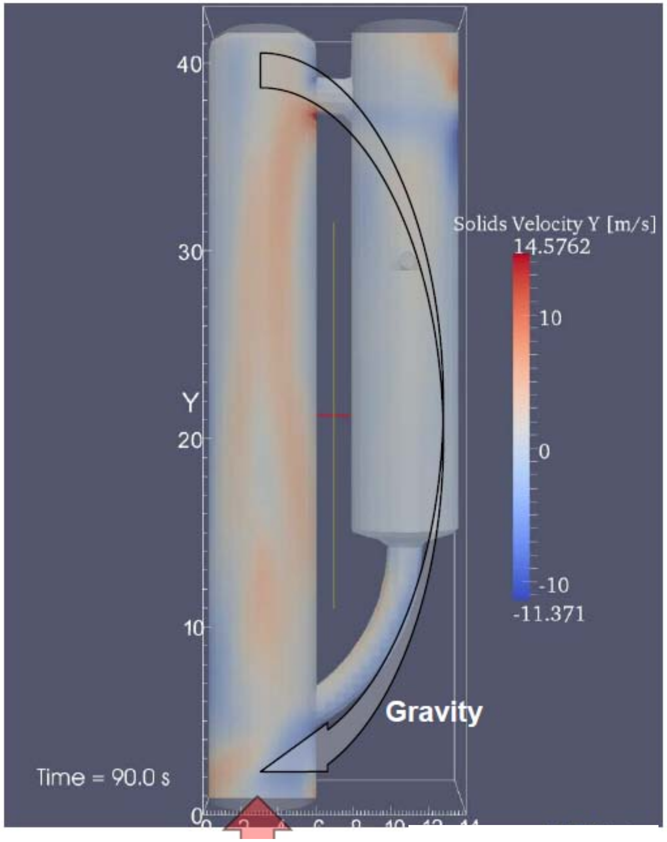






Prototype of full-scale device model demonstrated

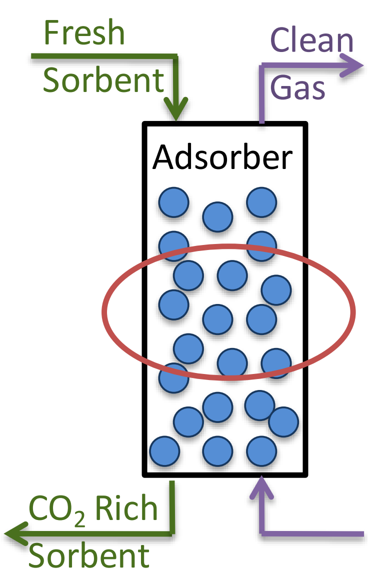
- Implemented a full-scale case in the open-source software MFIX
- Successfully ran initial simulations, to demonstrate physically reasonable results
- Device model for case A650.1 will be completed based on input from the process synthesis task



Method to generate surrogate models from detailed simulations developed

- 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®



Sample points

Build model

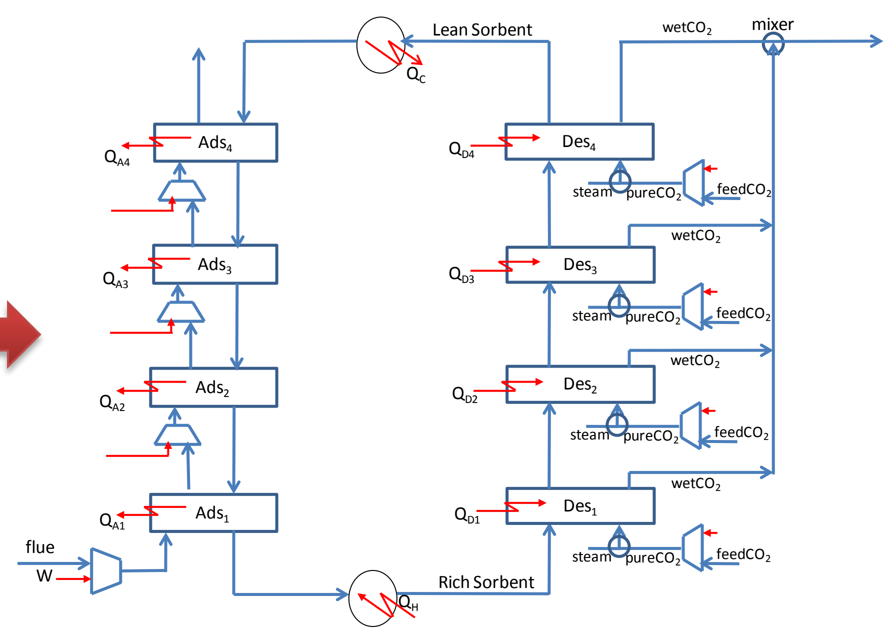
Adaptive sampling and **Model validation**

Done

$$f(x)$$

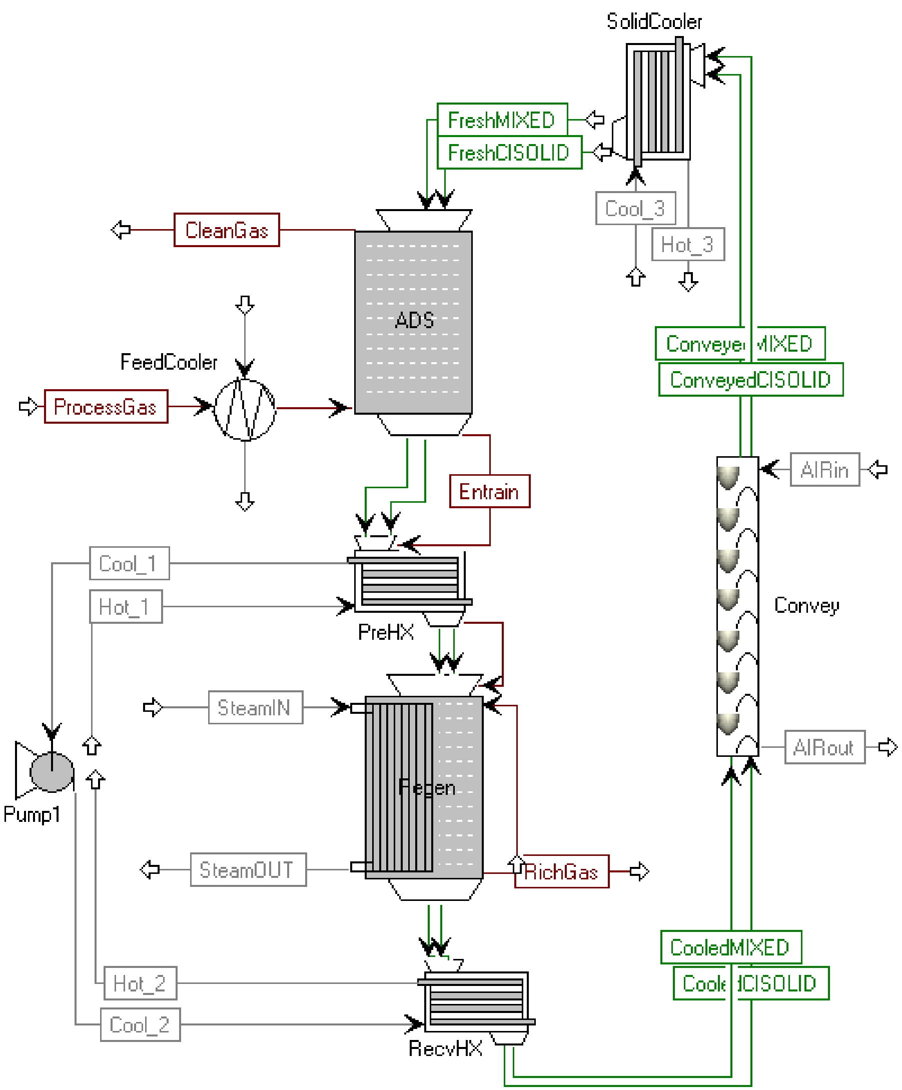
Algebraic Surrogate Model

Superstructure to determine optimal process configuration

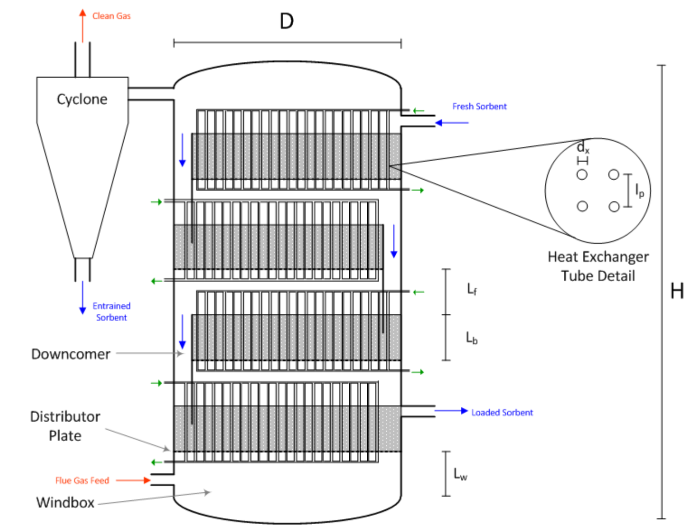


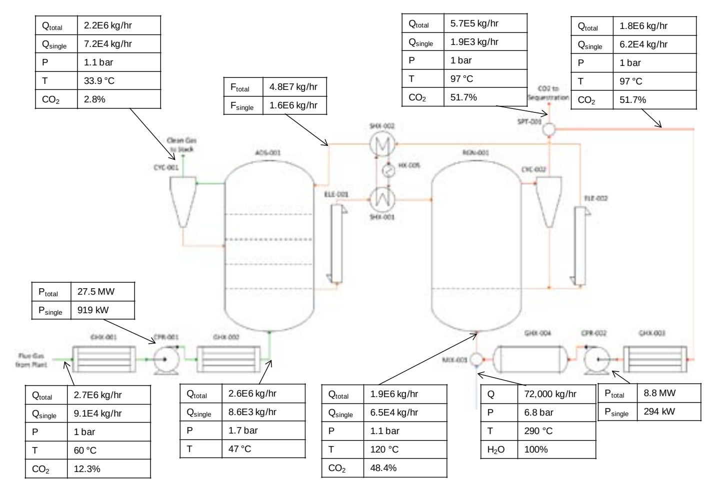
Preliminary detailed process designs

Moving Bed-Based Solid Sorbent Capture Process Simulation

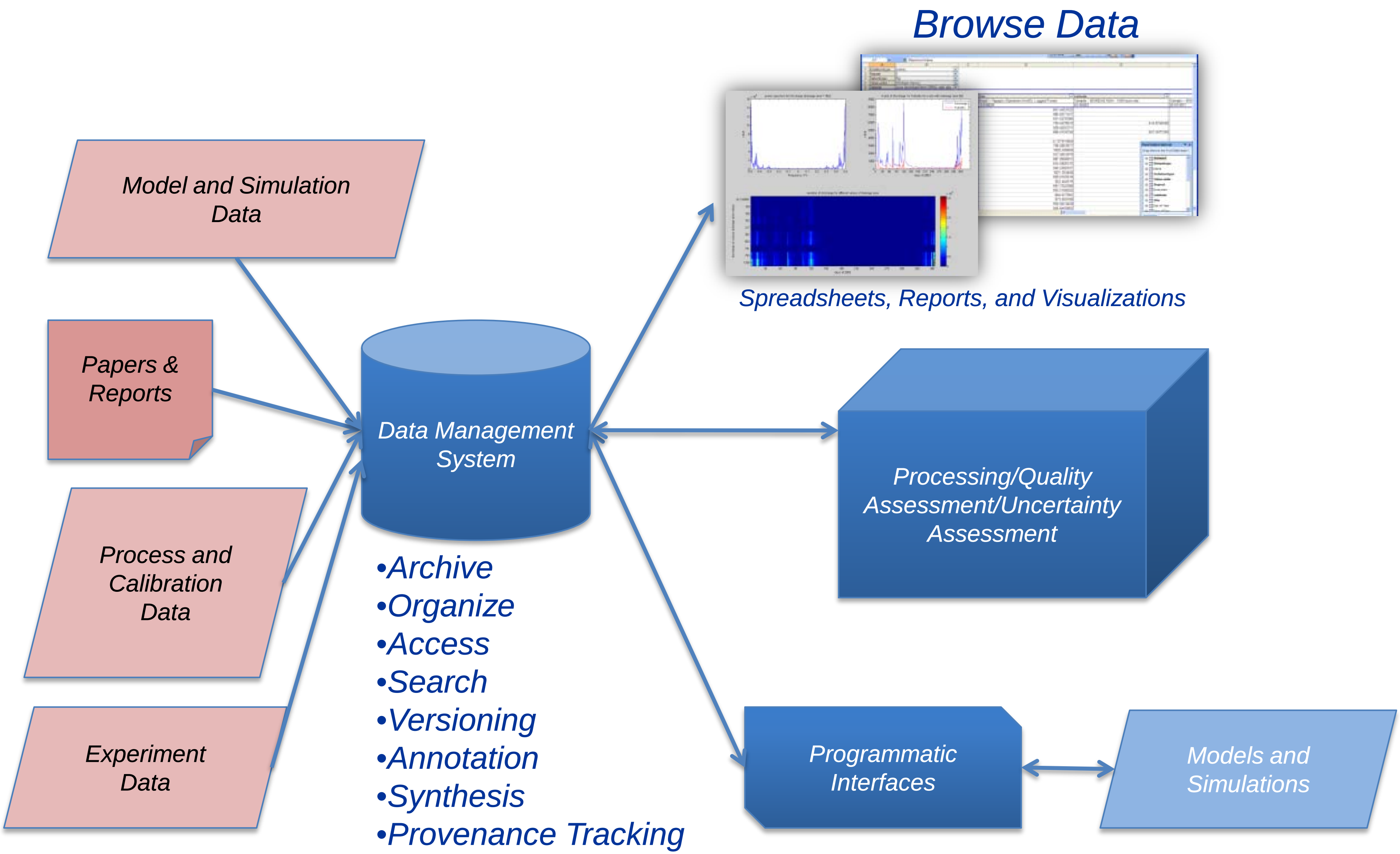


Multi-Stage Bubbling Bed Solid Sorbent Adsorber



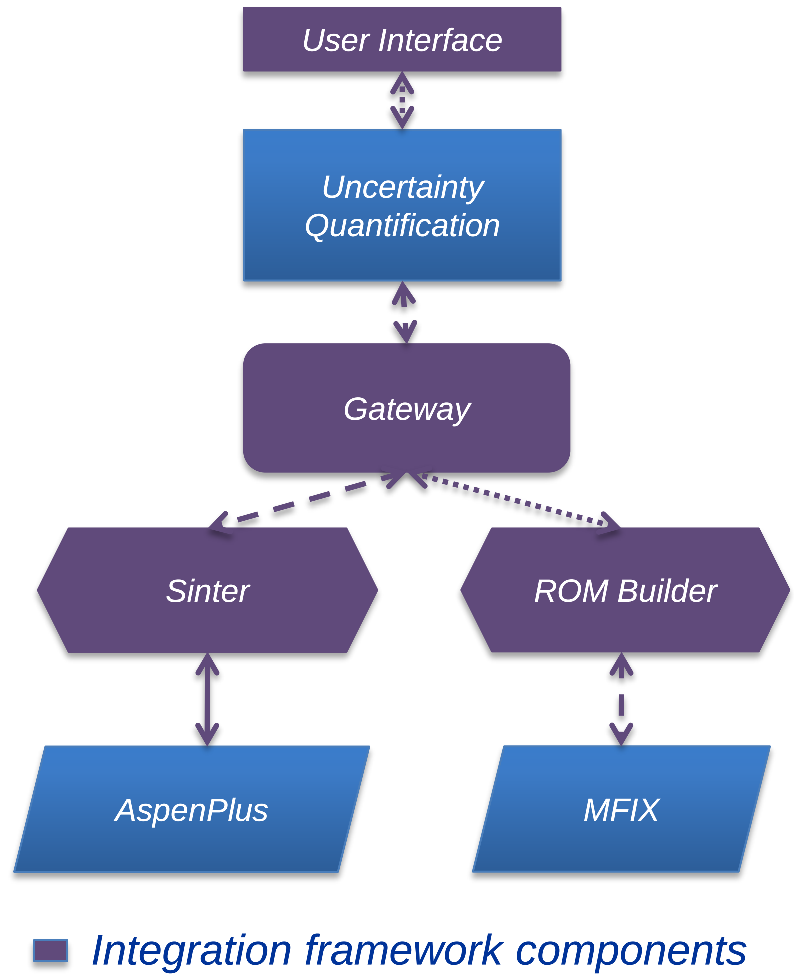


CCSI data management system is being defined



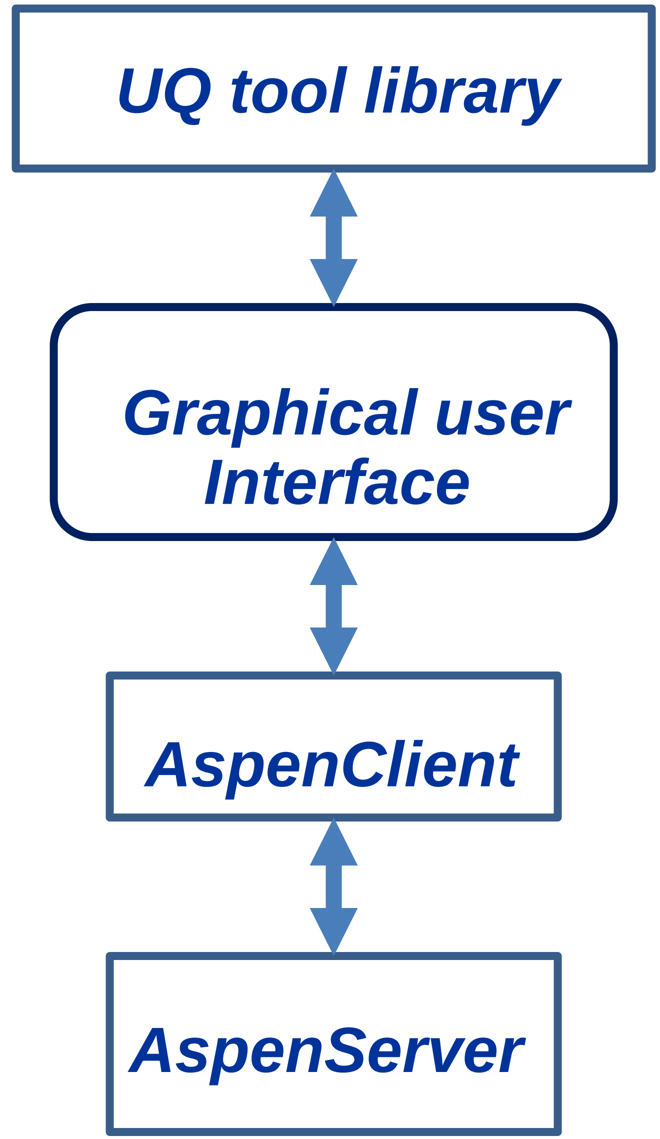
CCSI integration framework progress

- 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 MEA process simulations for UQ
- End-to-end connection of UQ through gateway and ROM development underway now
- Prototype UQ user interface designed – implementation underway



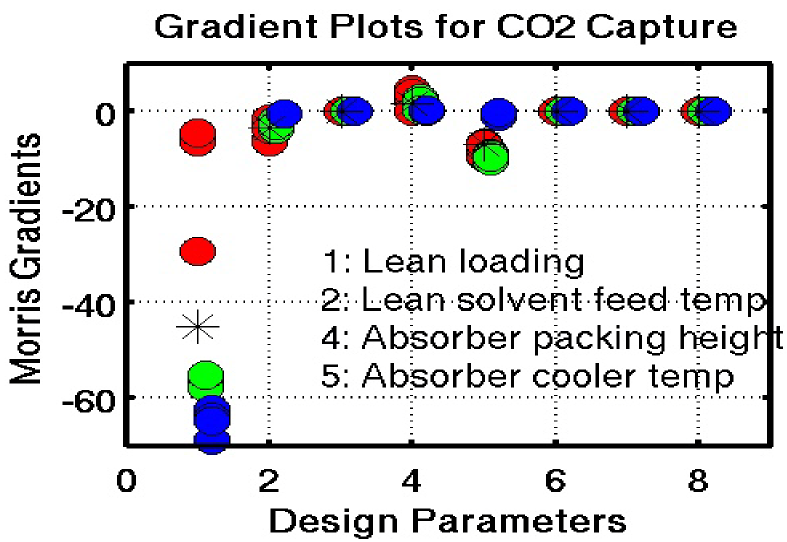
Uncertainty quantification progress

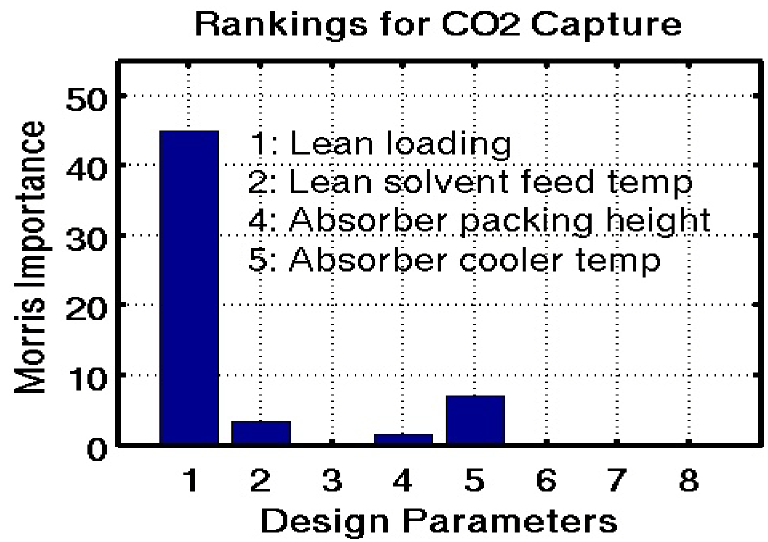
- Used an MEA capture model[1] in Aspen Plus to start the development of CCSI UQ framework
- Equilibrium constants and mass transfer coefficients identified as major sources of uncertainties
- Their uncertainty bounds are being defined from literature data
- Parameter ranking study conducted for design parameters with known ranges

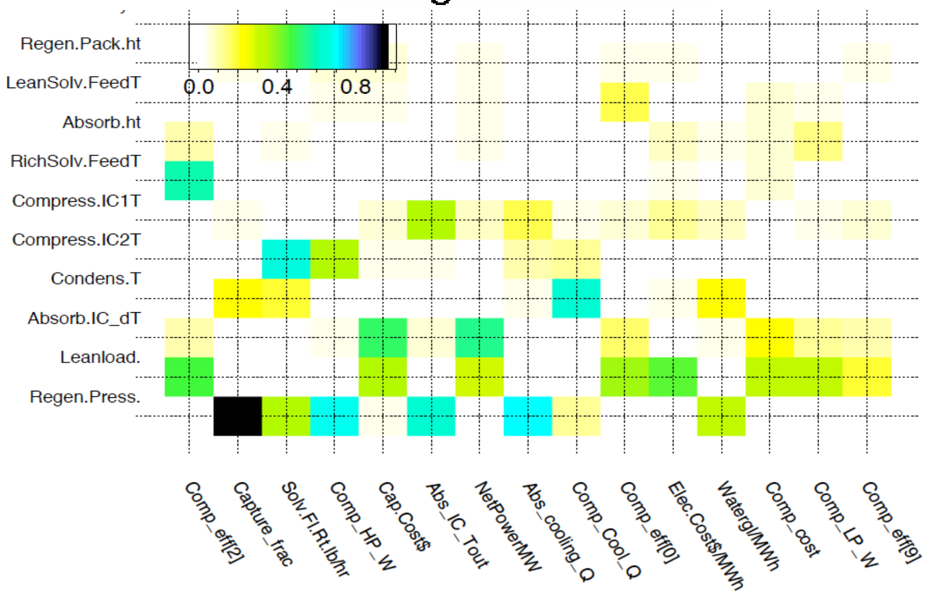


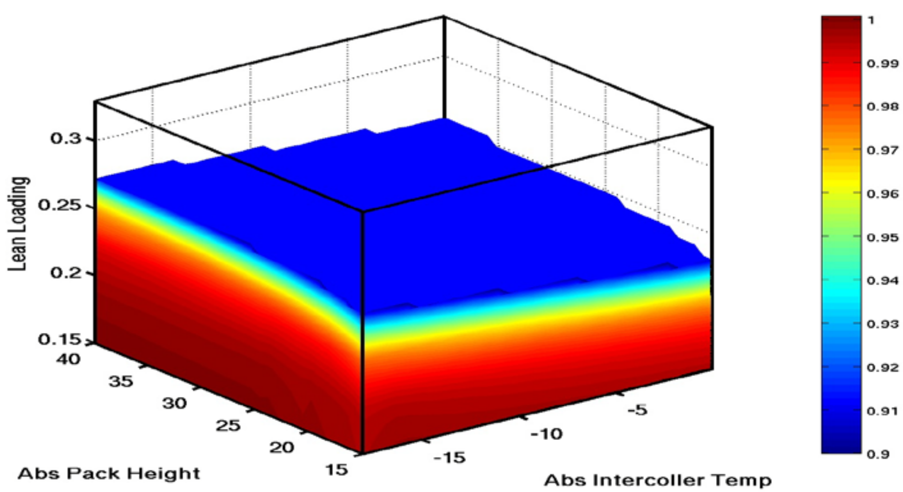
1. J. Eslick and D. Miller 2011

Design parameter ranking study





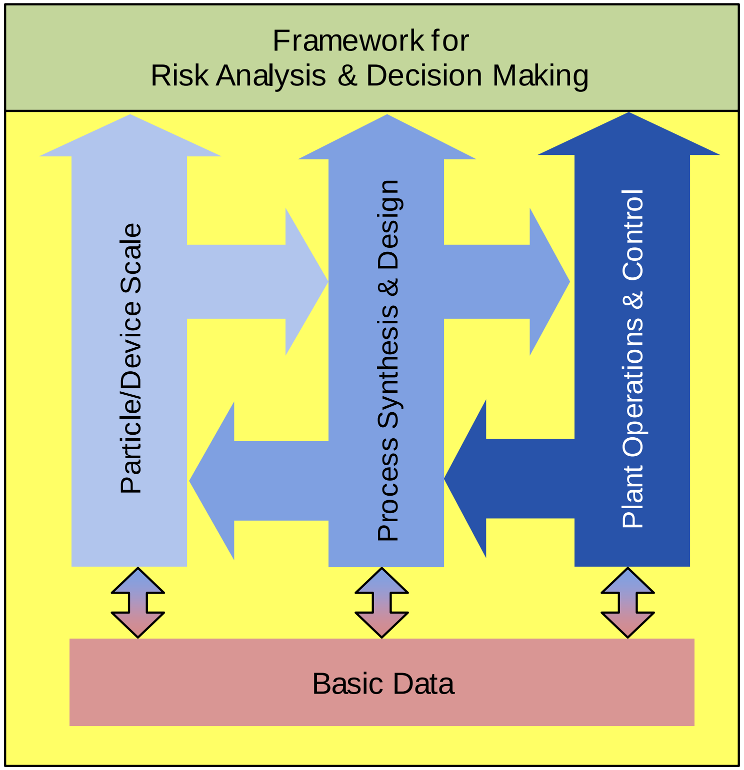




Colored region satisfies >= 90% CO_2 capture

Increase fidelity in integrated M&S for accelerating CCS technology development

- Part of DOE's CCS RD&D roadmap; experimental projects are potential sources of validation data
- Three industrial challenge problems: Solid-sorbents, Solvents, Oxy-combustion
- Embodies innovations in
  - Model Integration
  - UQ and Optimization
  - Technical Risk Analysis
- Promotes early adoption by integrating existing tools, widely used by the industry, into the CCSI Toolset



- Leverages core strengths of industry, academia, and national labs
- Primary users of CCSI Toolset
  - <u>Technology providers</u>: screening and optimizing designs
  - <u>Power generators</u>: evaluating technical risk of scale-up

Thank You!

On June 28-29, 2011 CCSI Team visited Boeing's Integrated Technology Development Lab and the Everett manufacturing plant to learn how they are successfully using simulation and modeling to accelerate the development of new aircraft, such as the 787.