CCSI

Carbon Capture Simulation Initiative

Project Overview

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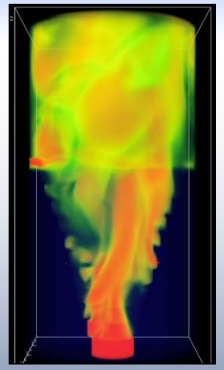
23 September 2014

U.S. DEPARTMENT OF ENERGY

CCSI For Accelerating 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

National Labs

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

Academia

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

Industry

ADA Environmental Solutions
Alstom
B&W
GE
EPRI Electric Power Research Institute
Fluor
Phillips 66
AEP American Electric Power
Southern California Edison An Edison International Company San Onofre Nuclear Generating Station
Southern Company
ExxonMobil
Chevron
URS
Air Products
Eastman
aspentech
ANSYS
Schneider Electric
PSE

CCSI Mission

- **Develop** new computational tools and models to enable industry to more rapidly develop and deploy new advanced energy technologies
  - Base development on industry needs/constraints

- **Demonstrate** the capabilities of the CCSI Toolset on non-proprietary case studies
  - Examples of how new capabilities improve ability to develop capture technology

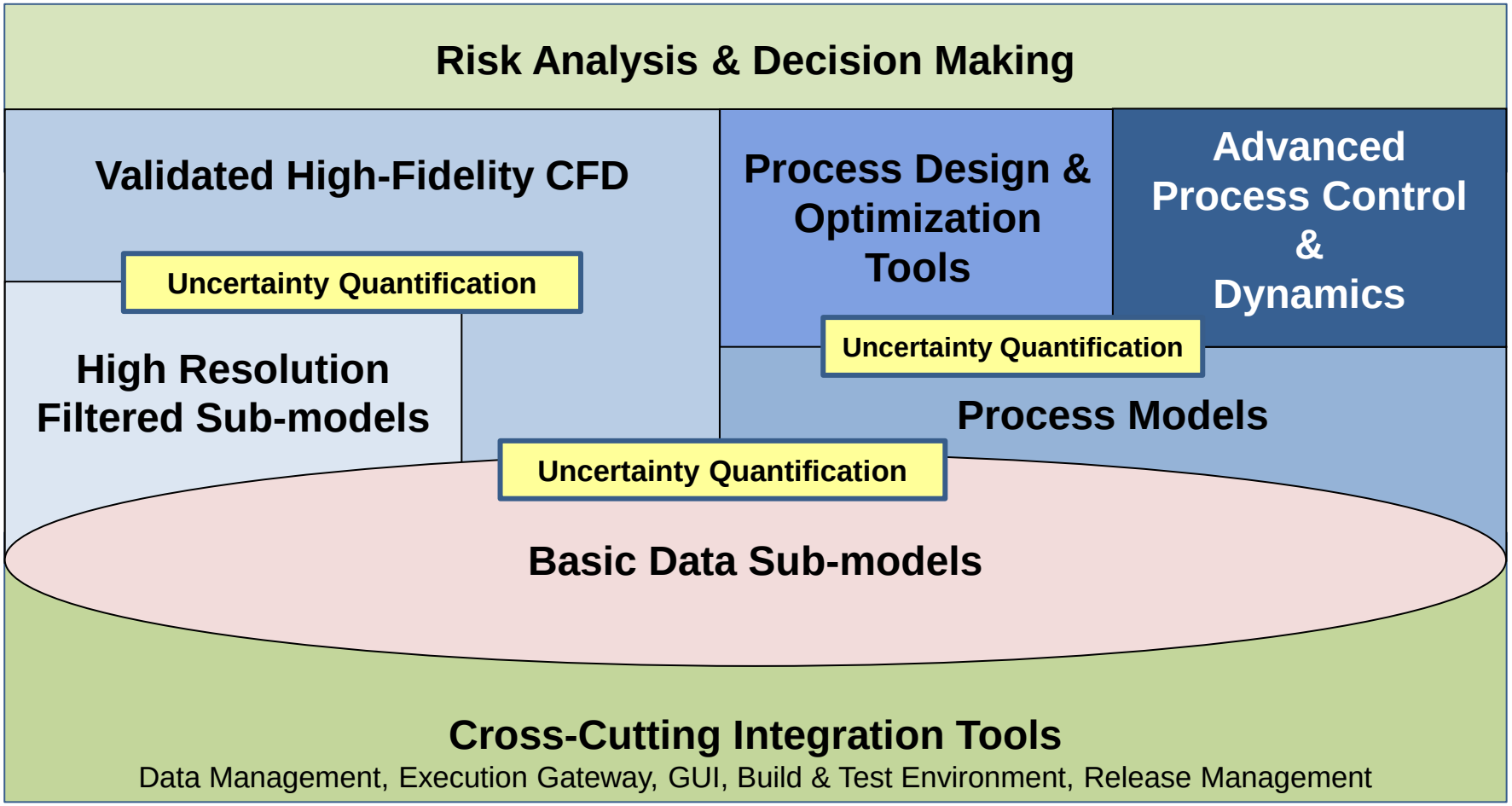
- **Deploy** the CCSI Toolset to industry
  - Support initial industry users
  - Obtain feedback on features and capabilities
  - Arrange for long term commercial licensing

CCSI Timeline

- Organizational Meetings: March 2010 - October 2010
- **Technical work initiated: Feb. 1, 2011**
- **Preliminary Release of CCSI Toolset: September 2012**
  - Initial licenses signed
- CCSI Year 3 starts Feb. 1, 2013
  - Began solvent modeling/demonstration component
- **2013 Toolset Release: October 31, 2013**
  - **Multiple tools and models released and being used by industry**

- **Future**
  - **2014 Toolset Release: October 31, 2014 – planned**
  - **Final release and workshop late 2015**
  - **Commercial licensing late 2015 or early 2016**

Advanced Computational Tools to Accelerate Carbon Capture Technology Development



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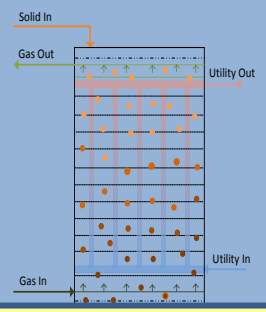
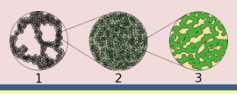
Tools to develop an optimized process using rigorous models

Process Models



Uncertainty

Basic Data Submodels



Uncertainty

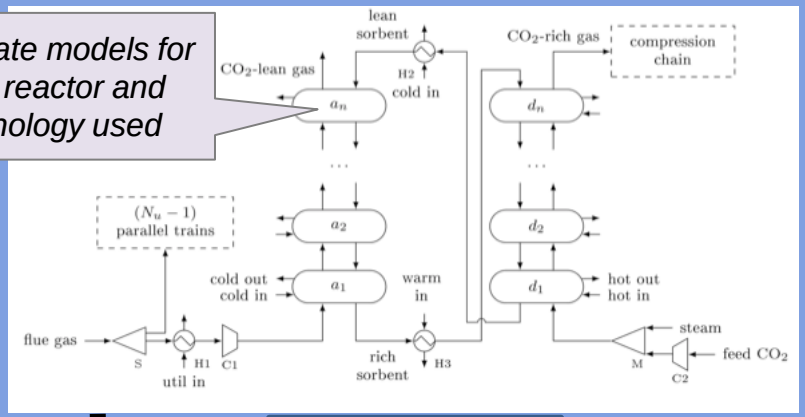
Algebraic Surrogate Models

ALAMO

Uncertainty

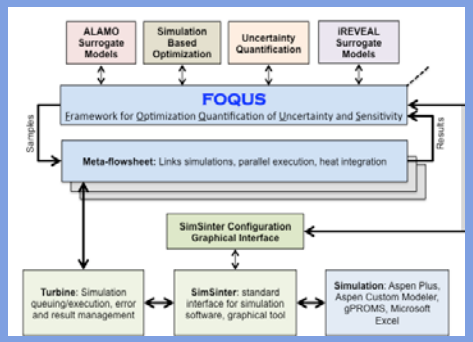
Surrogate models for each reactor and technology used

Superstructure Optimization



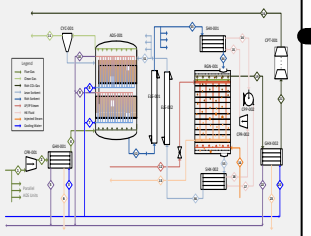
Uncertainty

Simulation-Based Optimization



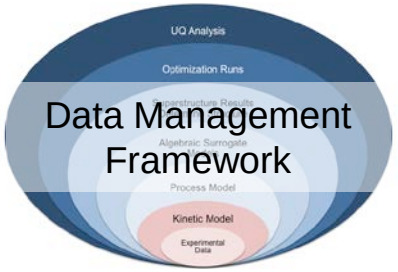
Uncertainty

Optimized Process



Uncertainty

Uncertainty Quantification



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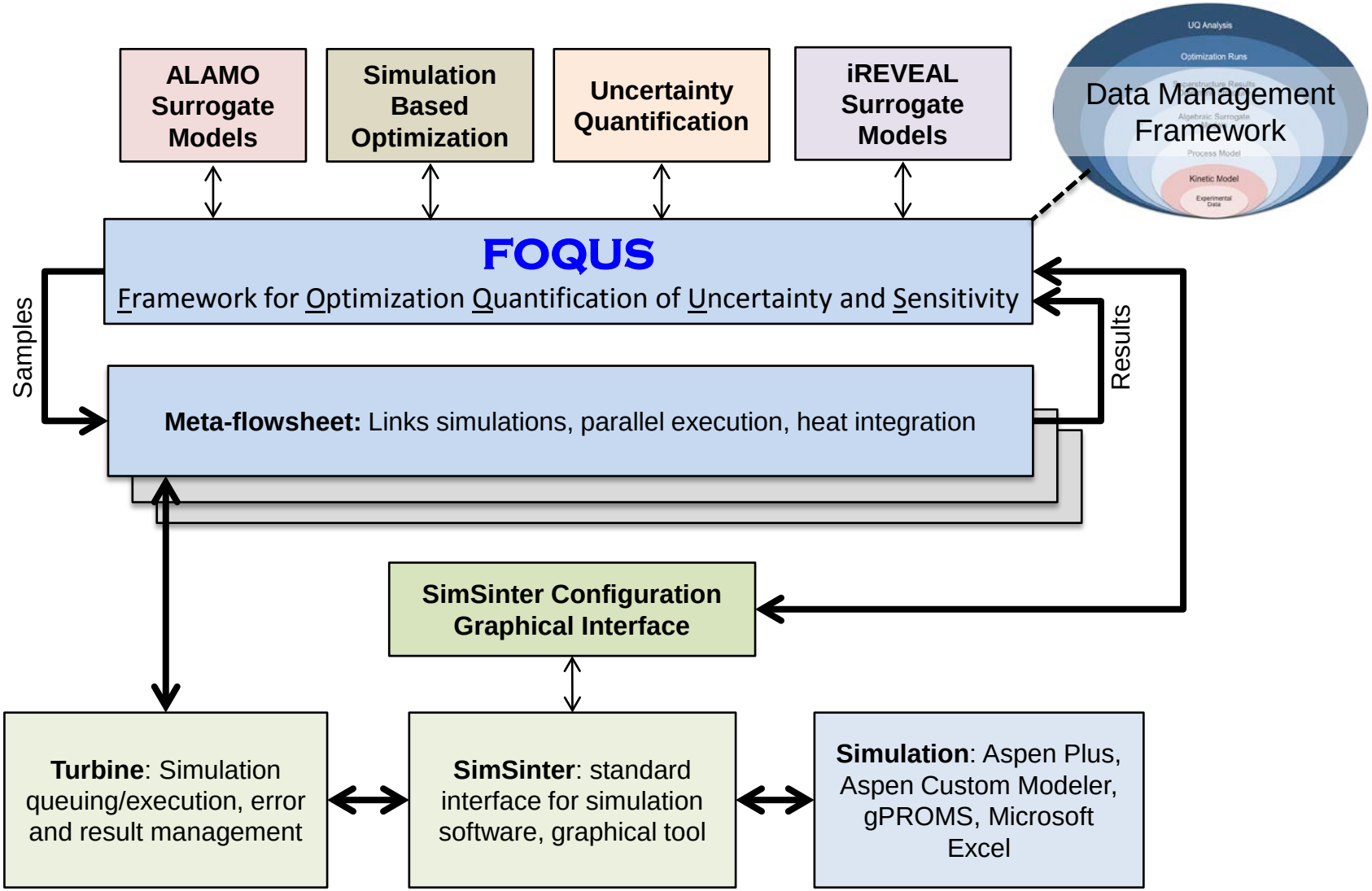
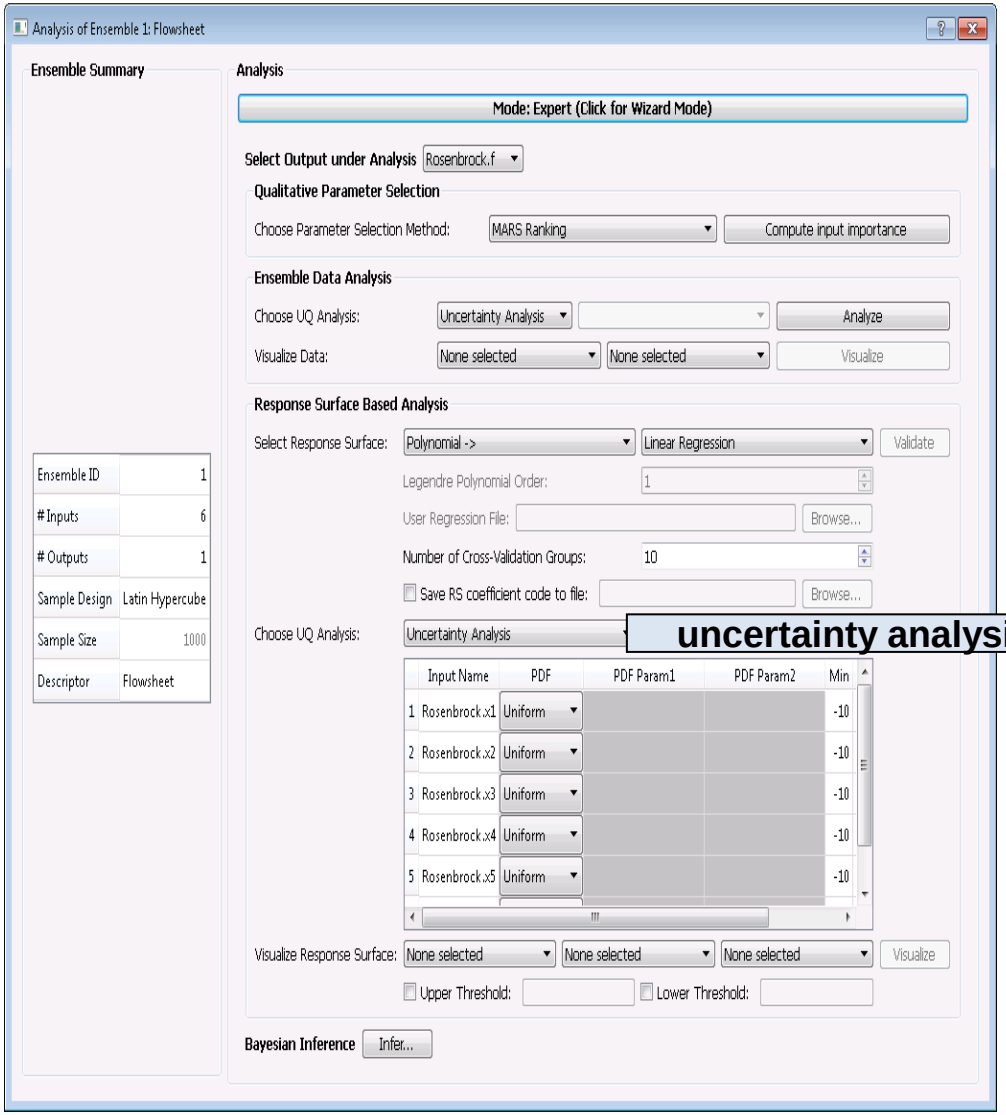
Framework for Optimization, Quantification of Uncertainty and Sensitivity

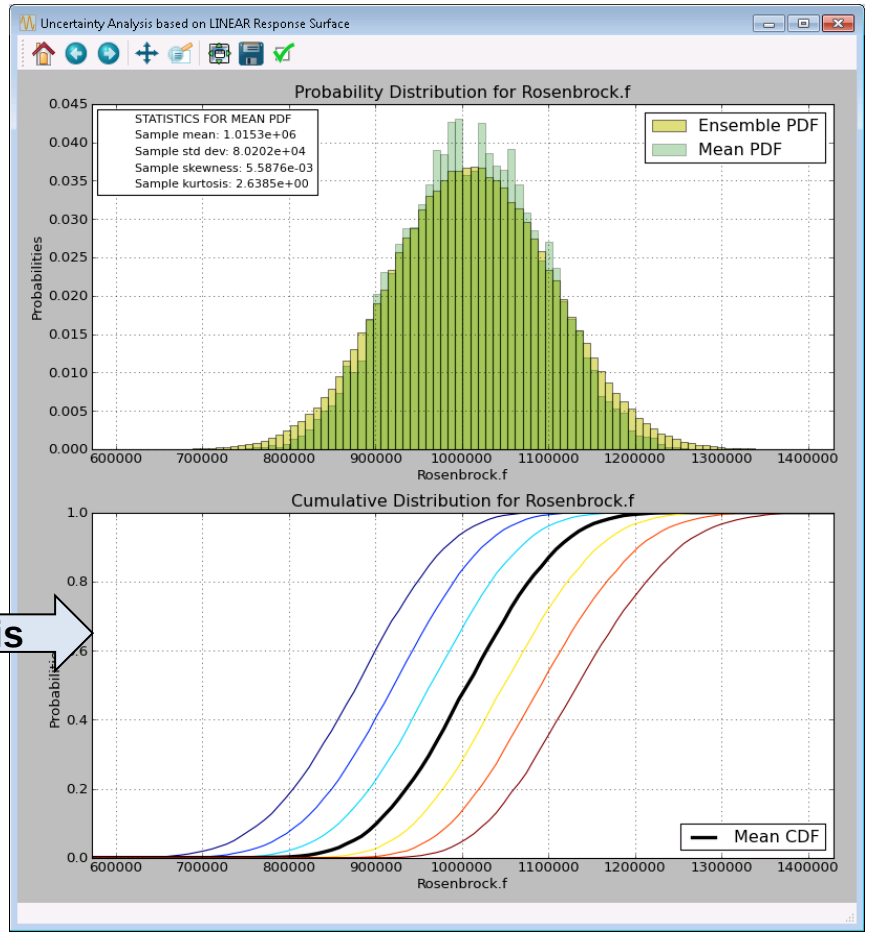


D. C. Miller, B. Ng, J. C. Eslick, C. Tong and Y. Chen, 2014, Advanced Computational Tools for Optimization and Uncertainty Quantification of Carbon Capture Processes. In *Proceedings of the 8th Foundations of Computer Aided Process Design Conference – FOCAPD 2014*. M. R. Eden, J. D. Siirola and G. P. Towler Elsevier.

Analyze output uncertainty with FOQUS



uncertainty analysis

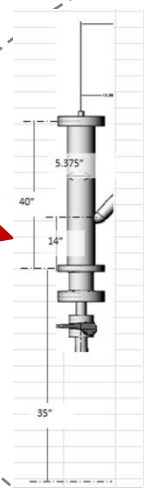


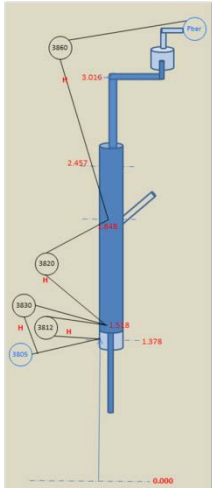
- **Raw data or response surface-based (RS) analysis**
- **Account for RS errors**
- **Different probability distributions**

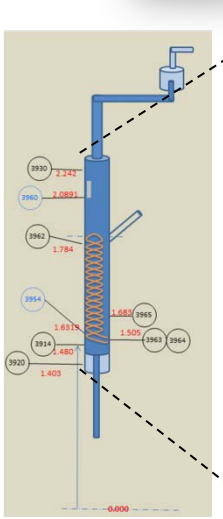
Simulation & Experiments to reduce time for design/troubleshooting

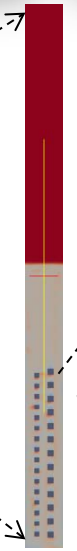
Experimental Validation

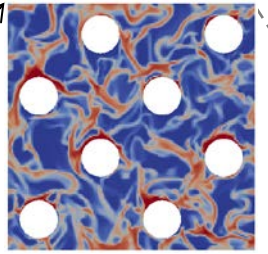
MFiX



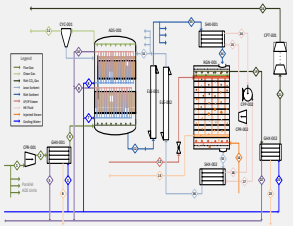




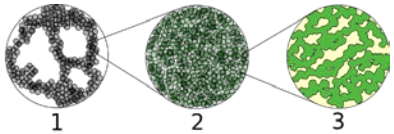


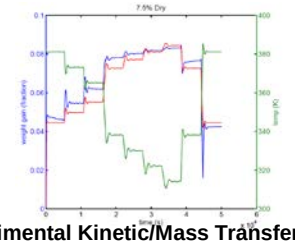


Process Models & Optimized Process

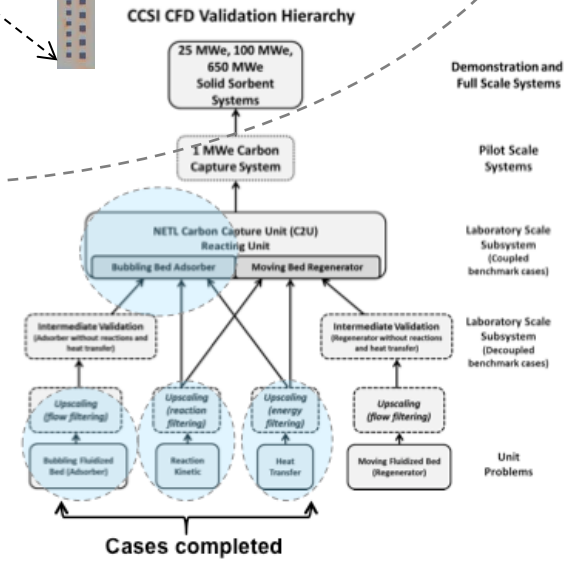


SORBENTFIT





Experimental Kinetic/Mass Transfer Data



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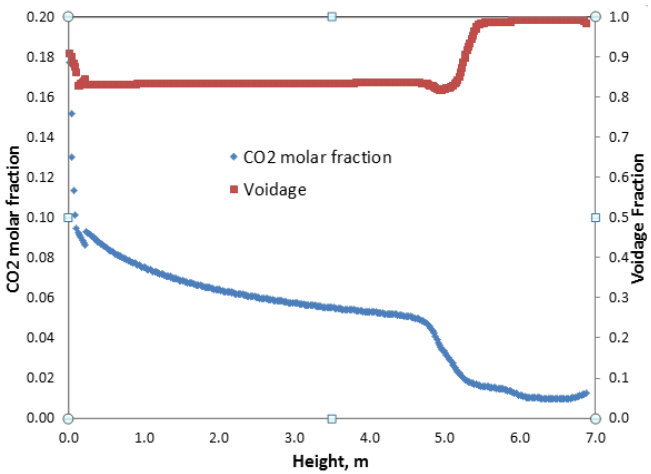
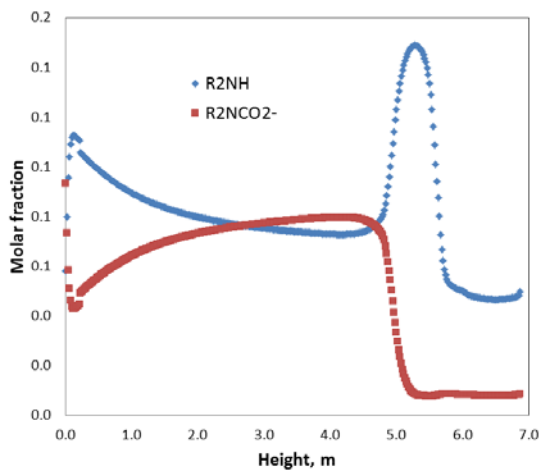
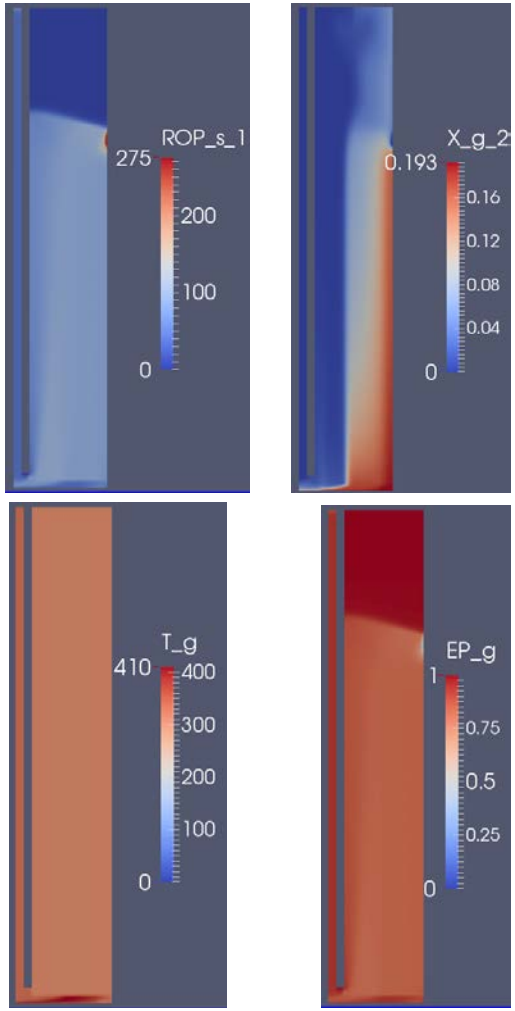
Predict Quantitative Confidence of 1MWe BFB Reactor

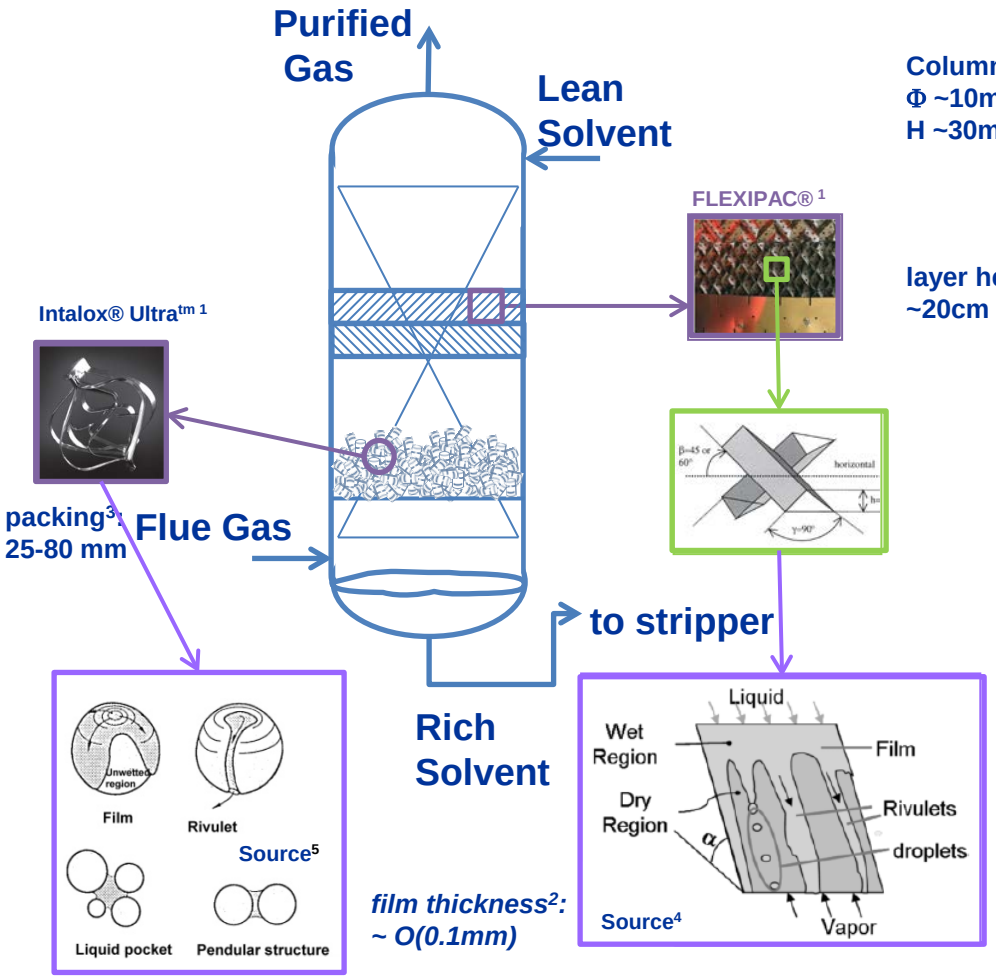
- Typical CFD results
  - Bed height 5.36 m (void fraction <0.95)
  - Temperature highest in the bottom where CO_2 adsorption rate highest
  - Sorbent amine molar fraction reduced to 6.5% at exit from 16%







Advanced Solvent System Scale Up



- Efficiency of CO_2 absorption is closely related to local flow behavior
- Cannot model entire column focusing in on all physical phenomenon
- Multi-scale approach required
- Developing closure models for **interphase interactions**

CCSI Release 2013.10.2	
Basic Data Submodels	High viscosity solvent model
	SorbentFit – Kinetic/diffusion basic data fitting tool with UQ
High Resolution Filtered Submodels	Attrition Model
	Cylinder Filtered Models with quantified uncertainty bounds
Validated high-fidelity CFD models & UQ tools	1 MW Adsorber and Regenerator CFD Models (validated)
	Large scale adsorber and regenerator CFD Models
	Statistical Model Validation Tool for Quantifying Predictions
	REVEAL: Reduced Order Modeling Tools for CFD and ROM Integration Tools
Process Models	Bubbling Fluidized Bed Reactor Model
	Moving Bed Reactor Model
	Multi-stage Centrifugal Compressor Model
	Membrane CO_2 Separation Model
	Reference Power Plant Model
Optimization and UQ Tools	FOQUS – Optimization & Quantification of Uncertainty
	ALAMO – Surrogate models for optimization
	Process Synthesis Superstructure
	Oxy-Combustion Process Optimization Model
Dynamics & Control	D-RM Builder
Risk Analysis Tools	Technical Risk Model
	Financial Risk Model
Crosscutting Integration Tools	SimSinter – Links simulation files to FOQUS/Turbine
	Turbine Science Gateway – Runs hundreds of thousands of simulations

Toolset Deployment

- Initial licensees: GE, ALSTOM, PHILLIPS 66
- Additional licensees: B&W, Chevron
- Others licenses in progress…. ExxonMobil, EPRI Electric Power Research Institute, Eastman, Southern Company
- CRADA: ADA Environmental Solutions in development GE
- Support: Help available for installation and use issues

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