Advanced Computational Tools to Accelerate the Development of Next Generation Technologies

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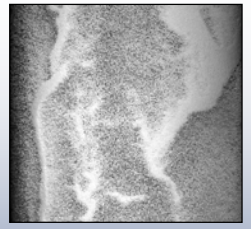
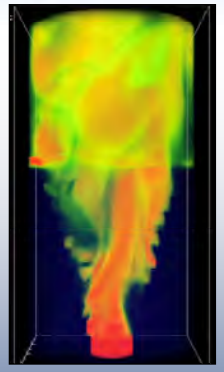
U.S. Department of Energy
National Energy Technology Laboratory

CCSI For Accelerating Technology Development

Carbon Capture Simulation Initiative


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
- Lawrence Livermore National Laboratory

Academia

- Carnegie Mellon
- Princeton University
- West Virginia University
- Boston University
- The University of Texas at Austin
- Institute for Clean and Secure Energy, The University of Utah

Industry

- Fluor
- ADA Environmental Solutions
- B&W
- GE
- EPRI Electric Power Research Institute
- Air Products
- Burns & McDonnell Since 1898
- AEP American Electric Power
- Southern California Edison, An Edison International Company, San Onofre Nuclear Generating Station
- Alstom
- Duke Energy
- URS
- Southern Company
- Boeing
- DuPont
- ExxonMobil
- Chevron
- Phillips 66
- WorleyParsons resources & energy
- Eastman

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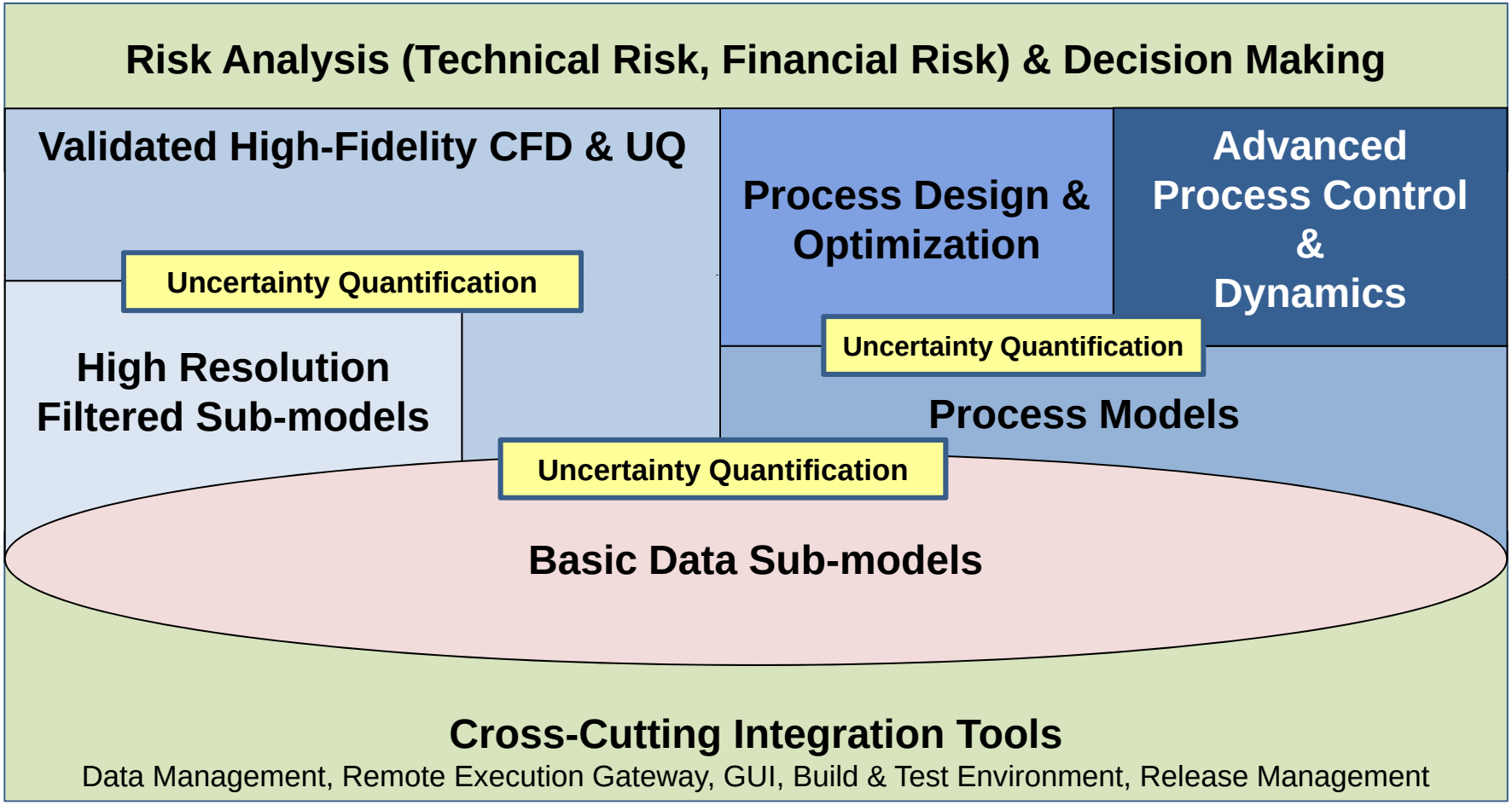

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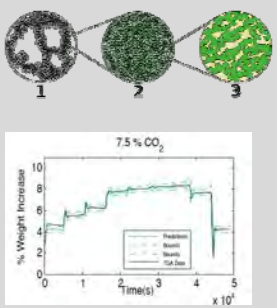
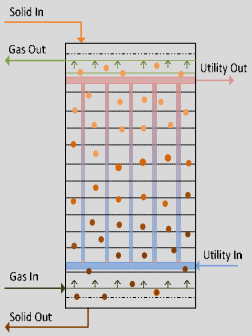
Advanced Process Systems Engineering Approaches

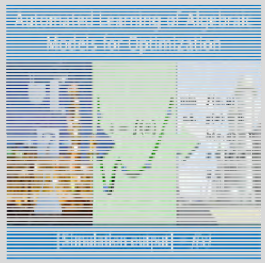
Basic Data Models



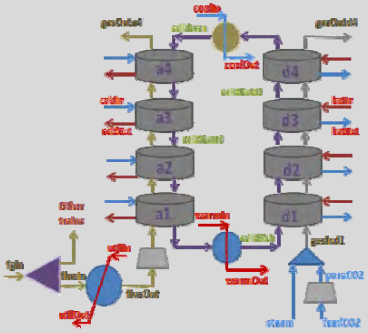
Process Models



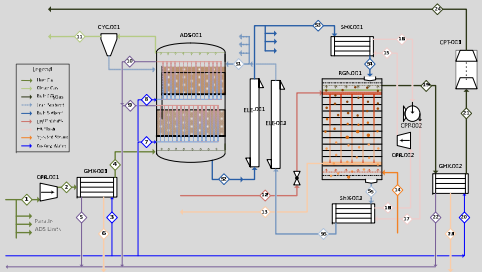
Algebraic Surrogate Models



Superstructure Optimization



Optimal Process



SORBENTFIT

aspentech

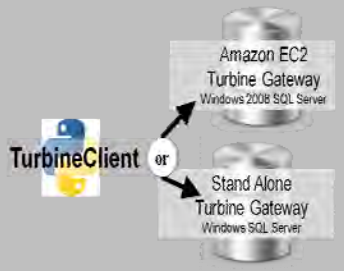
ALAMO

GAMS

gPROMS

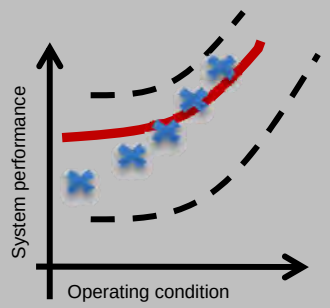
PSUADE

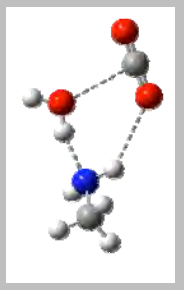
Simulation Gateway

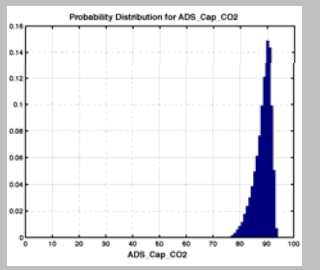


Simulation-Based DFO Framework

Uncertainty Quantification with Bayesian Calibration







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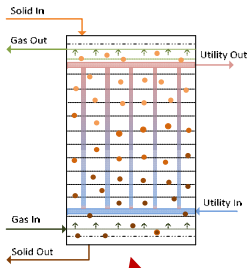
CFD models to reduce time for troubleshooting

Experimental Validation

Process Model



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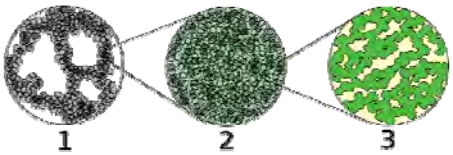
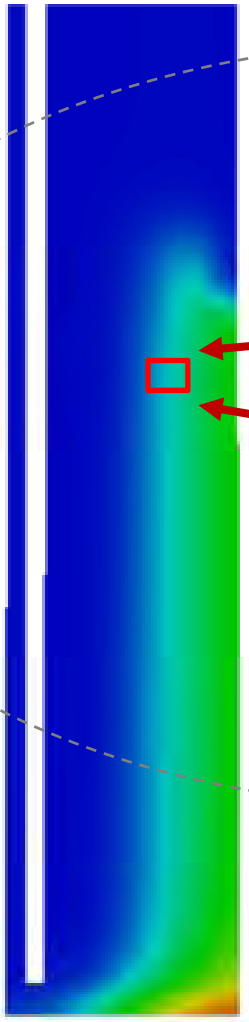
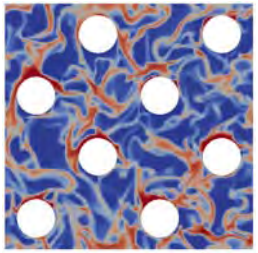




ANSYS FLUENT

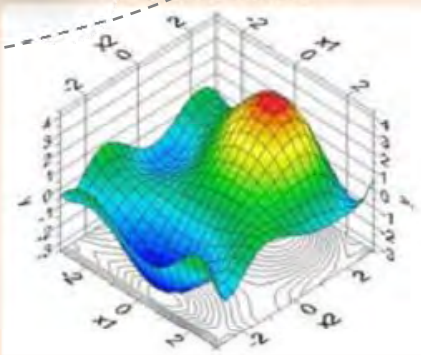
Heat-transfer-tube-scale hydrodynamics

$$f^*_{drag} = \beta^*\left(-v^*_s\left|v^*_s\right|\right) + \gamma^*$$



MFiX

Response Surface



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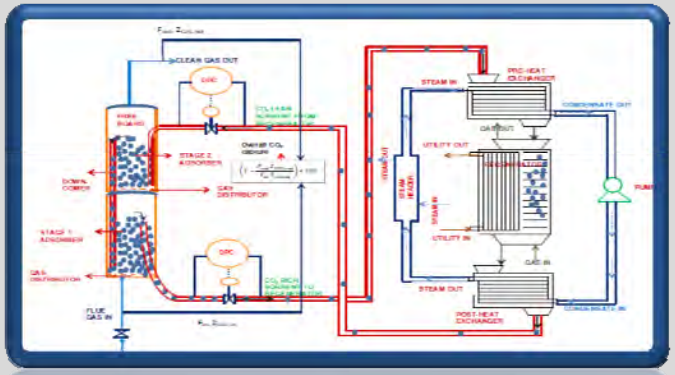
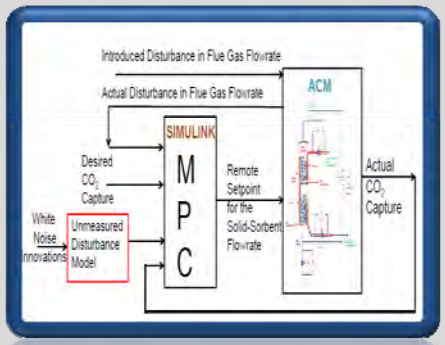
Dynamic Reduced Models & APC Framework

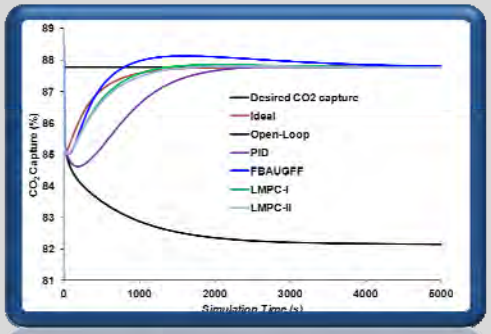
1-D Capture & Compression System Models



Dynamic Reduced Models

Advanced Process Control Framework





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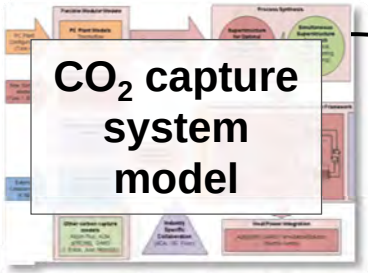
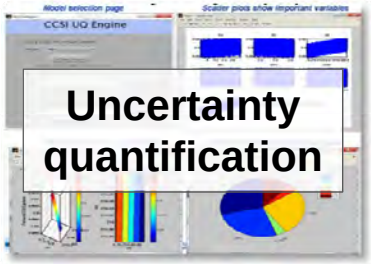
Risk analysis and decision making framework



CO_2 capture system model

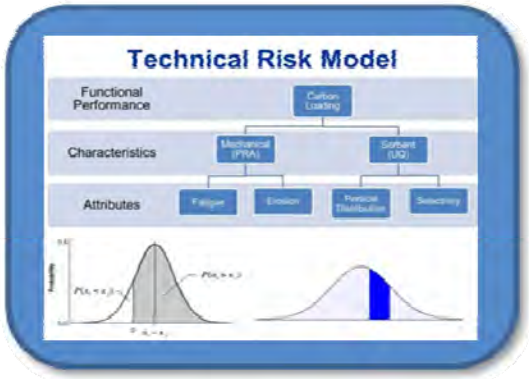


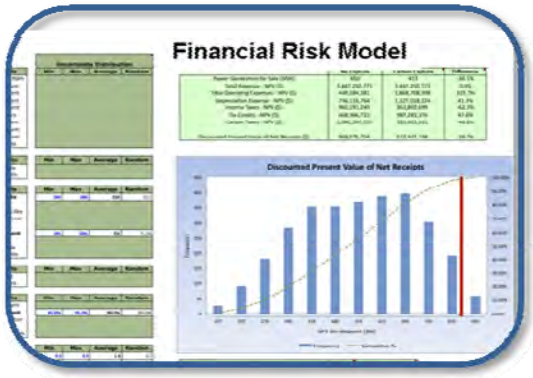
Uncertainty quantification

Risk factor expert elicitation

Technology maturity model

Combine technical risk and financial risk factors into an integrated decision analysis framework that naturally handles propagation of uncertainties into a variety of decision metrics.





Technical Risk Analysis

Financial Risk Analysis

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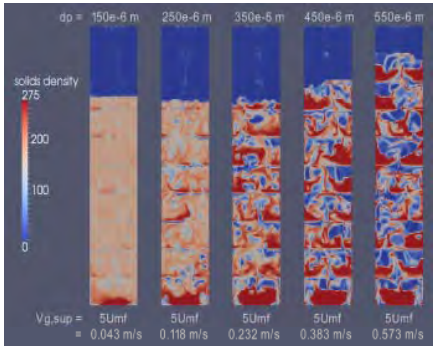
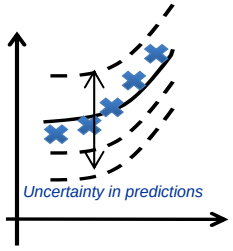
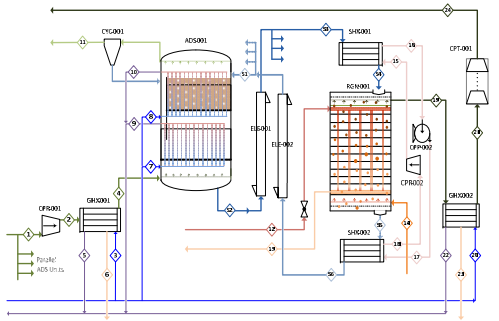
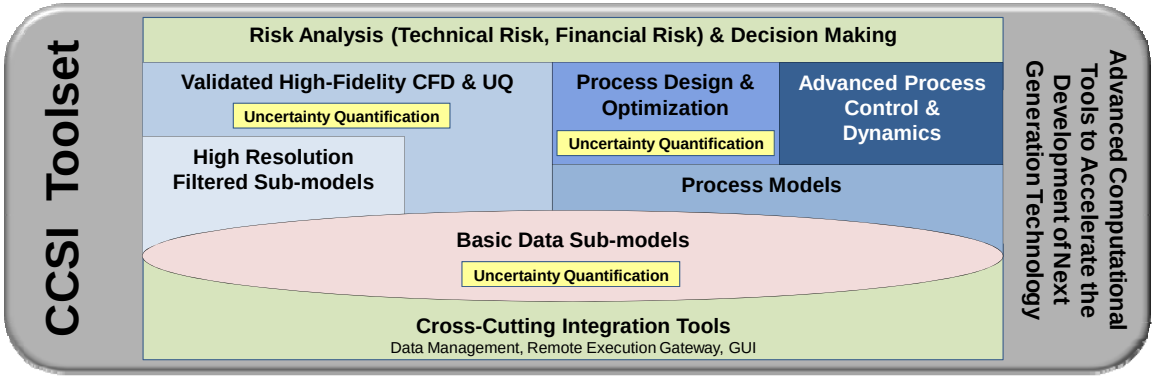
CCSI Deploys Initial Computational Toolset

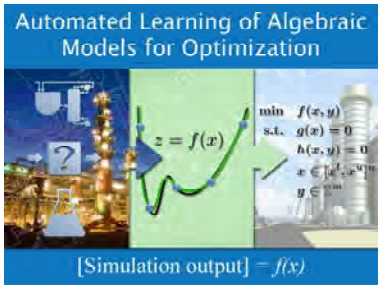
- Released 21 Toolset components Sept. 2012
  - Reaction kinetics model of solid sorbents
  - CFD models of 1 MW adsorber & regenerator
  - Process models of solid-sorbent capture, membrane, and compression systems
  - New optimization tools (ALAMO, superstructure, framework)
  - Advanced dynamic & control models (adsorber, compression
  - New integration tools (REVEAL, Turbine, Sinter)
  - Uncertainty Quantification Framework
  - Financial Risk Tool











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Thank you!