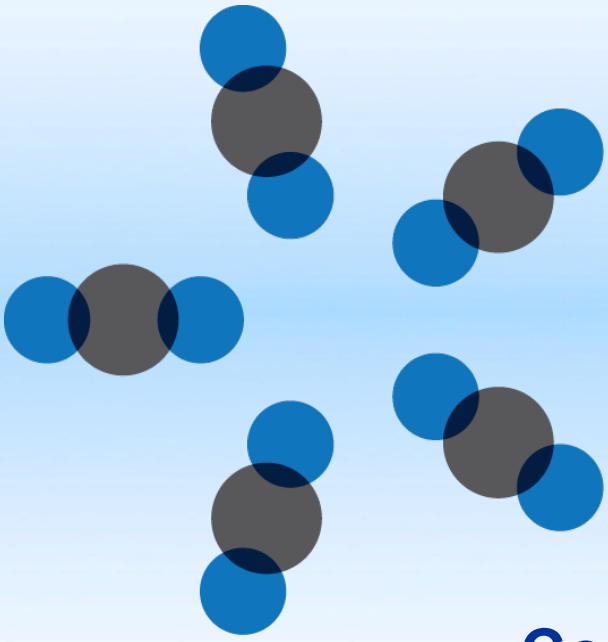

CCSI

Carbon Capture Simulation Initiative

Computational Tools to Accelerate Commercial Development

David C. Miller, Ph.D.
U.S. Department of Energy
National Energy Technology Laboratory

4 November 2013

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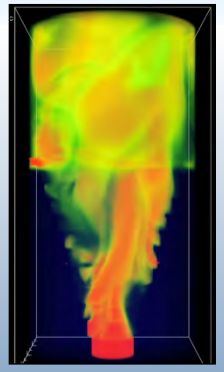
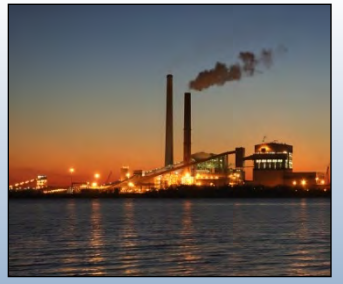
CCSI For Accelerating Technology Development

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

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- 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

Industry

- ADA Environmental Solutions
- Alstom
- B&W (The Babcock & Wilcox Company)
- GE
- EPRI Electric Power Research Institute
- Fluor
- Phillips 66
- AEP American Electric Power
- Southern California Edison (An Edison International Company)
- Southern Company
- Chevron
- URS
- ExxonMobil
- Air Products
- Eastman
- ANSYS
- aspentech
- invensys
- PSE

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Motivation and Timeline

- 2009: Carbon Regulations Imminent
- How can development & commercialization be accelerated while minimizing cost and risk?
- Role of advanced simulation & modeling in accelerating development, scale up and commercialization
  - Build on existing modeling & simulation tools used by industry
- 2010: Multi-lab - industry working group
- HQ organized Scientific Peer Review: Jan 25, 2011
- Preliminary Release of CCSI Toolset: September 2012
  - Five companies sign Test & Evaluation License
- 2013 Toolset Release: October 31, 2013

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Goals

- **Develop** new computational tools and models to enable industry to more rapidly develop and deploy new advanced energy technologies

- **Demonstrate** the capabilities of the CCSI Toolset on non-proprietary case studies
  - Solid sorbent
  - Solvent system

- **Deploy** the CCSI Toolset to industry
  - Support initial industry users
  - Feedback on features and capabilities

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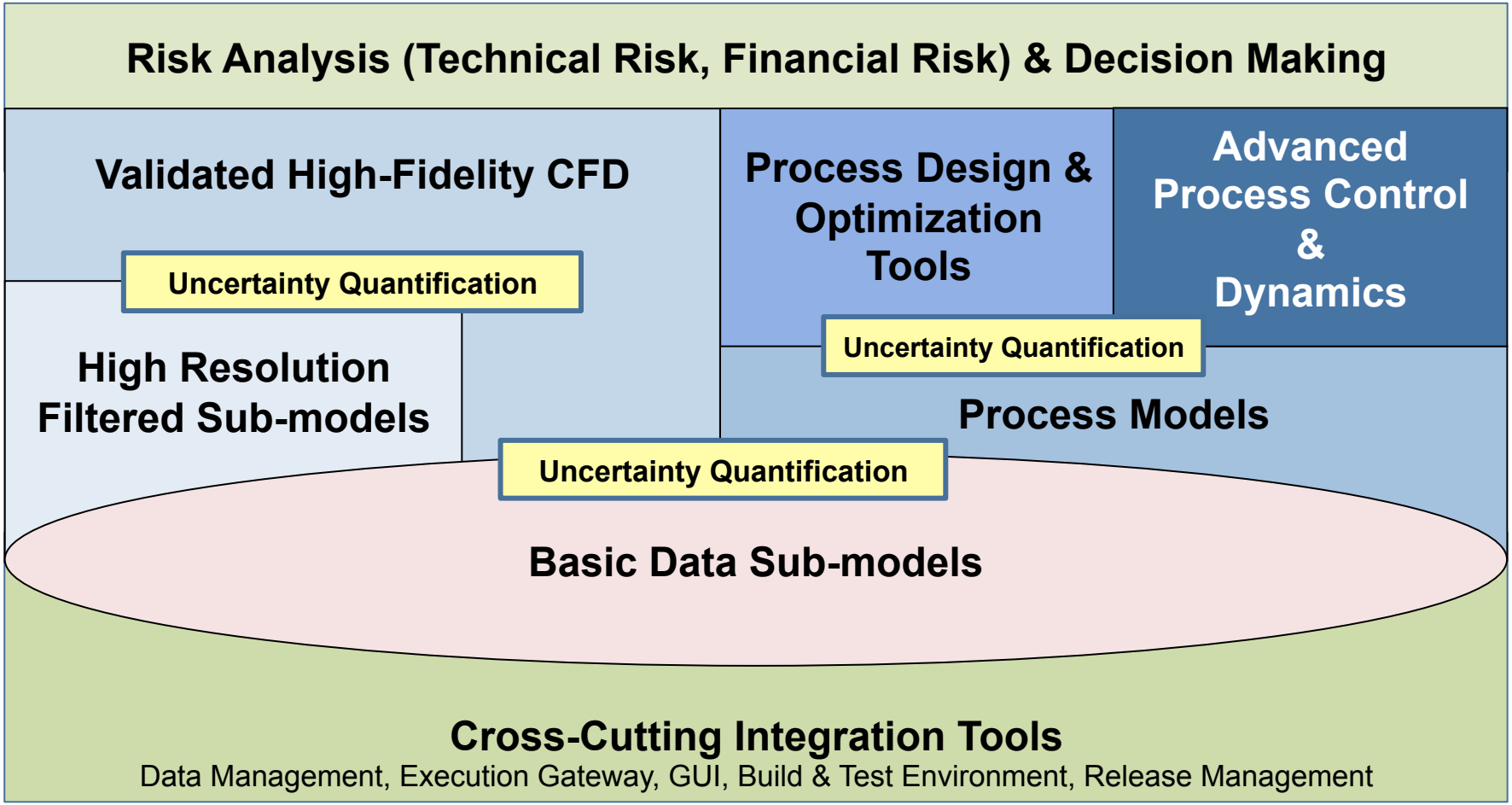
Challenges of Simulating Carbon Capture (and other) Processes

- **Multiple Scales**
  - **Particle**: individual adsorbent behavior, kinetics and transport
  - **Device**: fluid and heat flows within a sorbent bed
  - **Process**: integration of devices for a design of a complete sorbent system
- **Integration across scales**
  - Effective simplifications: Detailed tools too complex to integrate/optimize
- **Verification/Validation/Uncertainty**
  - Create confidence in predictions of models
- **Decision support**
  - Evaluate key process performance issues affecting choices of technology deployment/investment

Advanced Computational Tools to Accelerate Carbon Capture Technology Development



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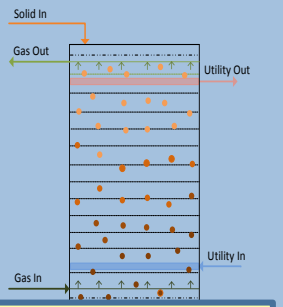
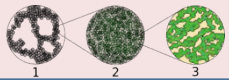
Tools to develop an optimized process using rigorous models

Process Models



Uncertainty

Basic Data Submodels



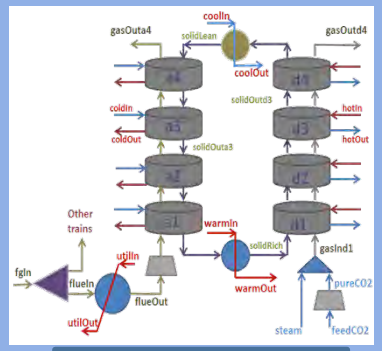
Uncertainty

Algebraic Surrogate Models

ALAMO

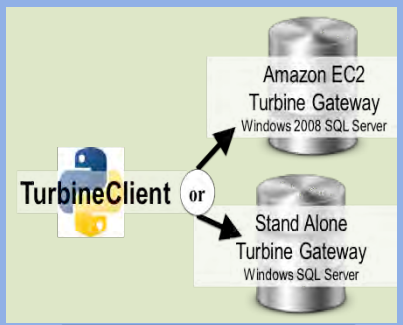
Uncertainty

Superstructure Optimization (Determine Configuration)



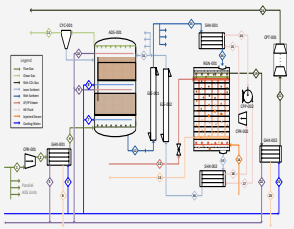
Uncertainty

Simulation-Based Optimization



Uncertainty

Optimized Process



Uncertainty

- Uncertainty Quantification
- Process Dynamics and Control
- CFD Device Models
- Risk Analysis

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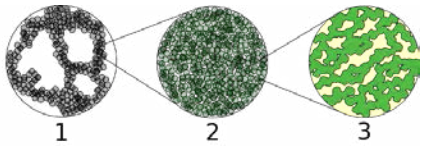
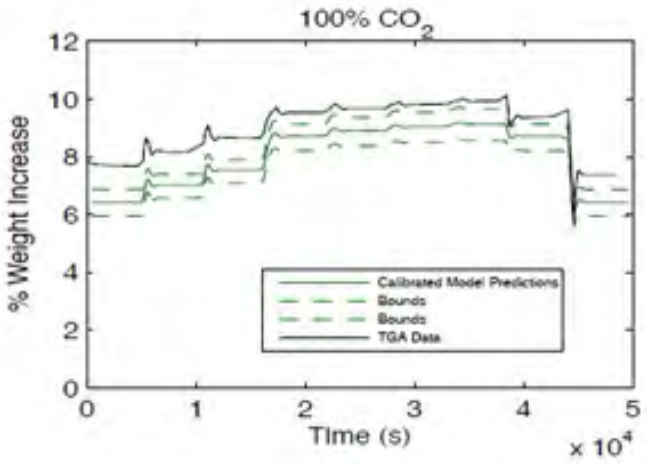
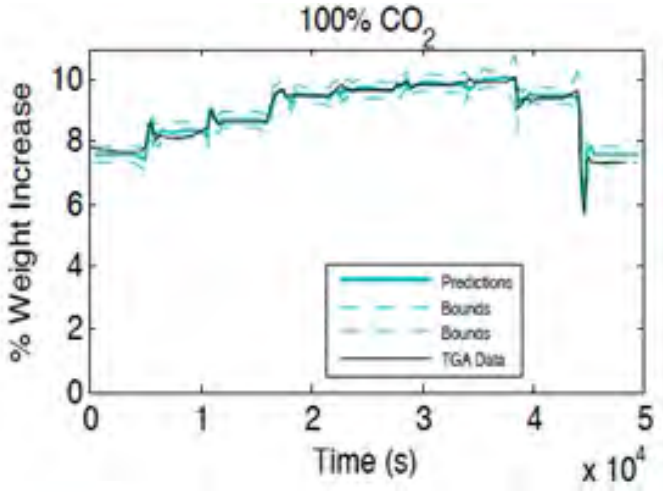
PEI-Impregnated Silica Sorbent Reaction Models

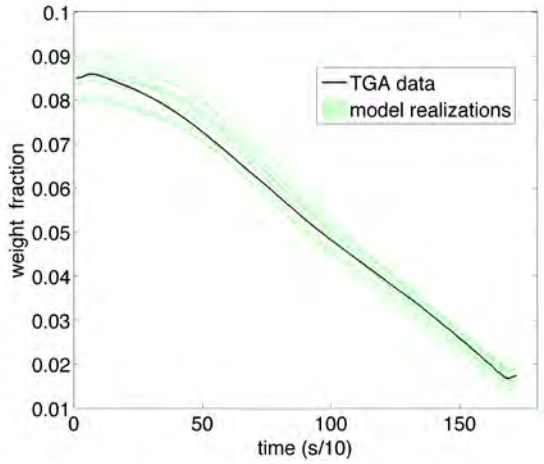


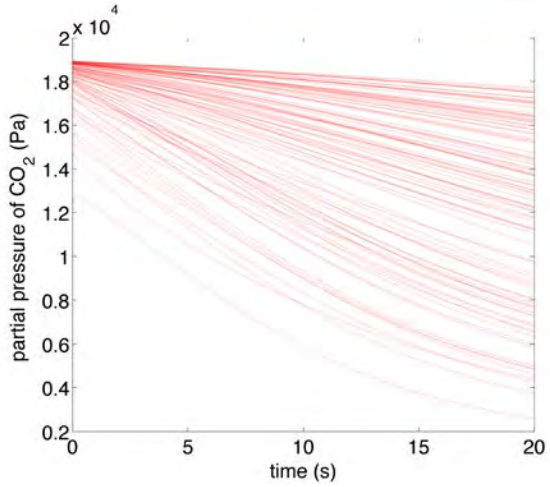
$$2R_2NH + CO_2(gas) \rightleftharpoons R_2NCO_2^- + R_2NH_2^+$$
$$R_2NH + H_2O(phys) + CO_2(gas) \rightleftharpoons HCO_3^- + R_2NH_2^+$$
$$H_2O(gas) \rightleftharpoons H_2O(phys)$$

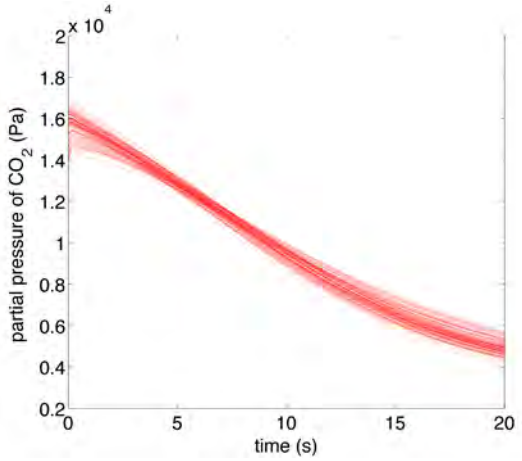


With Discrepancy









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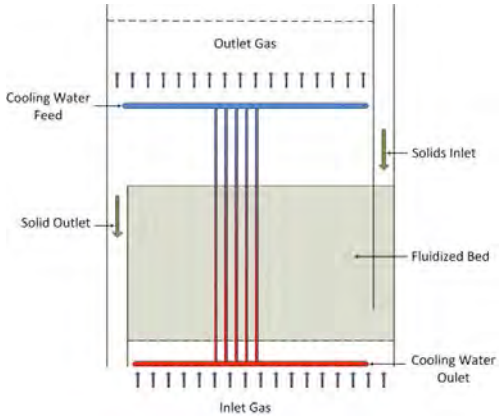
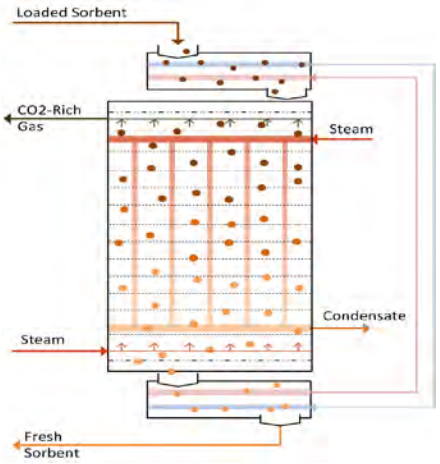
Process Models

Bubbling Fluidized Bed (BFB) Model

- 1-D, nonisothermal with heat exchange
- Unified steady-state and dynamic
- Adsorber and Regenerator
- Variable solids inlet and outlet location
- Modular for multiple bed configurations



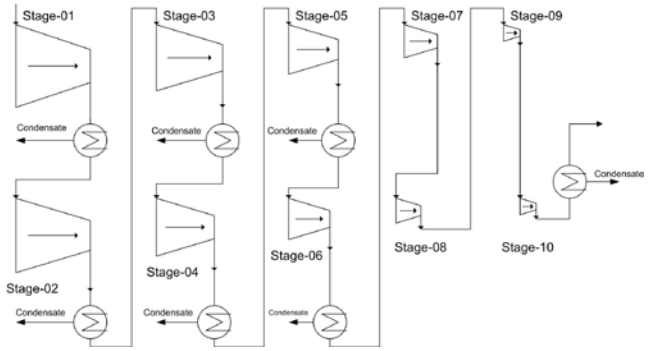


Moving Bed (MB) Model

- 1-D, nonisothermal with heat exchange
- Unified steady-state and dynamic
- Adsorber and Regenerator
- Heat recovery system

Compression System Model

- Integral-gear and inline compressors
- Determines stage required stages, intercoolers
- Based on impeller speed limitations
- Estimates stage efficiency
- CO_2 drying (TEG absorption system)
- Off-design performance.
- Includes surge control algorithm



816c: Moving Bed, Kim, Modekurti, Miller, Bhattacharyya, Zitney, Friday, Nov. 8 @ 12:30 pm in Union Square 12
774b: Dynamic Model, Modekurti, Bhattacharyya, Zitney, Miller, Friday, Nov. 8 @ 8:55 am in Mason B

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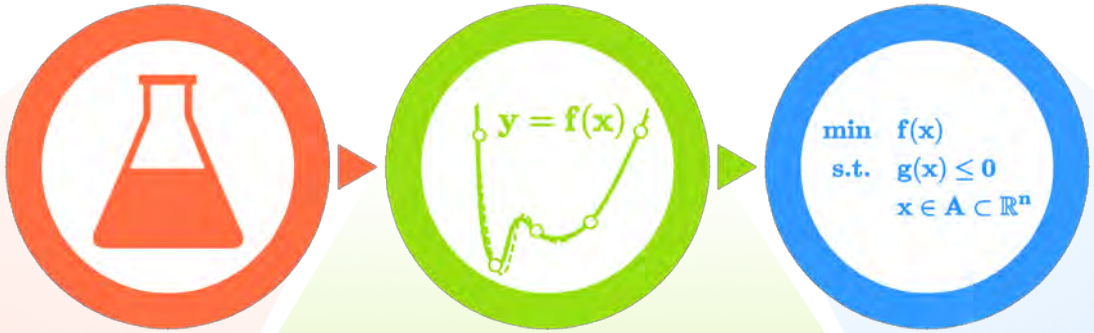
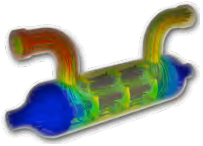
ALAMO

Automated Learning of Algebraic Models for Optimization

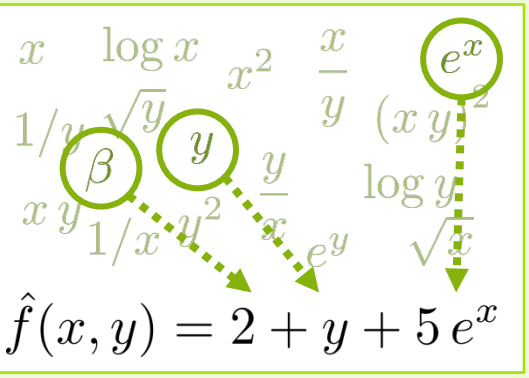
Simplifying the balance between optimal decision-making and model fidelity through tailored simple surrogate models



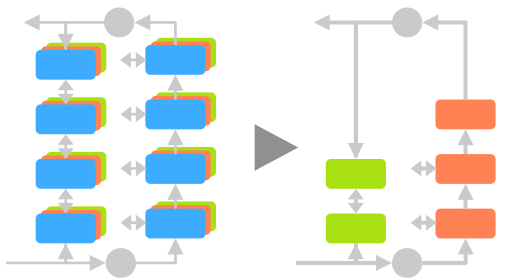
High-fidelity simulations and experiments



Algebraic surrogate models



Superstructure optimization



Technology selection

287e: Algebraic Surrogates, Sahinidis, Tuesday, Nov 5 @ 2:10 pm in Continental 8
589b: ALAMO, Cozad, Sahinidis, Miller. Thursday, Nov 7 @ 8:50 in Continental 7
554d: Superstructure, Yuan, Sahinidis, Miller, Wednesday, Nov 6 @ 4:15 in Union Square 11.

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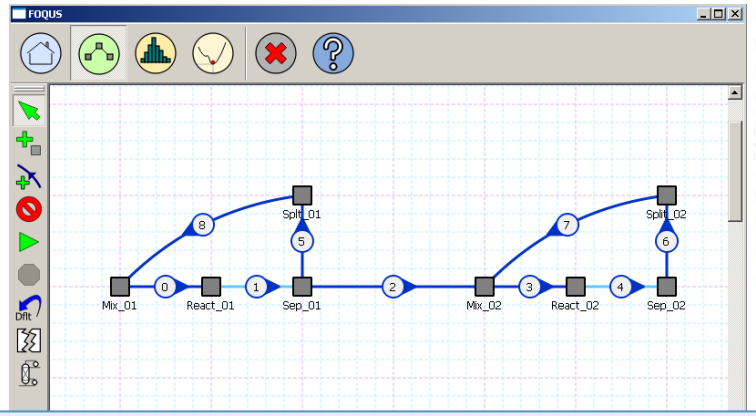
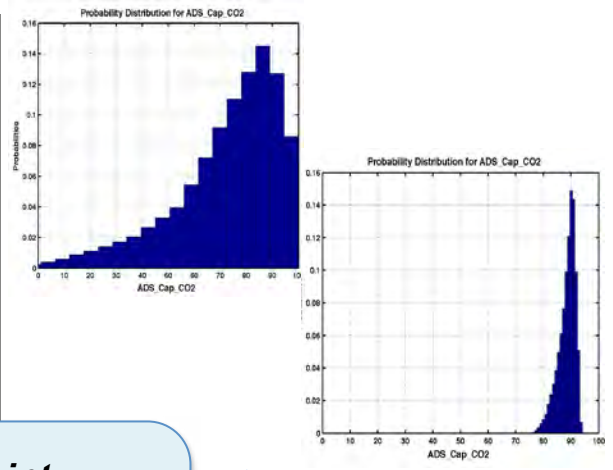
Framework for Optimization and Quantification of Uncertainty and Sensitivity

FOQUS





Derivative Free Optimization or Uncertainty Quantification Sample Generation

Sample Set

Result Set

Parallel Flowsheet Execution

Meta-Flowsheet

Meta-Flowsheet

Meta-Flowsheet

- Connects to Turbine/SimSinter to run simulations.

Heat Integration

538d: Chen, Eslick, Grossmann, Miller, Wednesday, Nov. 6 @ 4:21 pm in Continental 9

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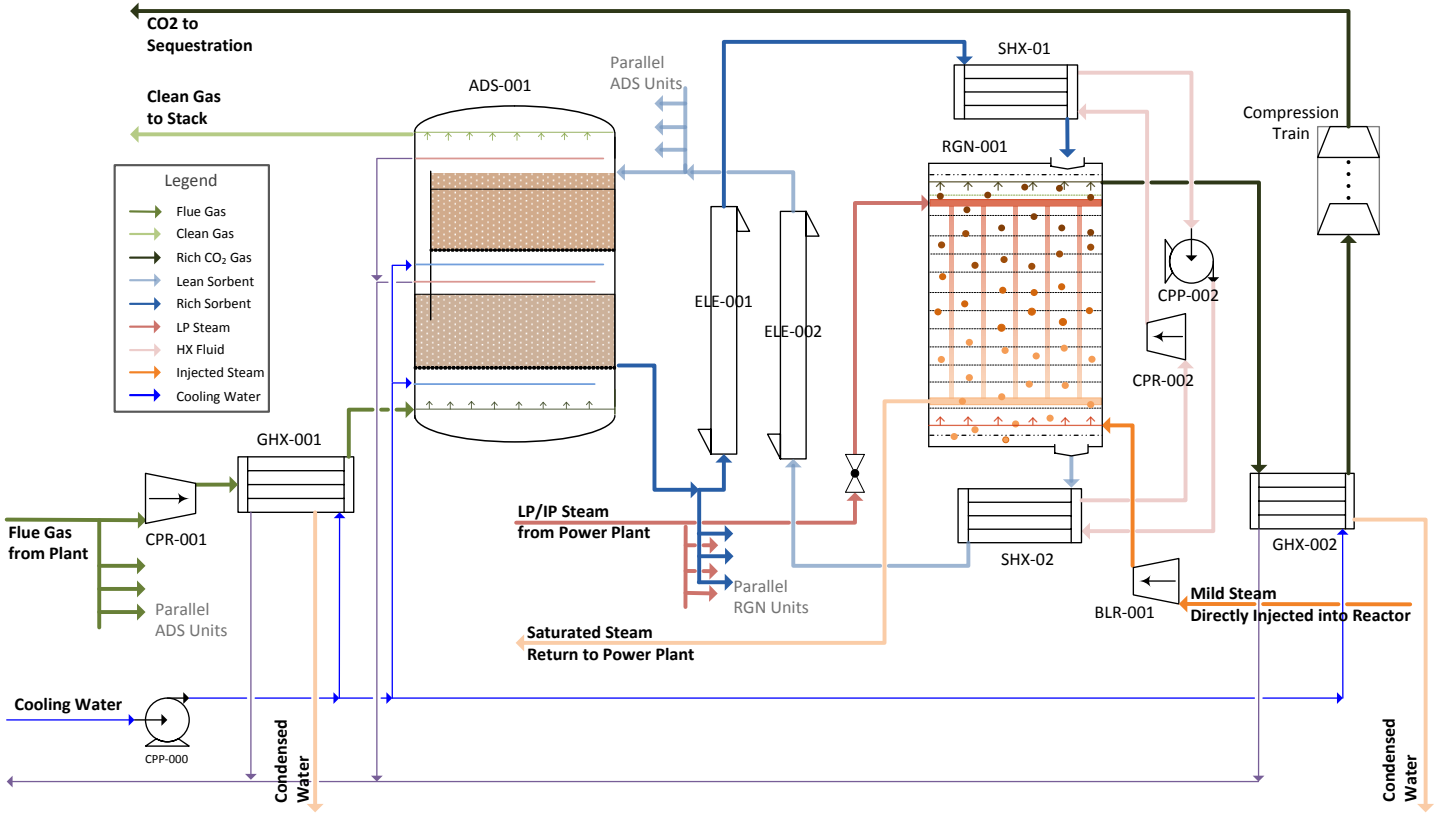
Optimized Process Developed using CCSI Toolset



ΔLoading
1.8 mol CO2/kg
0.66 mol H2O/kg

	Solid Sorbent	MEA (D10°C HX)	MEA (D5°C HX)
Q_Rxn (GJ/tonne CO2)	1.82	1.48	1.48
Q_Vap (GJ/tonne CO2)	0	0.61	0.74
Q_Sen (GJ/tonne CO2)	0.97	1.35	0.68
Total Q	2.79	3.44	2.90

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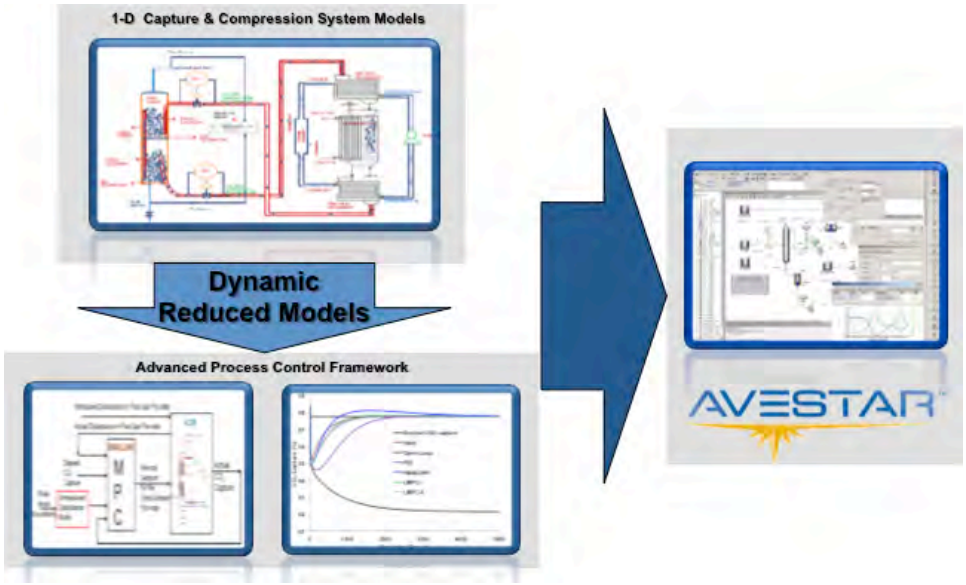
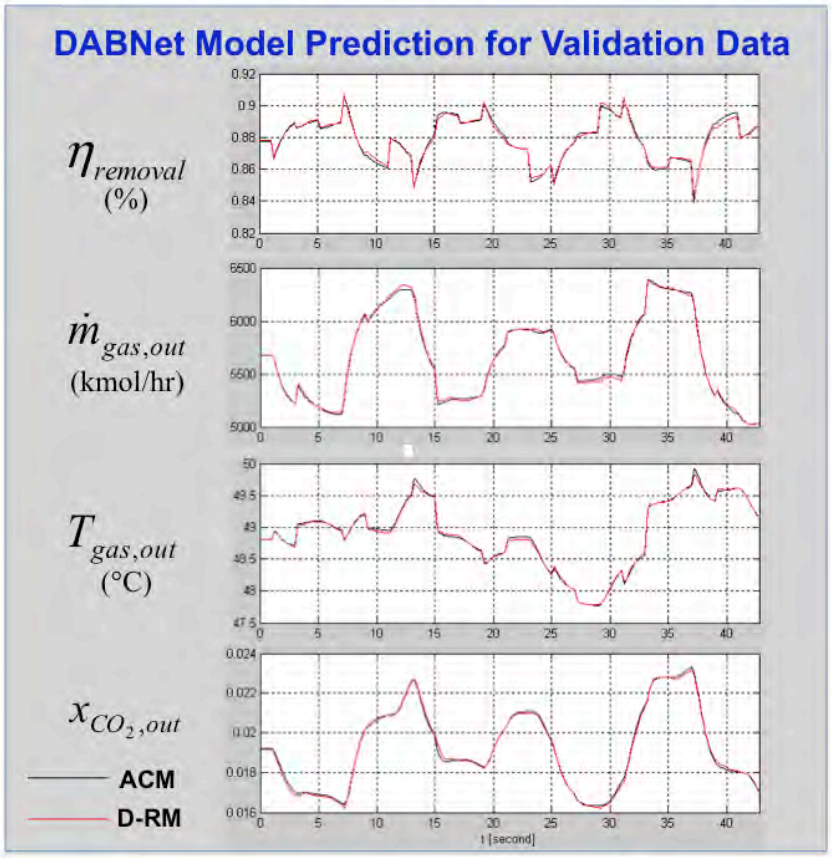
Dynamic Reduced Model Builder



Example (BFB Reactor/Adsorber)



- **Automatic D-RM Generation**
  - Use high-fidelity ACM/APD models embedded in Simulink to create data-driven black-box D-RMs as MATLAB script files (.m files)
- **GUI Driven Workflow**
- **Data-driven Black-Box Methods**
  - Nonlinear Autoregressive Moving Average (NARMA) based on Neural Networks
  - Decoupled A-B Net (DABNet)

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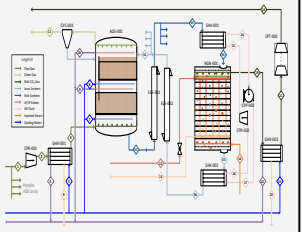
Simulation & Experiments to reduce time for design/troubleshooting

Experimental Validation

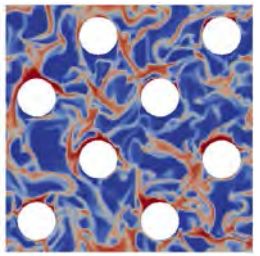
Process Models & Optimized Process



ANSYS FLUENT

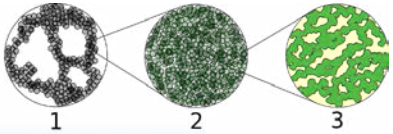
Heat-transfer-tube-scale hydrodynamics

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

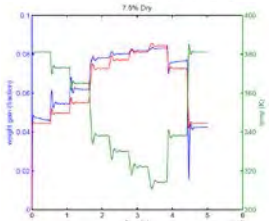


MFIX Multiphase Flow with Interphase eXchanges

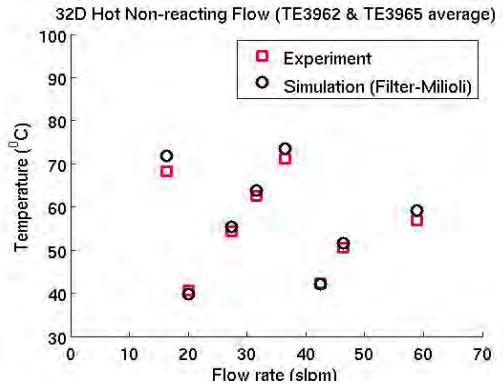
SORBENTFIT



Void Fraction along vertical center plane



Experimental Kinetic/Mass Transfer Data



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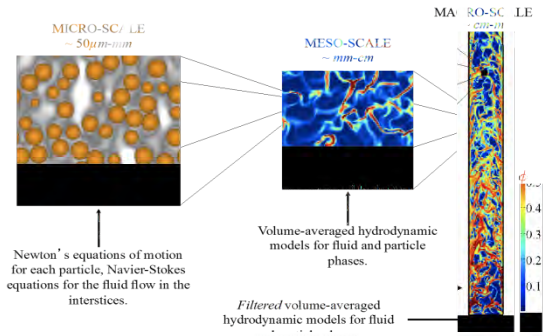
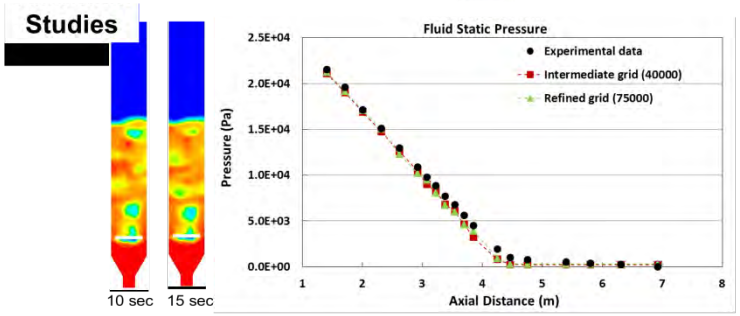
High Resolution, Validated Multi-scaleCFD Models

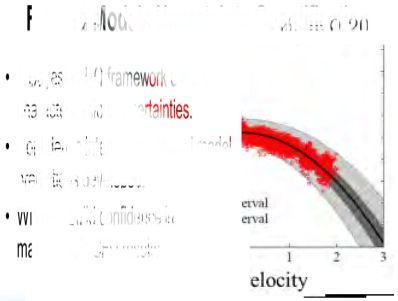
Filtered Models for Gas-Particle Flows

Filtered Models for Gas-Particle Flows

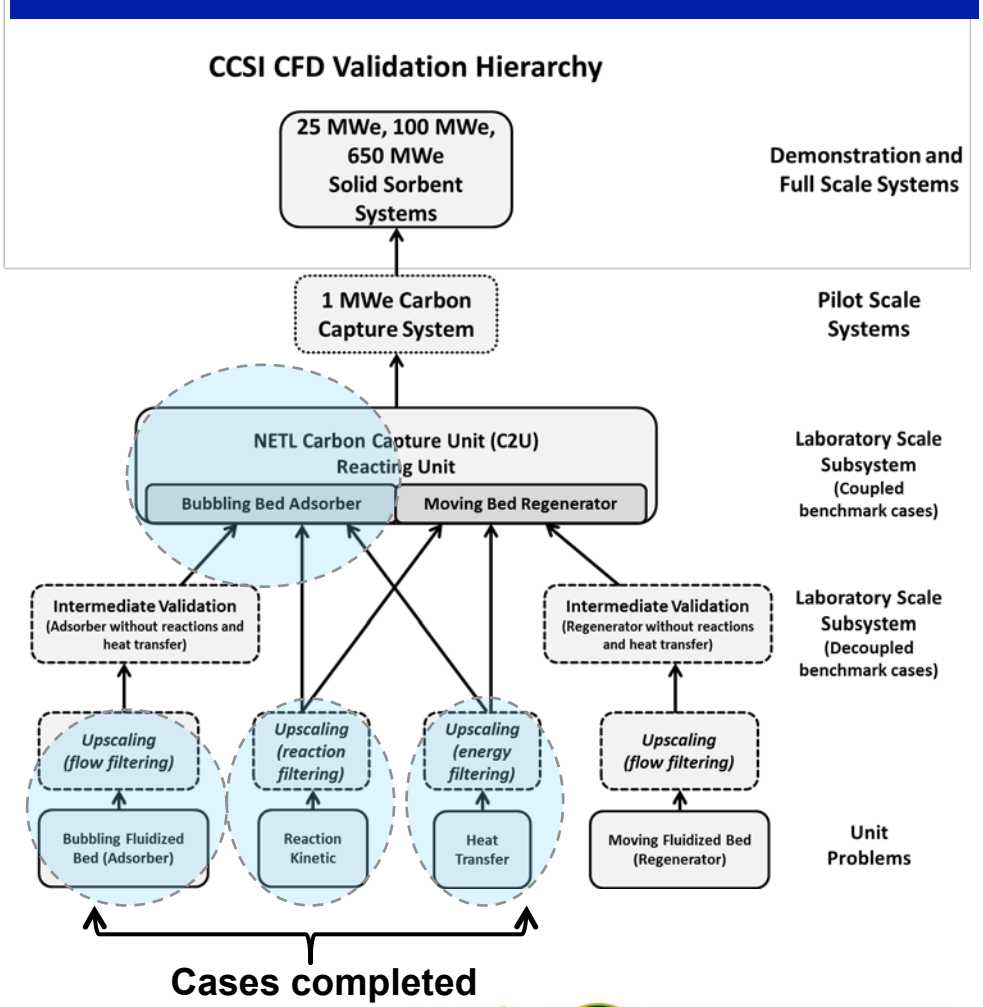




Validation and UQ of Filtered Models



Objective: To provide quantitative confidence on device-scale (CFD) model predictions for devices that are yet to be built.



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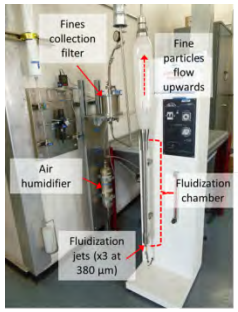
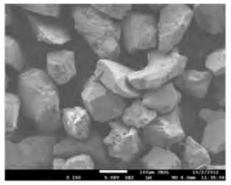
CFD Modeling of Carbon Capture Sorbent Particle Attrition

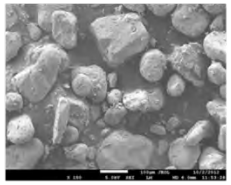
Experimental Attrition Observation



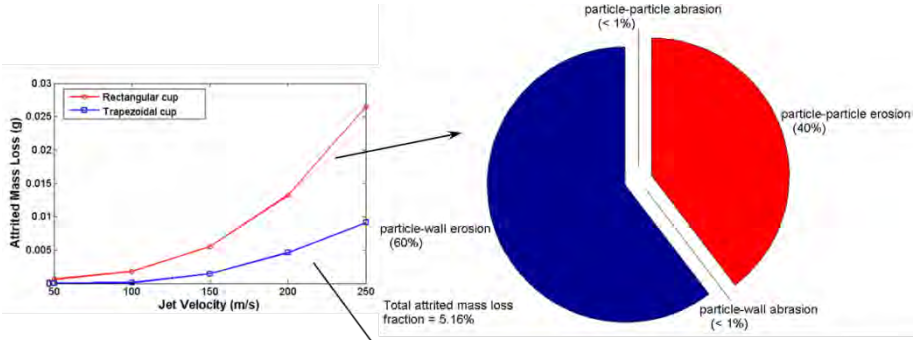
ASTM-5757 Attrition Test Unit

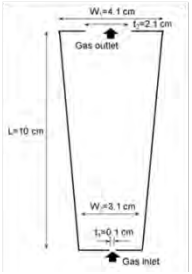
SEM images show evidence of particle abrasion (rounding and fines)

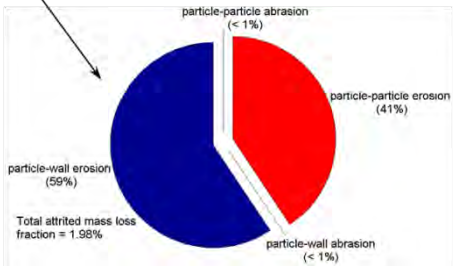

Hematite (fresh)


Hematite (post-attrition)

Jet Cup Modeling: Understanding the Mechanisms of Attrition

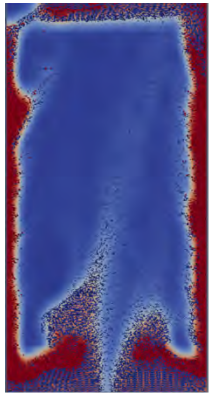


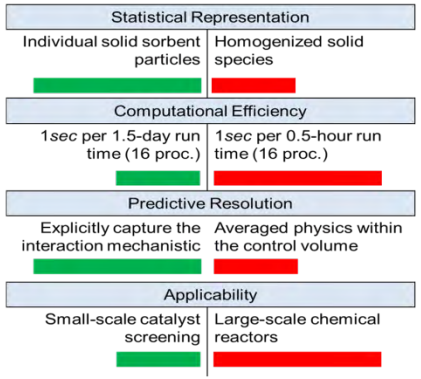




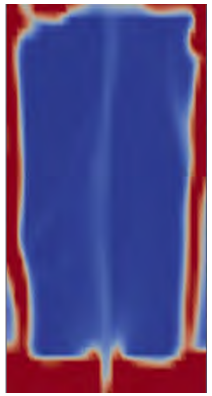
Attrition Models

CFD Discrete Element Model





Population Balance Model



- Dominant attrition mechanism: erosive chipping
- Major attrition source: particle-wall interaction
- Critical operating factors: jet velocity and sorbent density

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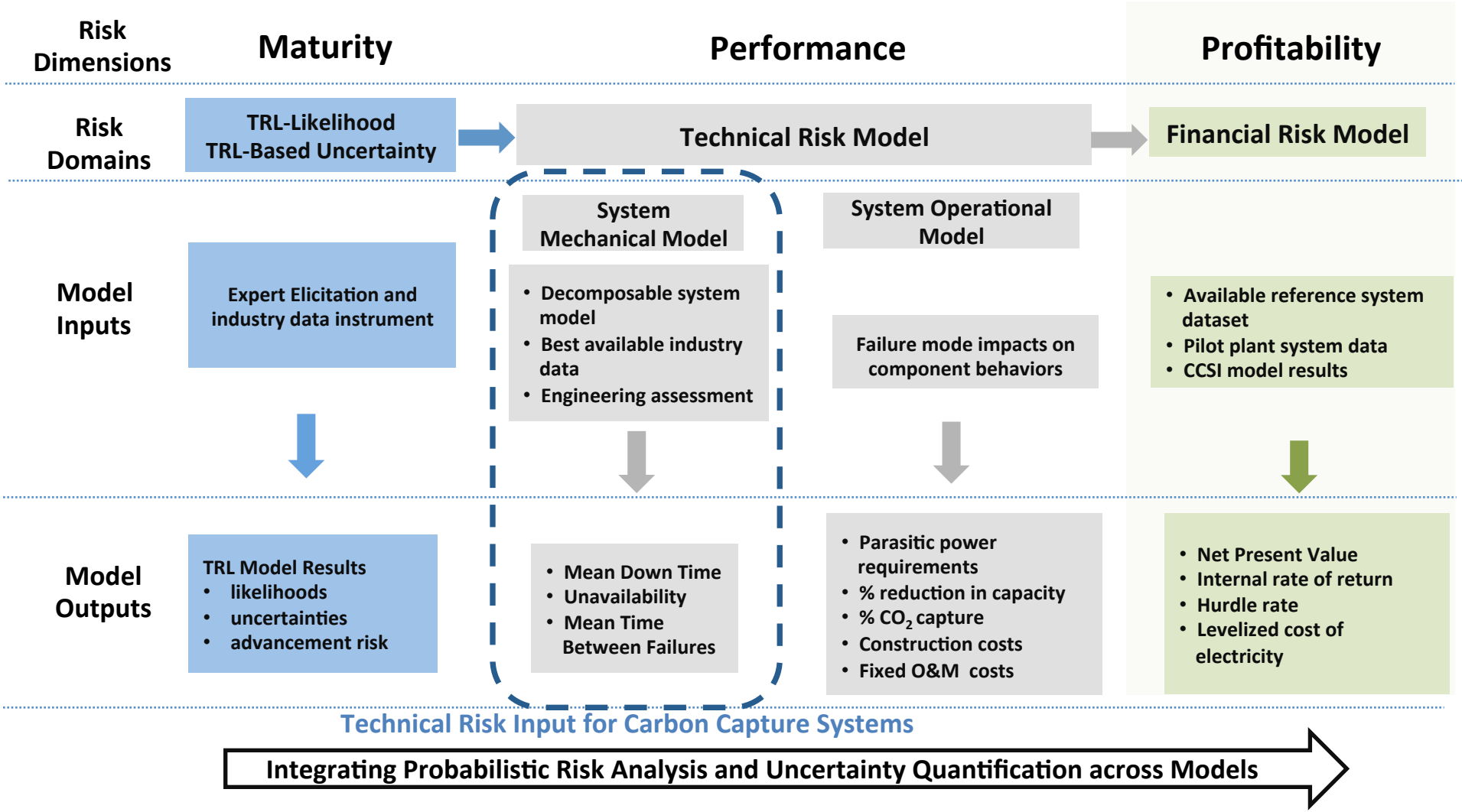
Risk Integration Across Models



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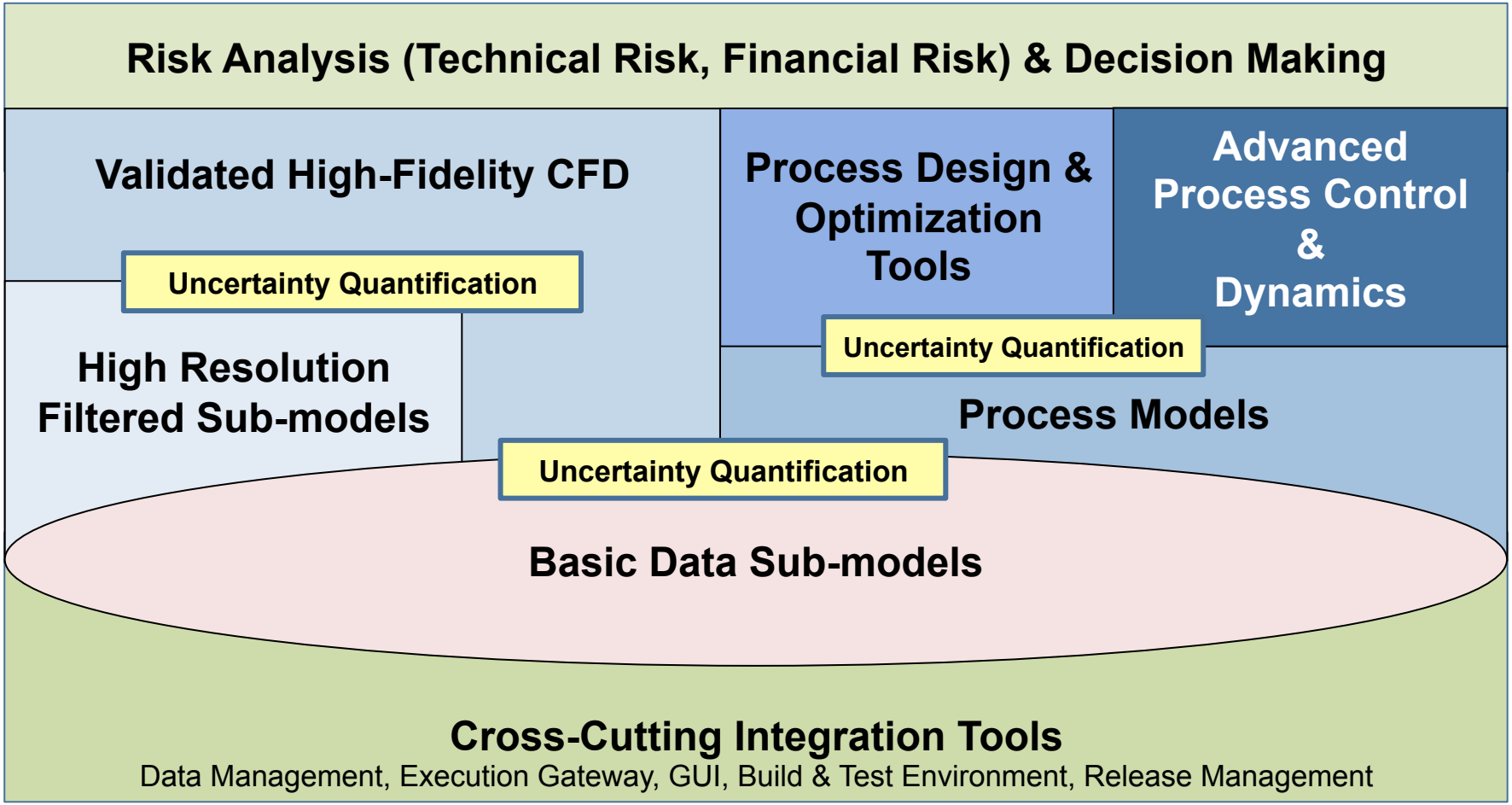
Advanced Computational Tools to Accelerate Carbon Capture Technology Development



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