CCSI
Carbon Capture Simulation Initiative

Advanced Computational Tools for Optimization and Quantification of Uncertainty

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National Energy Technology Laboratory
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  - David Mebane

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Outline

- **DOE/FE Mission & Carbon Capture Challenge**
- Carbon Capture Simulation Initiative
- Optimization & Quantification of Uncertainty
- Summary

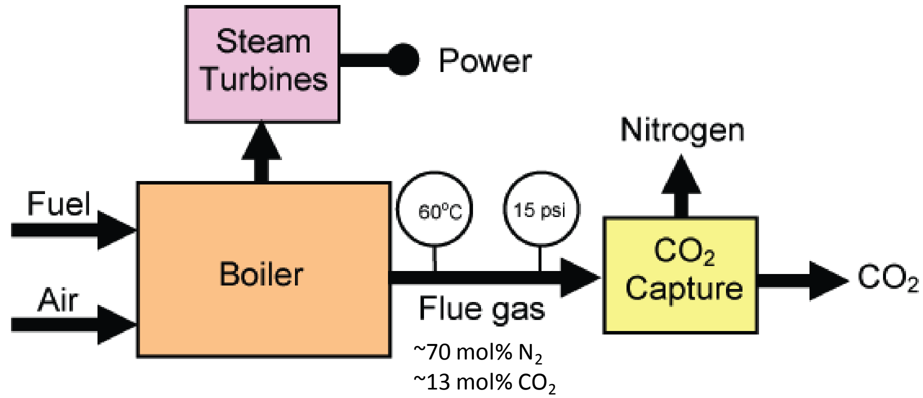
Mission

- RD&D of cutting edge fossil energy technologies to ensure a secure, affordable, low-carbon energy future.
  - Collaborative partnerships with industry
  - International collaboration

- The Cross-cutting Research activity serves as a bridge between basic and applied research by fostering the development and deployment of innovative systems for improving efficiency and environmental performance.
  - Includes development of computation, simulation, and modeling tools focused on optimizing plant design and shortening developmental timelines.

Challenges associated with carbon capture

- Fossil energy generates:
  - 67% of the US electricity
    - 42% coal, 25% natural gas
  - 65% worldwide electricity



- Large-scale problem
  - 2 billion tons/year CO_2 emitted from coal by 2020 in US
  - Flue gas: 5 million lb/hr for 550MW PC plant (630 kg/s)

- No existing economical solution
  - Cost of capture plant
  - De-rate of power plant

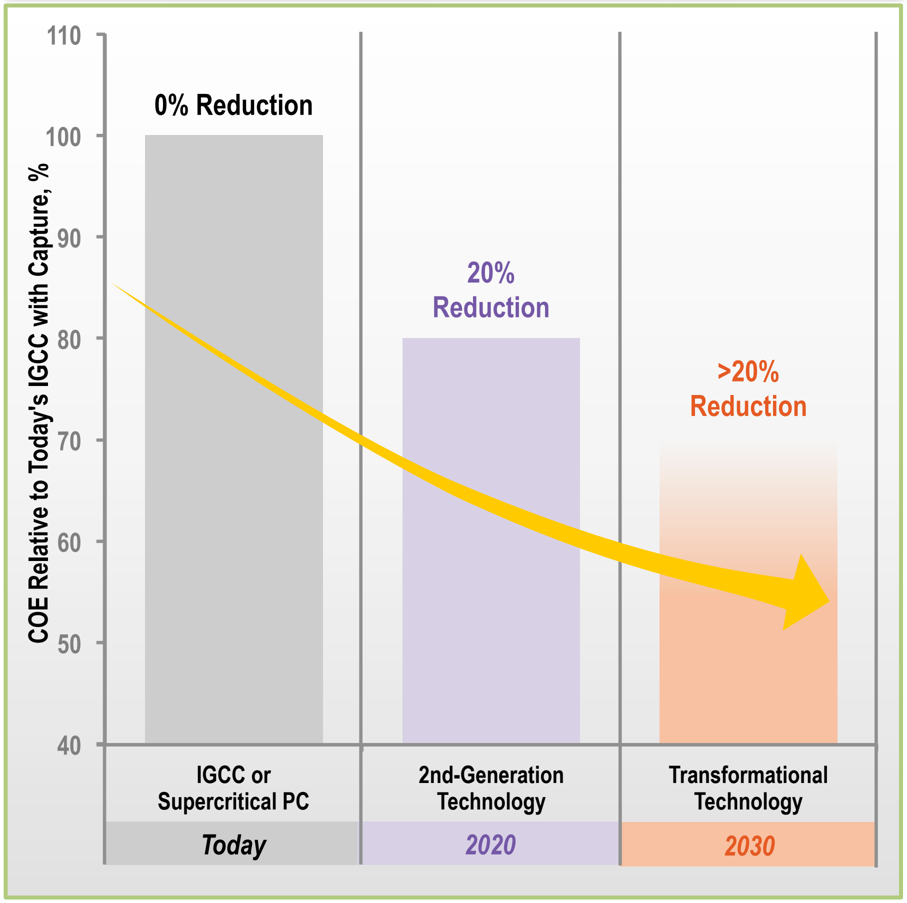
- Need for system optimization to fully evaluate technology options

U.S. Energy Information Administration, Annual Energy Outlook 2013 Early Release Overview. Report Number: DOE/EIA-0383ER(2013), http://www.eia.gov/forecasts/aeo/er/pdf/0383er%282013%29.pdf (2013).
U.S. Energy Information Administration, International Energy Outlook 2011. Report Number: DOE/EIA-0484(2011), http://www.eia.gov/forecasts/ieo/pdf/0484%282011%29.pdf (2011).

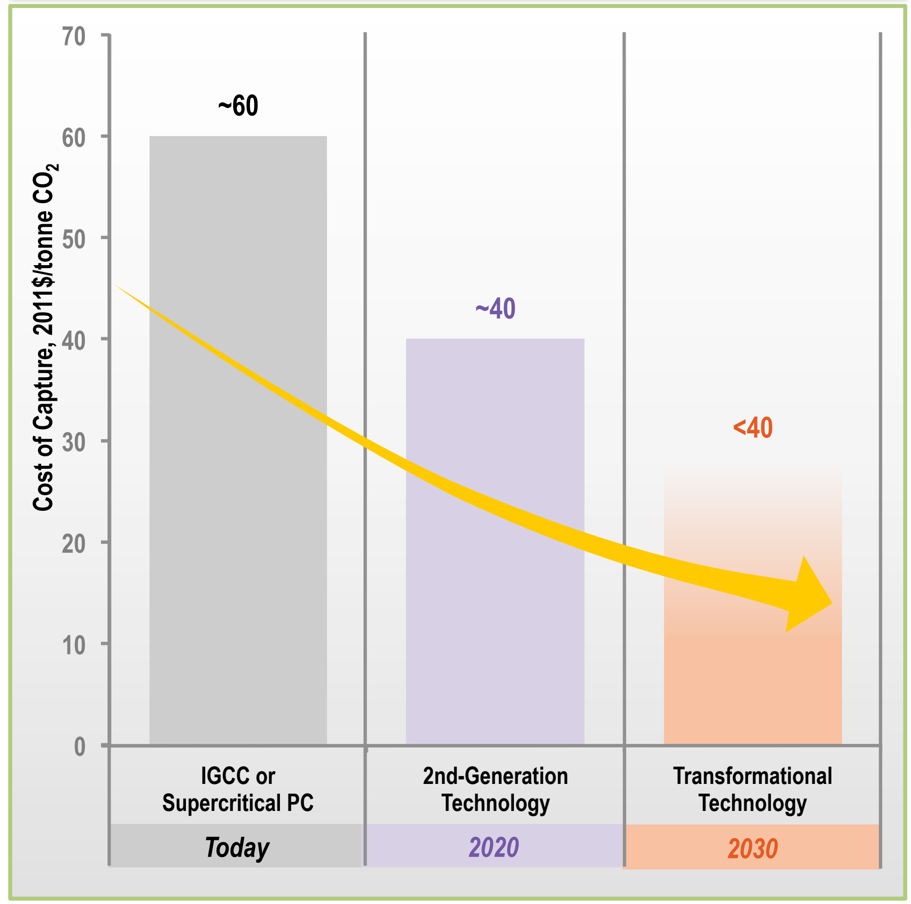
Clean Coal Research Program Goals

Driving Down the COE and Cost of Coal Power CCS

Cost of Electricity Reduction Targets



Corresponding Cost of CO_2 Capture Targets



Goals shown are for greenfield plants. Costs are for nth-of-a-kind plants, during first year of plant operation, and include compression to 2215 psia but exclude CO_2 transport and storage costs. Today's capture costs are relative to Today's SCPC without CO_2 capture. 2020 and 2030 capture costs are relative to an A-USC PC without CO_2 capture.

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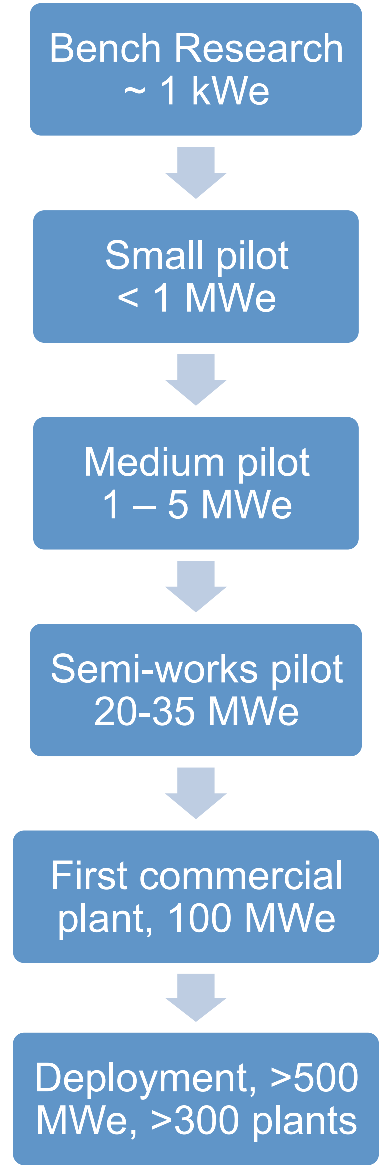
Development Challenges

- The traditional pathway from discovery to commercialization of energy technologies can be quite long, i.e., ~ 2-3 decades[1]
- President's plan requires that barriers to the widespread, safe, and cost-effective deployment of CCS be overcome within 10 years[2]
- 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
- Accelerate the development of CCS technology, from discovery through deployment, with the help of advanced computations tools and models



1. International Energy Agency Report: Experience Curves for Energy Technology Policy," 2000. 2. http://www.whitehouse.gov/the-press-office/presidentialmemorandum-a-comprehensive-federal-strategy-carbon-capture-and-storage

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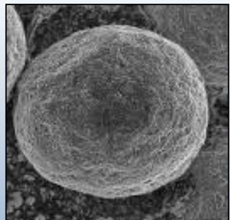
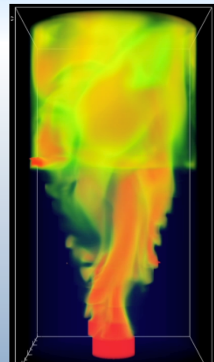
For Accelerating Technology Development






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, the babcock&wilcox company
- 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

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Goals & Objectives of CCSI

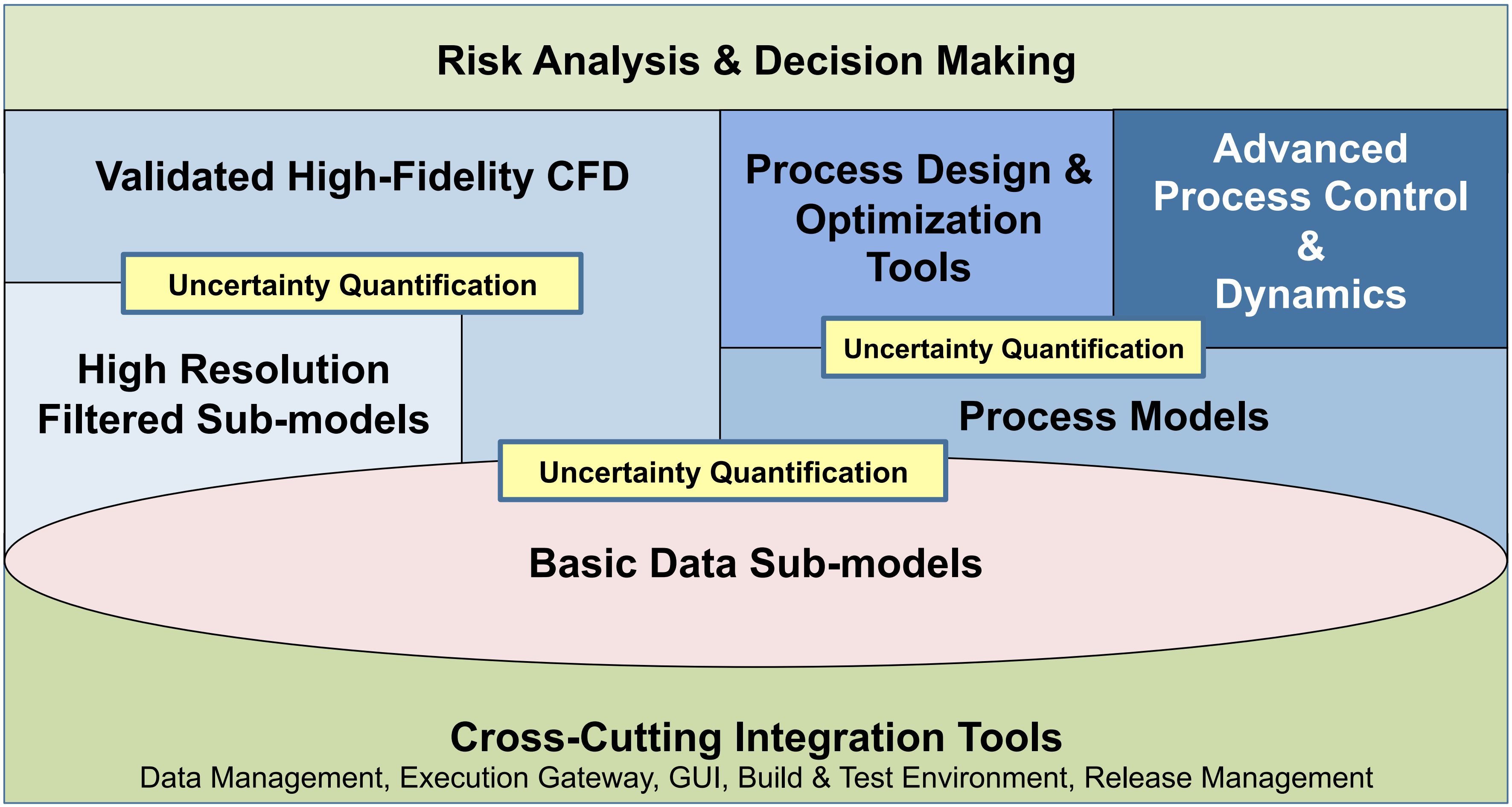
- **Develop** new computational tools and models to enable industry to more rapidly develop and deploy new advanced energy technologies
  - Base development on industry needs/constraints
- **Demonstrate** the capabilities of the CCSI Toolset on non-proprietary case studies
  - Examples of how new capabilities 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
  - <u>Began solvent modeling/demonstration component</u>
- **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



Carbon Capture (and other process) Simulation Grand Challenges

- **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

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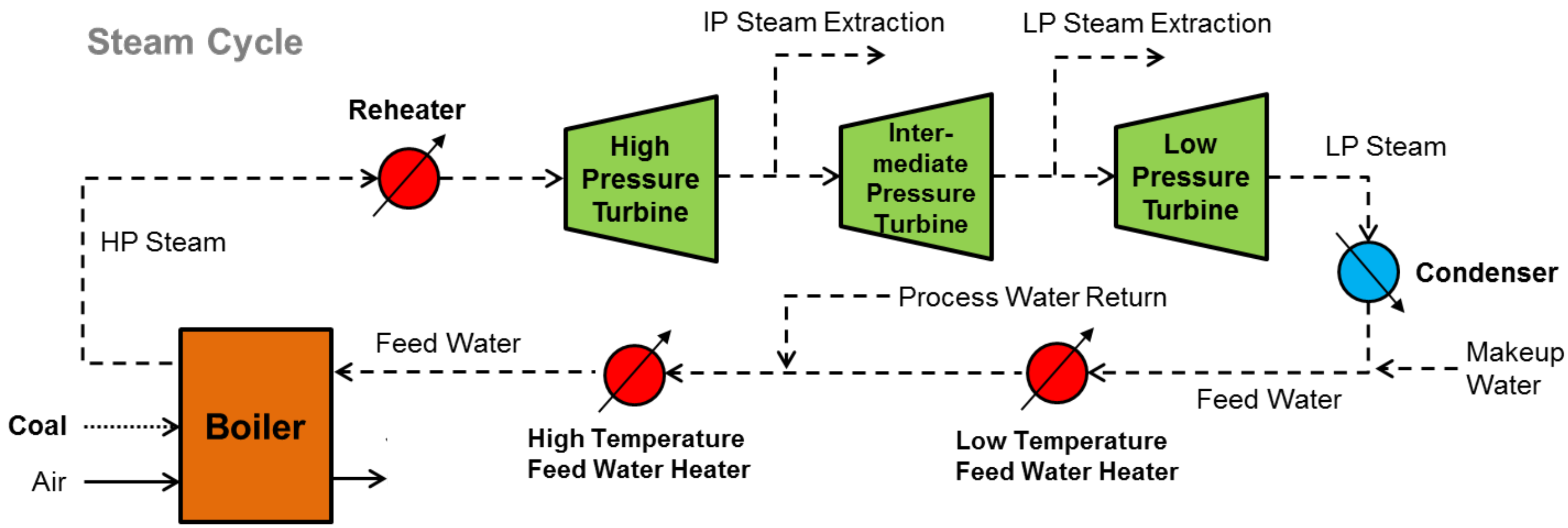
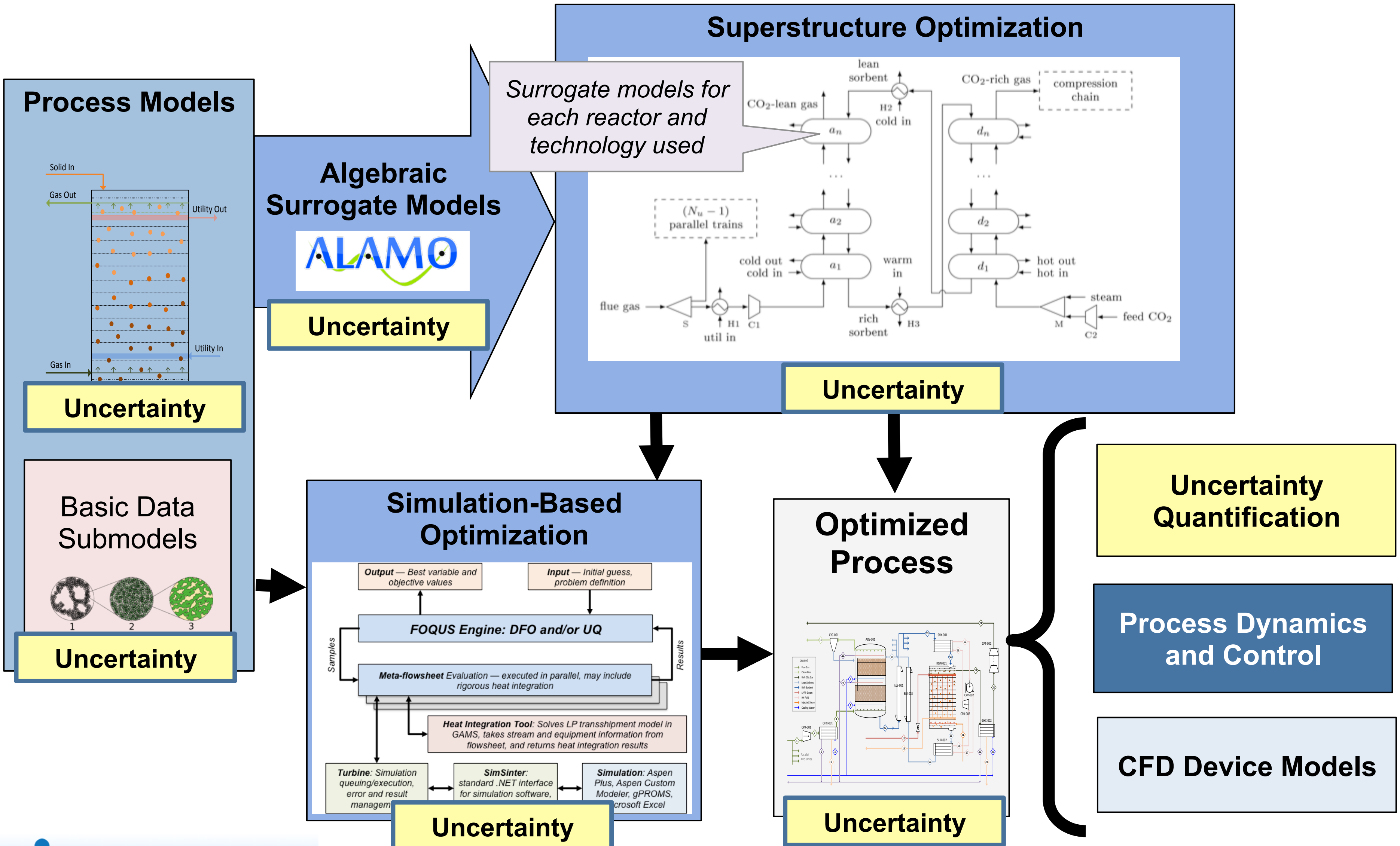

Steam Cycle
IP Steam Extraction
LP Steam Extraction
Reheater
High Pressure Turbine
Inter-mediate Pressure Turbine
Low Pressure Turbine
LP Steam
HP Steam
Condenser
Process Water Return
Feed Water
Makeup Water
Feed Water
Coal
Boiler
Air
High Temperature Feed Water Heater
Low Temperature Feed Water Heater

Tools to develop an optimized process using rigorous models



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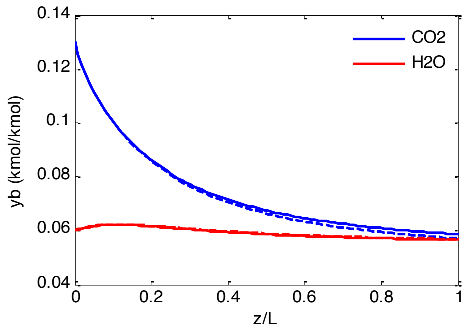
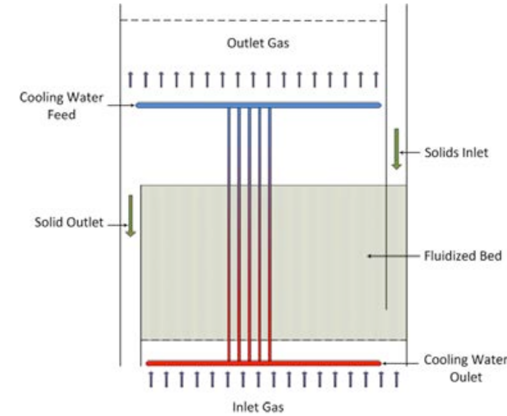
Process Models

Bubbling Fluidized Bed (BFB) Model

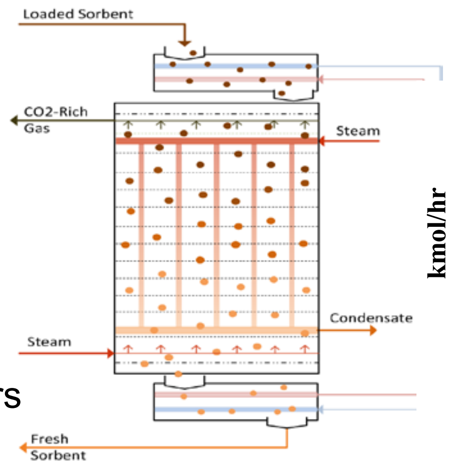
- 1-D, nonisothermal with heat exchange
- Unified steady-state and dynamic
- Adsorber and Regenerator
- Variable solids inlet and outlet location
- Modular for multiple bed configurations

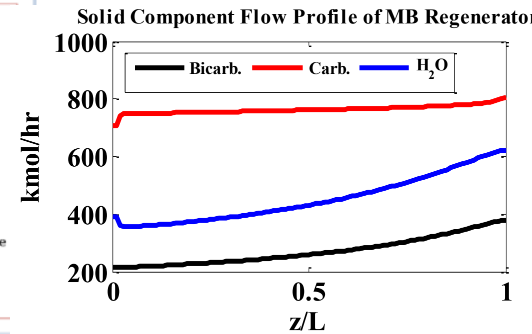




Moving Bed (MB) Model

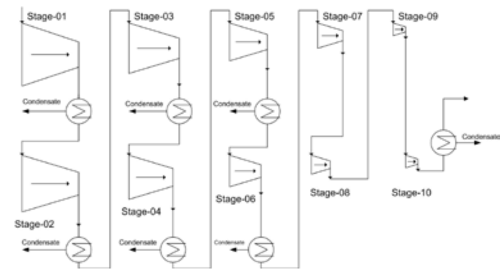
- 1-D, nonisothermal with heat exchange
- Unified steady-state and dynamic
- Adsorber and Regenerator
- Heat recovery system





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



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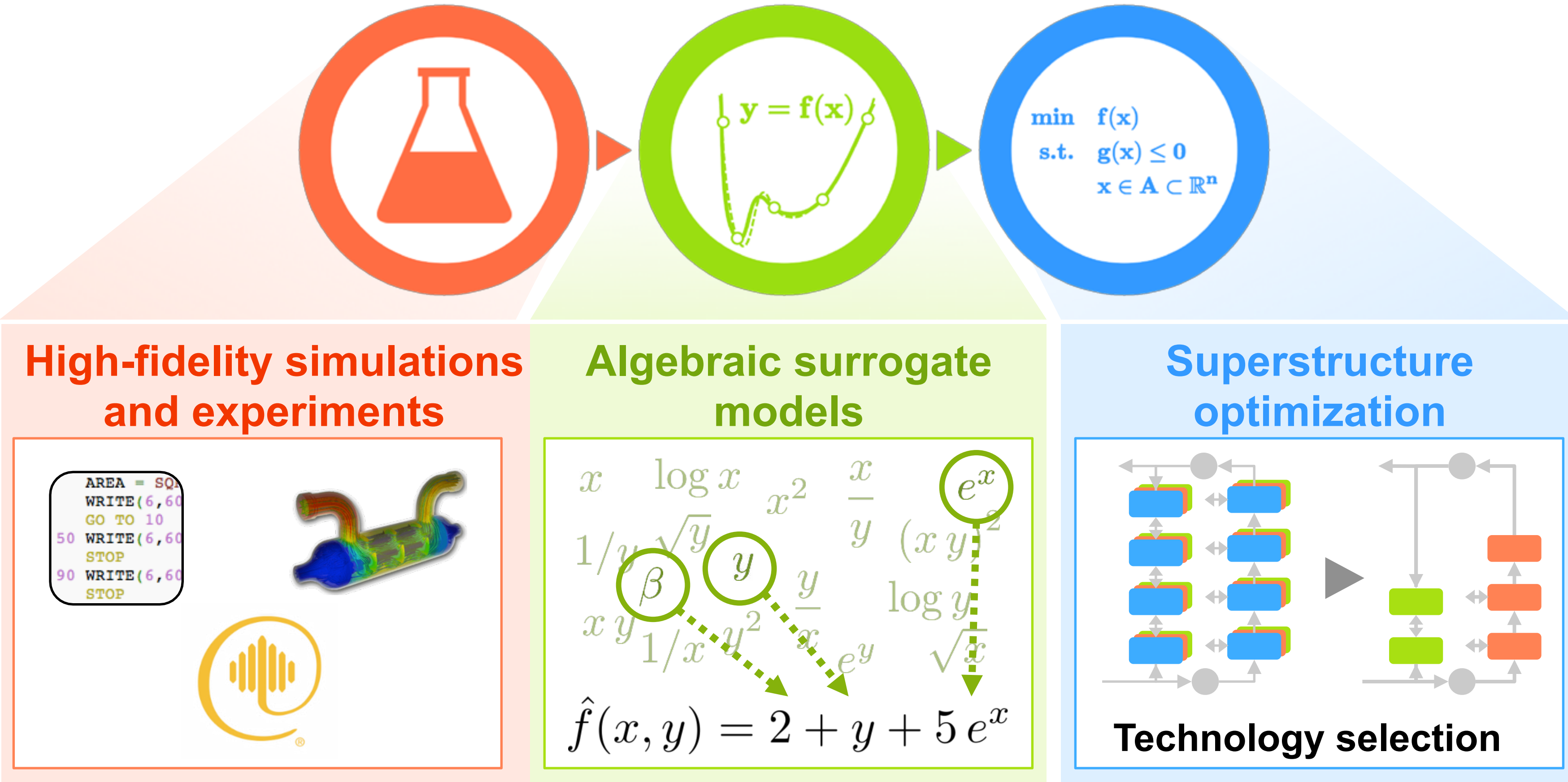
ALAMO

Automated Learning of Algebraic Models for Optimization

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



A. Cozad, N. V. Sahinidis and D. C. Miller, 2014, "Learning surrogate models for simulation-based optimization." *AIChE Journal* **60**(6): 2211-2227.

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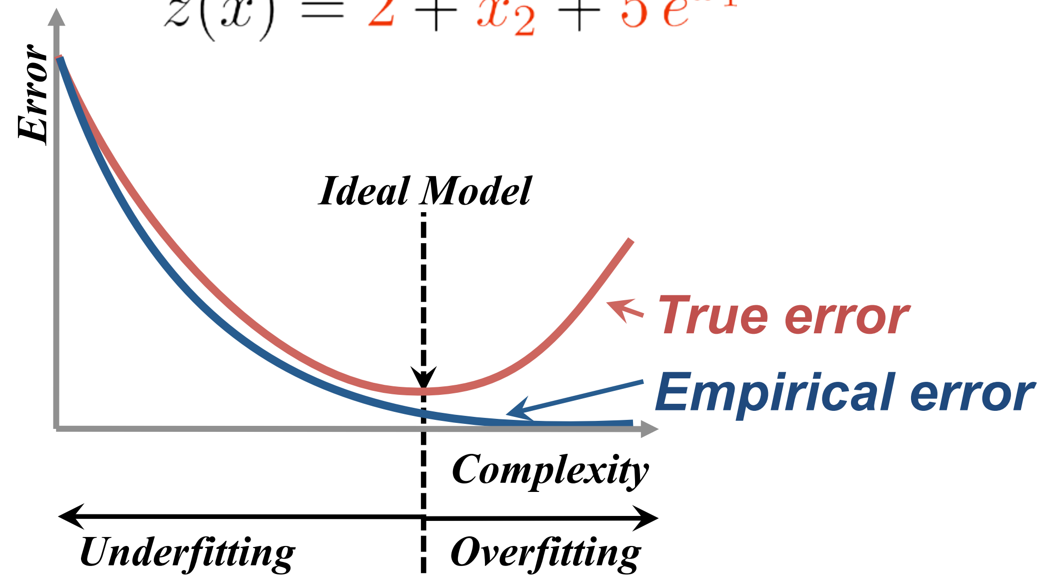
ALAMO: Model Development & Overfitting

- Step 1: Define a large set of potential basis functions

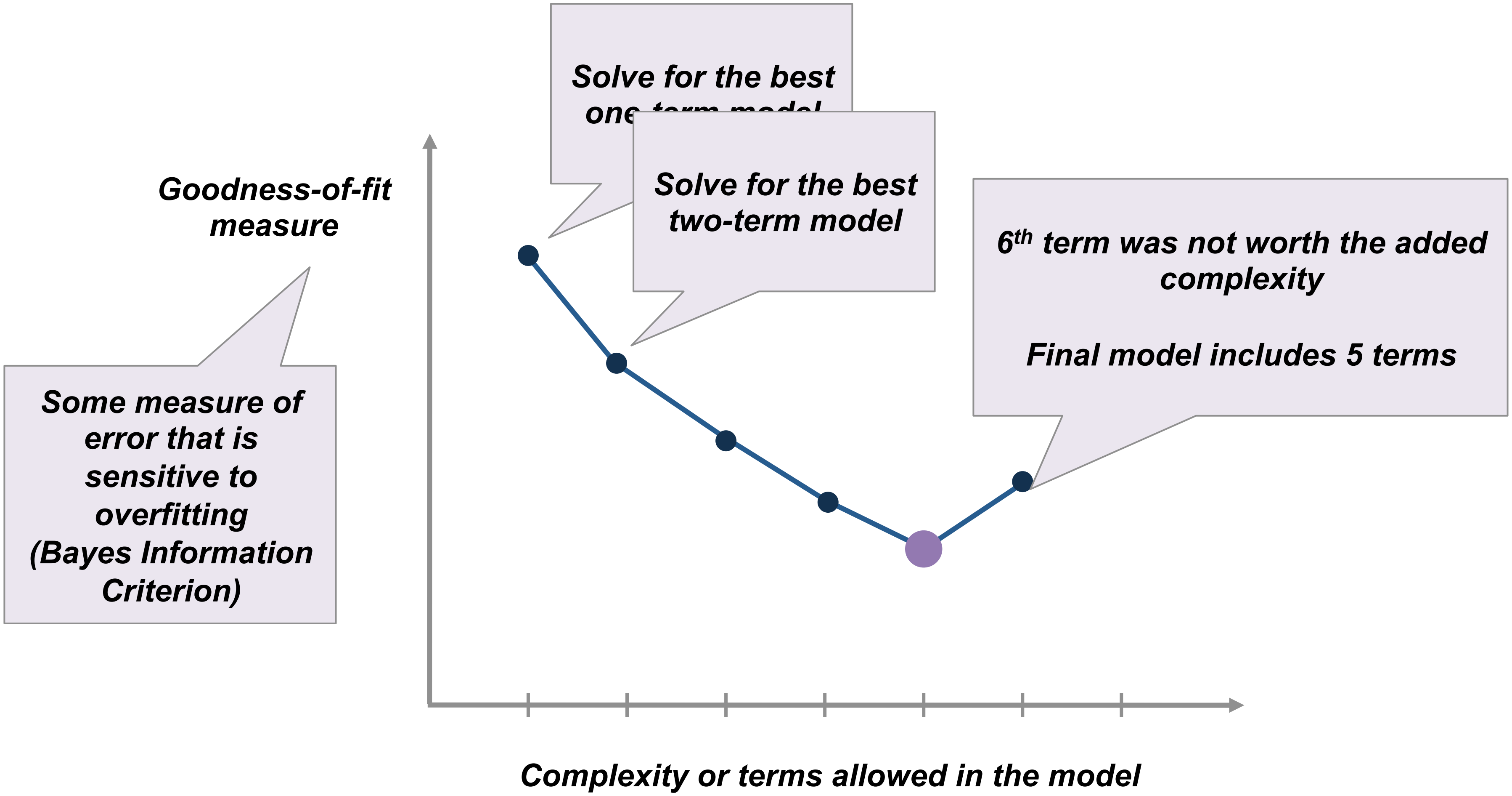
$$\hat{z}(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \beta_4 e^{x_1} + \beta_5 e^{x_2} + \ldots$$

- Step 2: Model reduction

$$\hat{z}(x) = 2 + x_2 + 5\,e^{x_1}$$

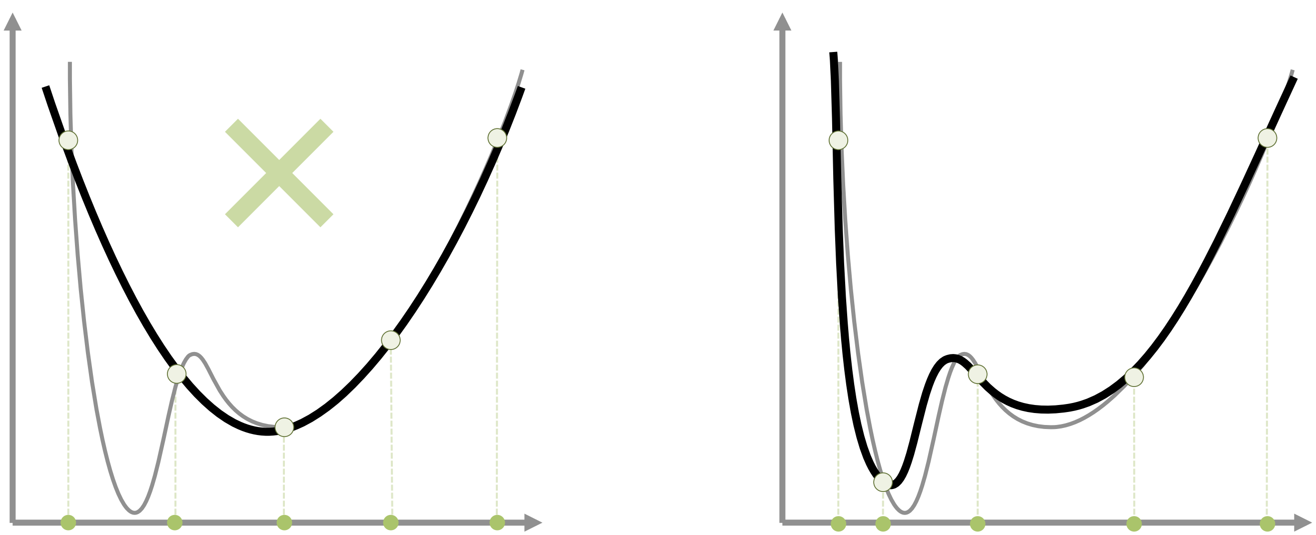


ALAMO: Surrogate Model Development



Adaptive Sampling Improves Surrogate Model

- We use an iterative design of experiments to
  - Sample better or sample fewer data points
- Two models given the same data set size:

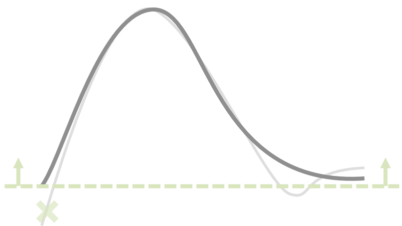


Even sampling *Stronger sampling*

Constrained Regression Improves Surrogates

Response bounds

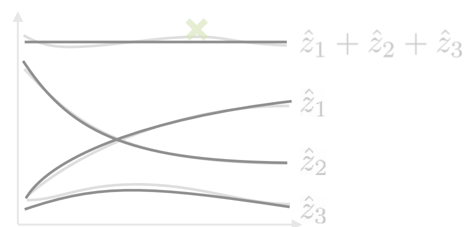
$$[\hat{A}]_t \geq 0$$



pressure, temperature, compositions

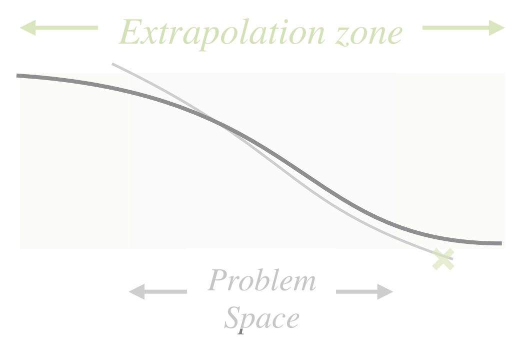
Multiple responses

$$\hat{z}_1 + \hat{z}_2 + \hat{z}_3 = 1$$



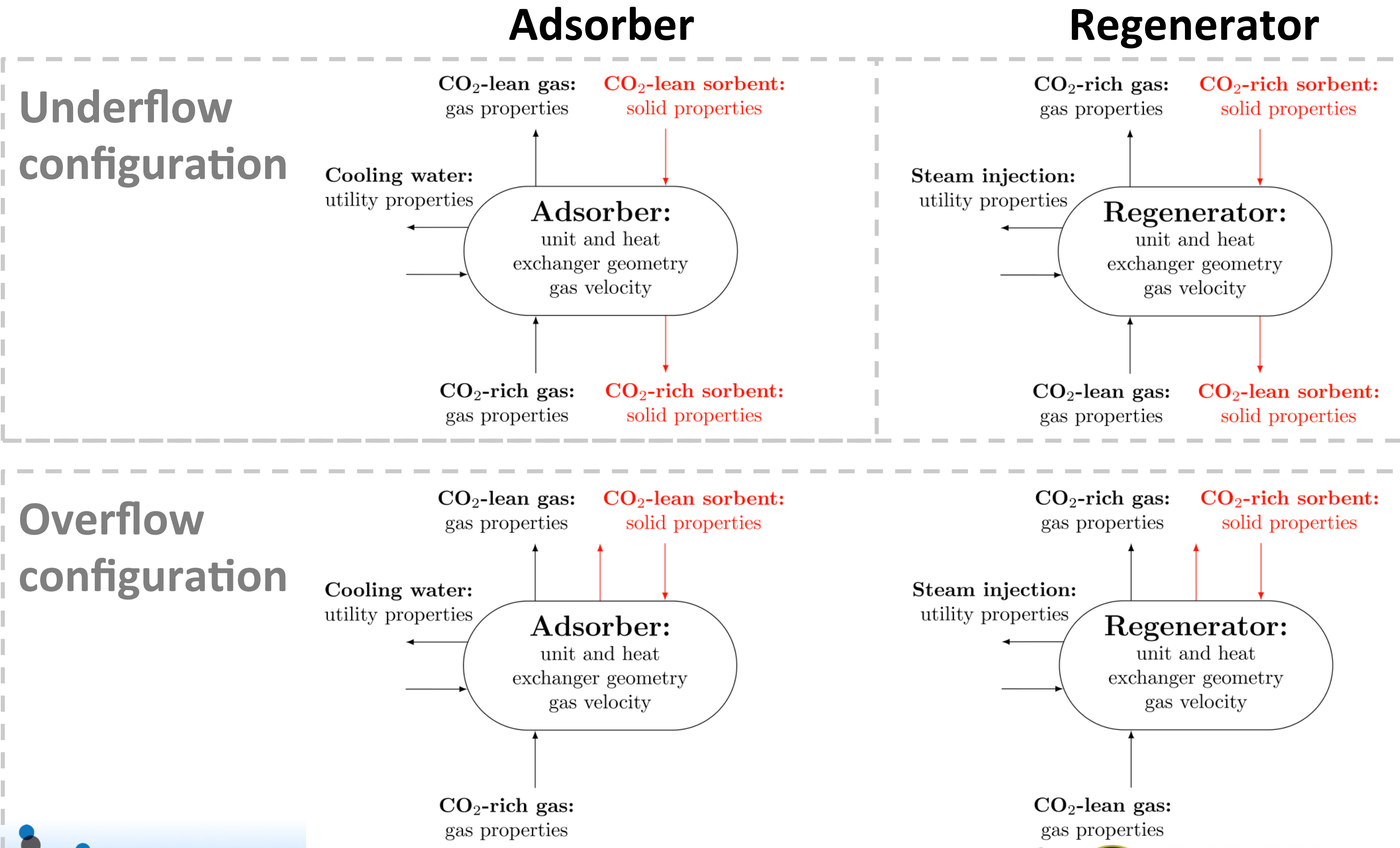
mass balances, sum-to-one, state variables

Alternative domains

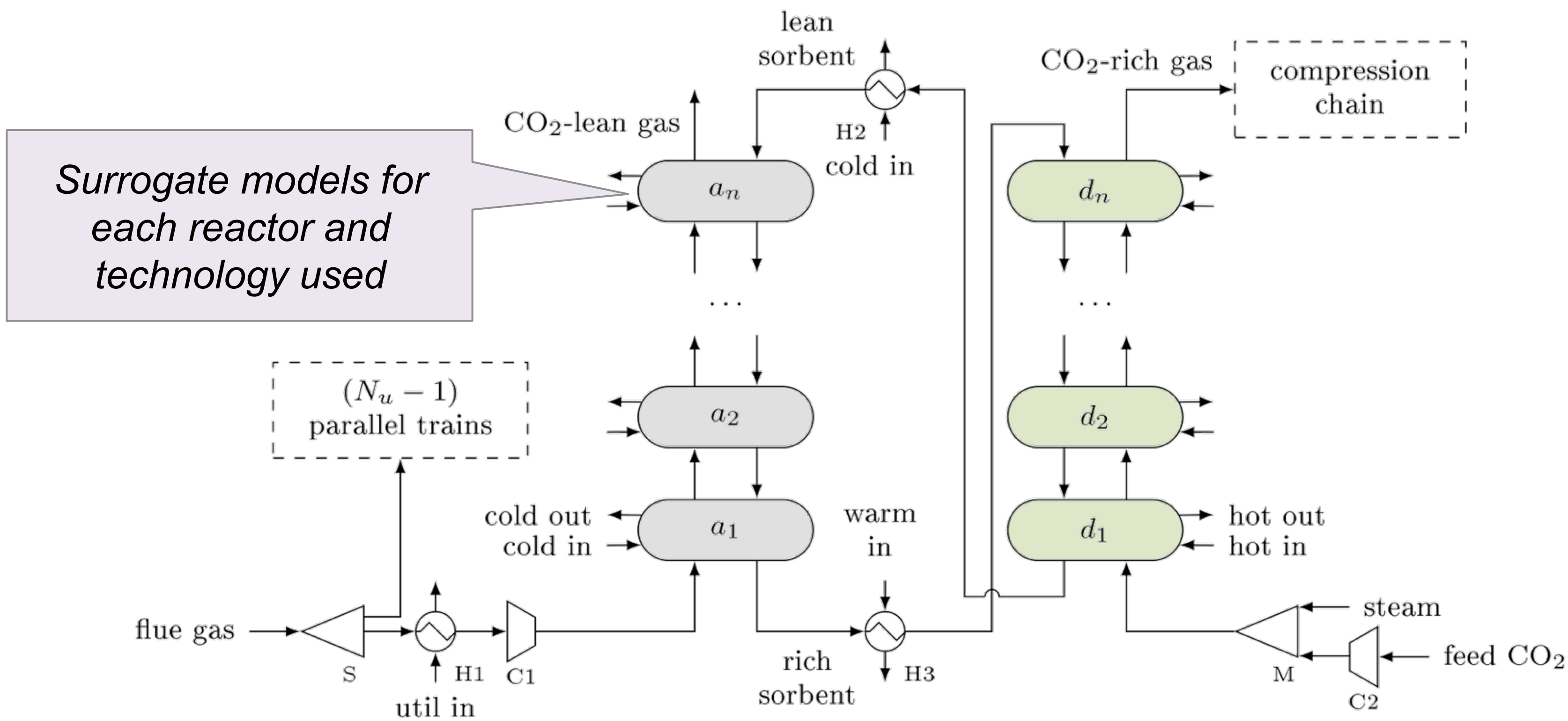


safe extrapolation, boundary conditions

Carbon Capture Reactors

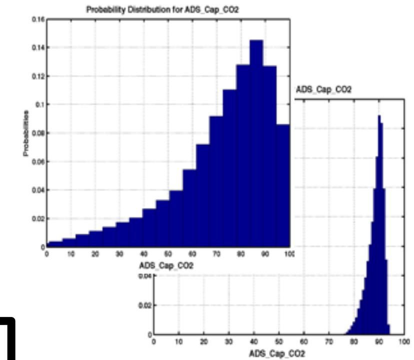


Carbon Capture System Configuration



- Discrete decisions: How many units? Parallel trains? What technology used for each reactor?
- Continuous decisions: Unit geometries
- Operating conditions: Vessel temperature and pressure, flow rates, compositions

Framework for Optimization, Quantification of Uncertainty and Sensitivity



Input *— Initial guess, problem definition*

Output *— Best variable and objective values*

FOQUS Engine: DFO and/or UQ

Samples

Results

Meta-flowsheet *Evaluation — executed in parallel, may include rigorous heat integration*

Heat Integration Tool*: Solves LP transshipment model in GAMS, takes stream and equipment information from flowsheet, and returns heat integration results*

Turbine*: Simulation queuing/execution, error and result management*

SimSinter*: standard interface for simulation software, graphical tool*

Simulation*: Aspen Plus, Aspen Custom Modeler, gPROMS, Microsoft Excel*

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.

Sinter: Generic Connectivity for Simulations

- Links simulations to FOQUS/Turbine

- Support for
  – gPROMS
  – Aspen Plus
  – Aspen Custom Modeler
  – Excel
    - Costing
    - Generic connectivity (i.e., Thermoflex)

- Explicitly links to any input/output variables via GUI
  – JSON structure

Turbine: Simulation Execution Management

- Works with Aspen, gPROMS, Excel
- Supports large number of simulation executions
  – Manages failed simulations
- Scalable
  – Amazon Cloud
    - Up to 500 parallel simulations tested
    - Over 100,000 simulations run
  – Cluster at NETL (coming online 2014)
  – Local desktop
- Challenge: Licensing of commercial simulation tools

FOQUS: DFO Example with Heat Integration

Objective Function: Maximize **Net efficiency**

Constraint: **CO_2 removal** ratio ≥ 90%
Flowsheet evaluation (via process simulators)
Minimum utility target (via heat integration tool)

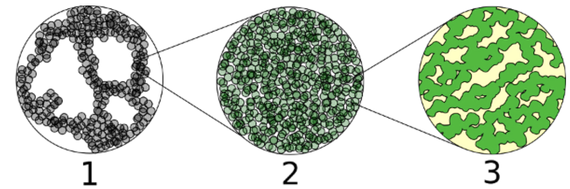
Decision Variables (17): Bed length, diameter, sorbent and steam feed rate

FOQUS Optimization Results

	Simultaneous	Sequential	w/o heat integration
Net power efficiency (%)	**32.6**	**31.8**	**30.0**
Net power output (MW_e)	504.3	491.5	463.9
CO_2 removal ratio (%)	**91.9**	**90.2**	**90.2**
Electricity consumption (MW_e)	86.9	75.1	75.1
IP steam (kg/s)	0	0	0
LP steam (kg/s)	93.9	125.3	139.0
Cooling water consumption (m^3/s)	12.8	10.4	20.7
Heat addition to feed water (MW_{th})	135.4	139.8	0

Base case w/o CCS: 650 MW_e, **42.1 %**

Uncertainty in Kinetic Parameters

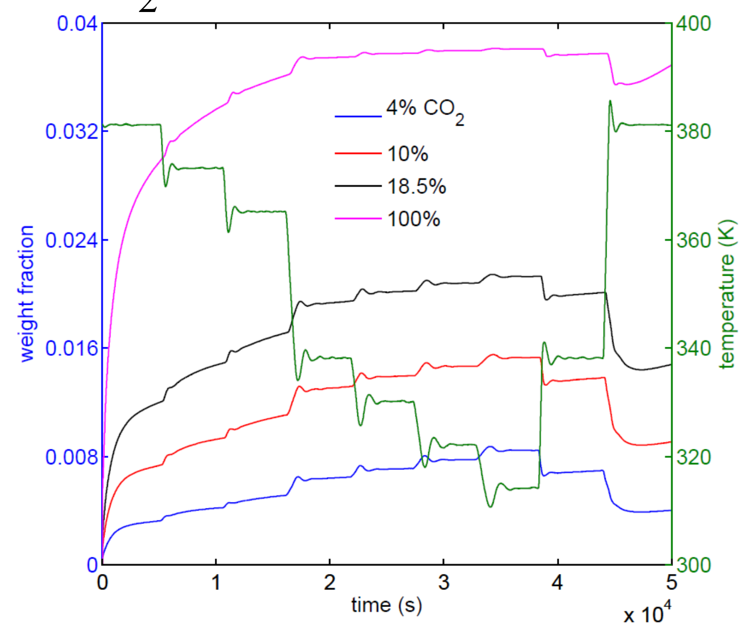


$$H_2O_{(g)} \rightleftharpoons H_2O_{(phys)}$$

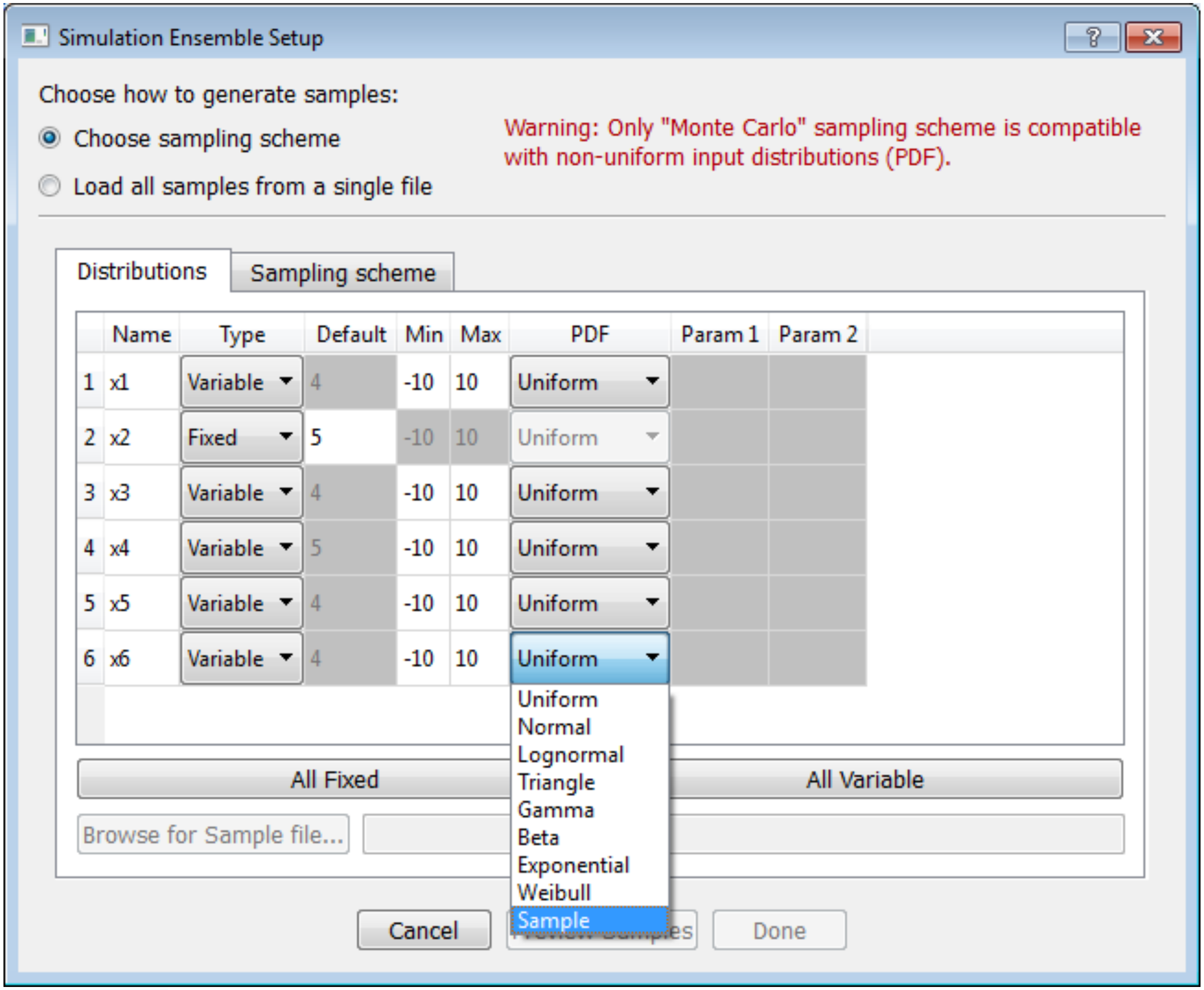
$$R_2NH + CO_{2,(g)} + H_2O_{(phys)} \rightleftharpoons R_2NH_2^+ + HCO_3^-$$

$$2R_2NH + CO_{2,(g)} \rightleftharpoons R_2NH_2^+ + R_2NCO_2^-$$

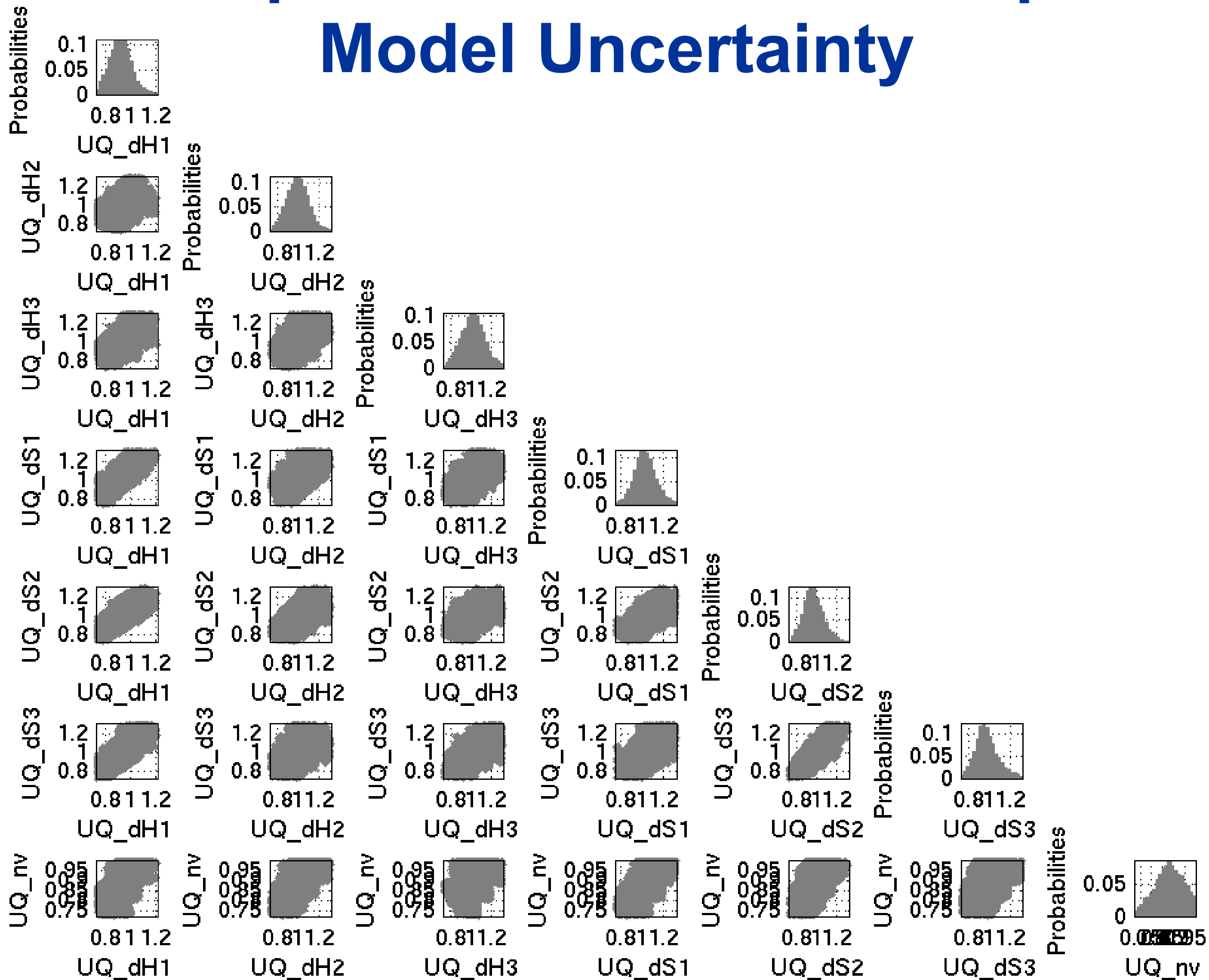
$$K_i = \exp\left(\frac{\Delta S_i}{R}\right)\exp\left(\frac{-\Delta H_i}{RT}\right)\Big/ P$$



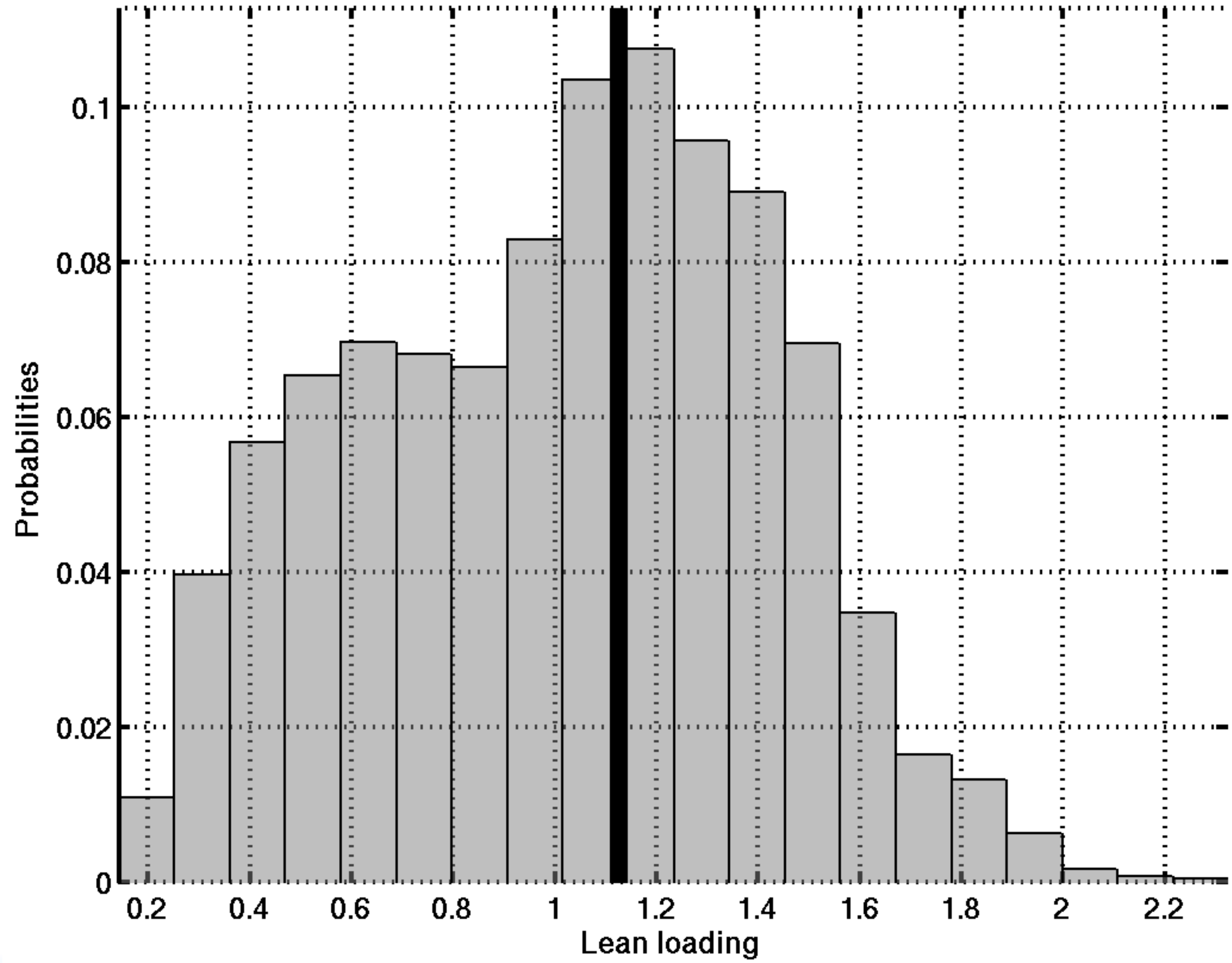
UQ Sampling


Simulation Ensemble Setup
Choose how to generate samples:
Choose sampling scheme
Load all samples from a single file
Warning: Only "Monte Carlo" sampling scheme is compatible with non-uniform input distributions (PDF).
Distributions
Sampling scheme
Name Type Default Min Max PDF Param 1 Param 2
1 x1 Variable 4 -10 10 Uniform
2 x2 Fixed 5 -10 10 Uniform
3 x3 Variable 4 -10 10 Uniform
4 x4 Variable 5 -10 10 Uniform
5 x5 Variable 4 -10 10 Uniform
6 x6 Variable 4 -10 10 Uniform
Uniform
Normal
Lognormal
Triangle
Gamma
Beta
Exponential
Weibull
Sample
All Fixed
All Variable
Browse for Sample file...
Cancel
Done

Feasible Input Distributions for Equilibrium Model Uncertainty



Probability distribution for the loading exiting the regeneration system



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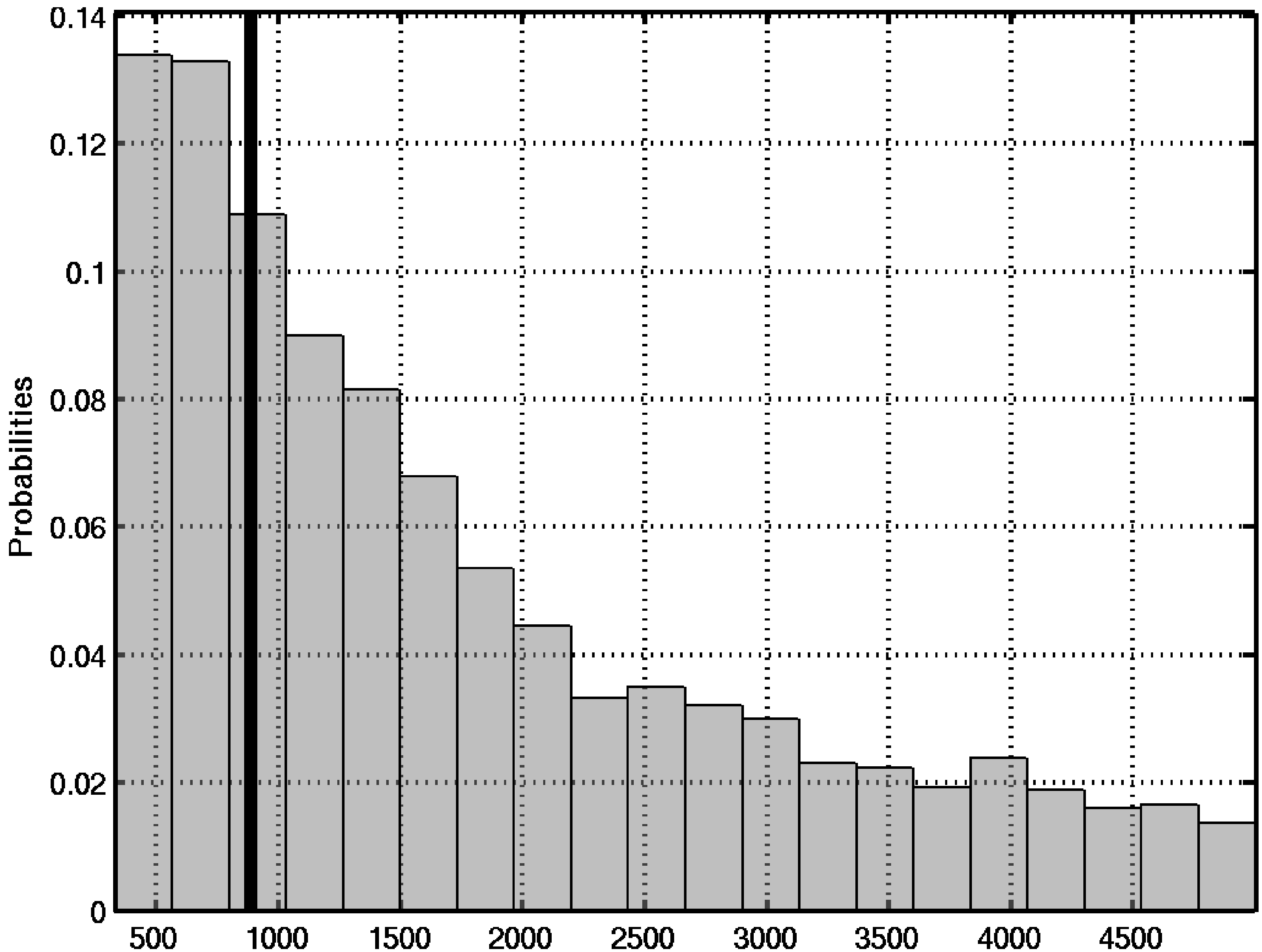
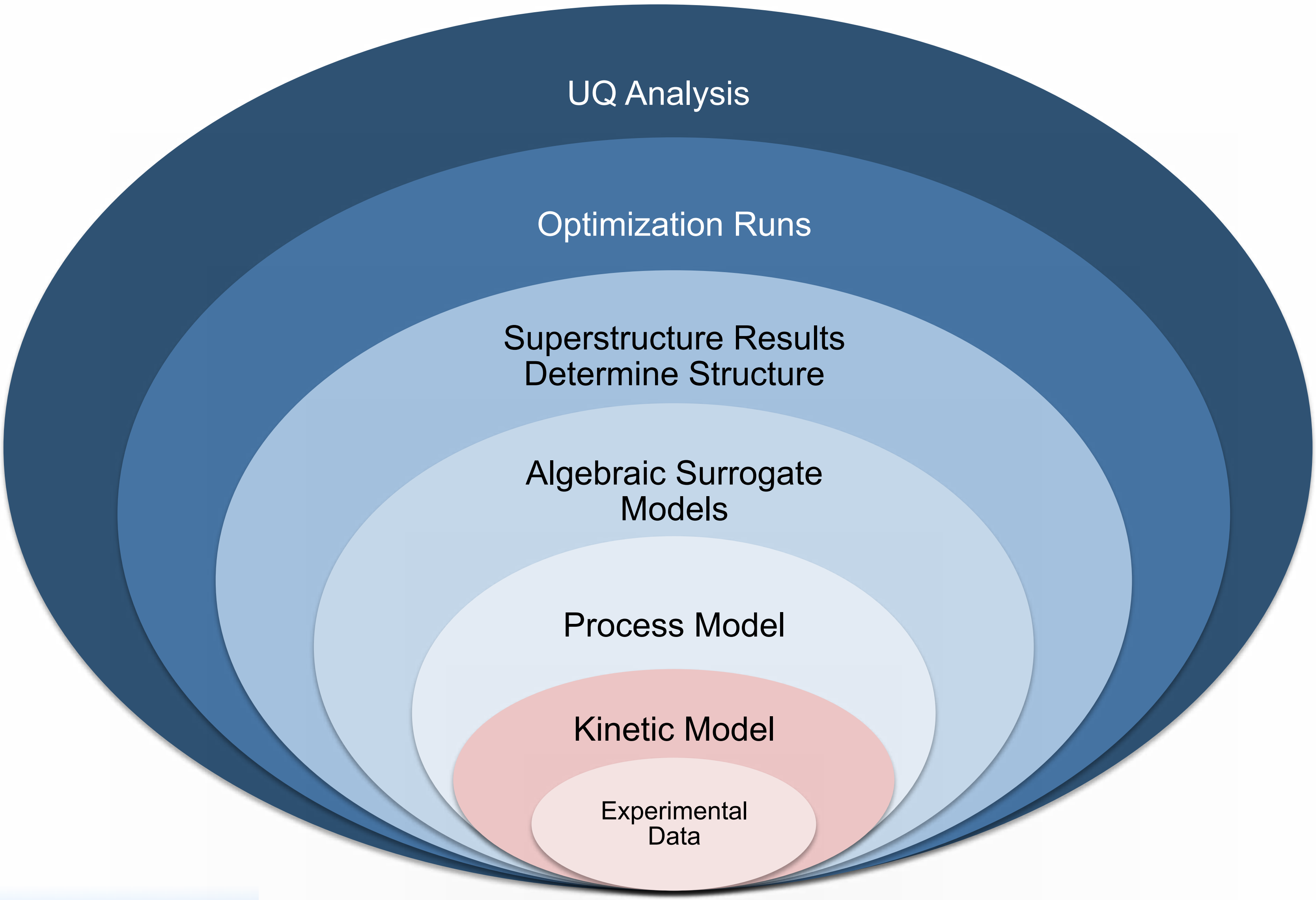
Required new steam flow to meet product specs



Data Management: Provenance



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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:
- Additional licensees:
- Others licenses in progress….
- CRADA: in development

Carbon Capture Simulation Initiative: A Case Study in Multiscale Modeling and New Challenges

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Emily Ryan,[11] Dave Engel,[9] and Crystal Dale[4]

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