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Carbon Capture Simulation Initiative

FOQUS: A Framework for Optimization and Quantification of Uncertainty

Extending the Capabilities of Aspen Plus and Aspen Custom Modeler

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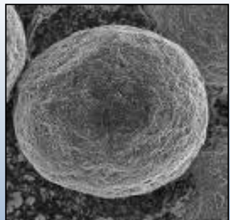
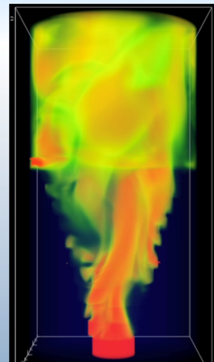
For Accelerating Technology Development





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

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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
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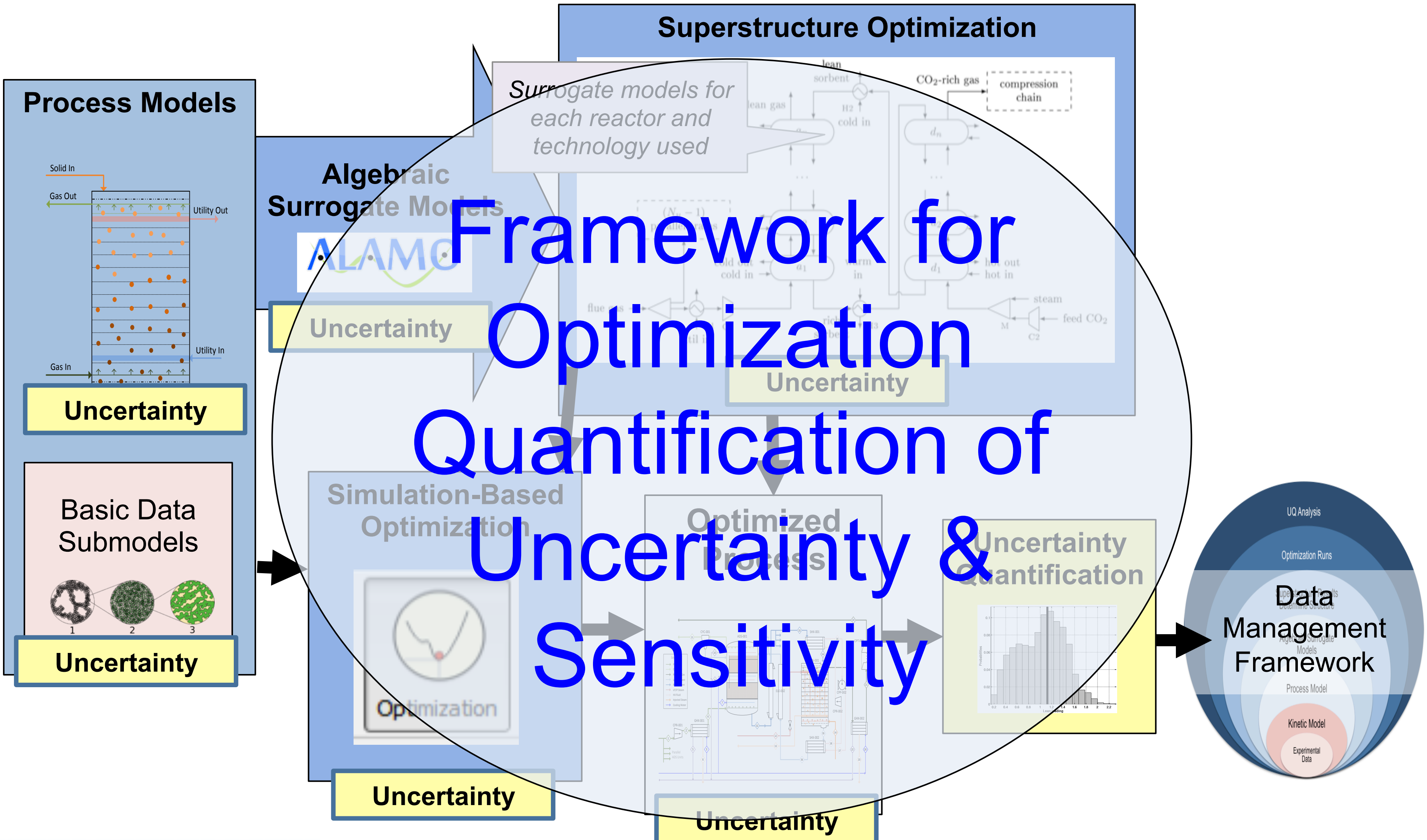
Eastman
aspentech
ANSYS
Schneider Electric
PSE

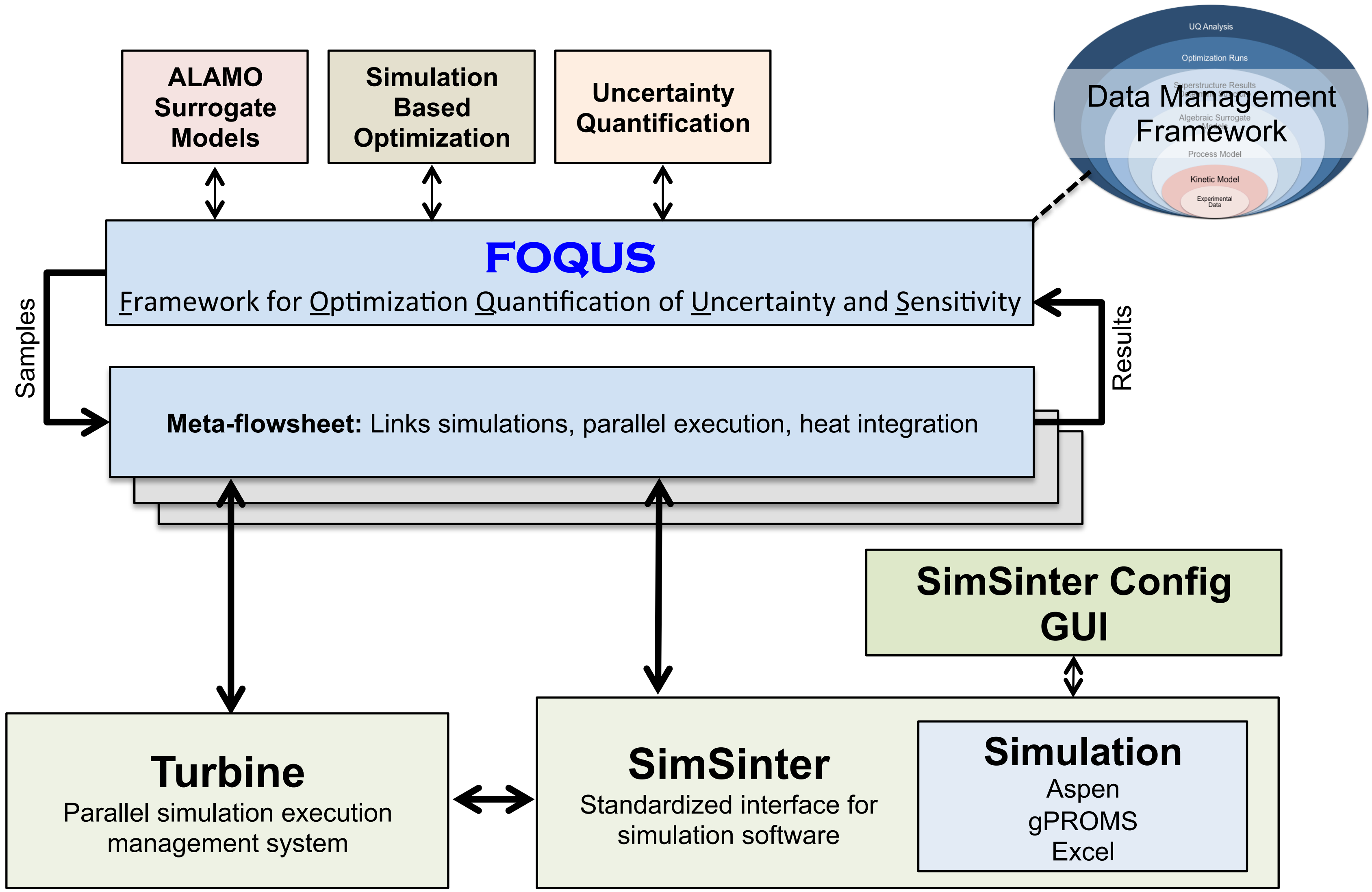
Goals & Objectives of CCSI

- **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
  - Initial licensees

Tools to develop an optimized process using rigorous models



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.

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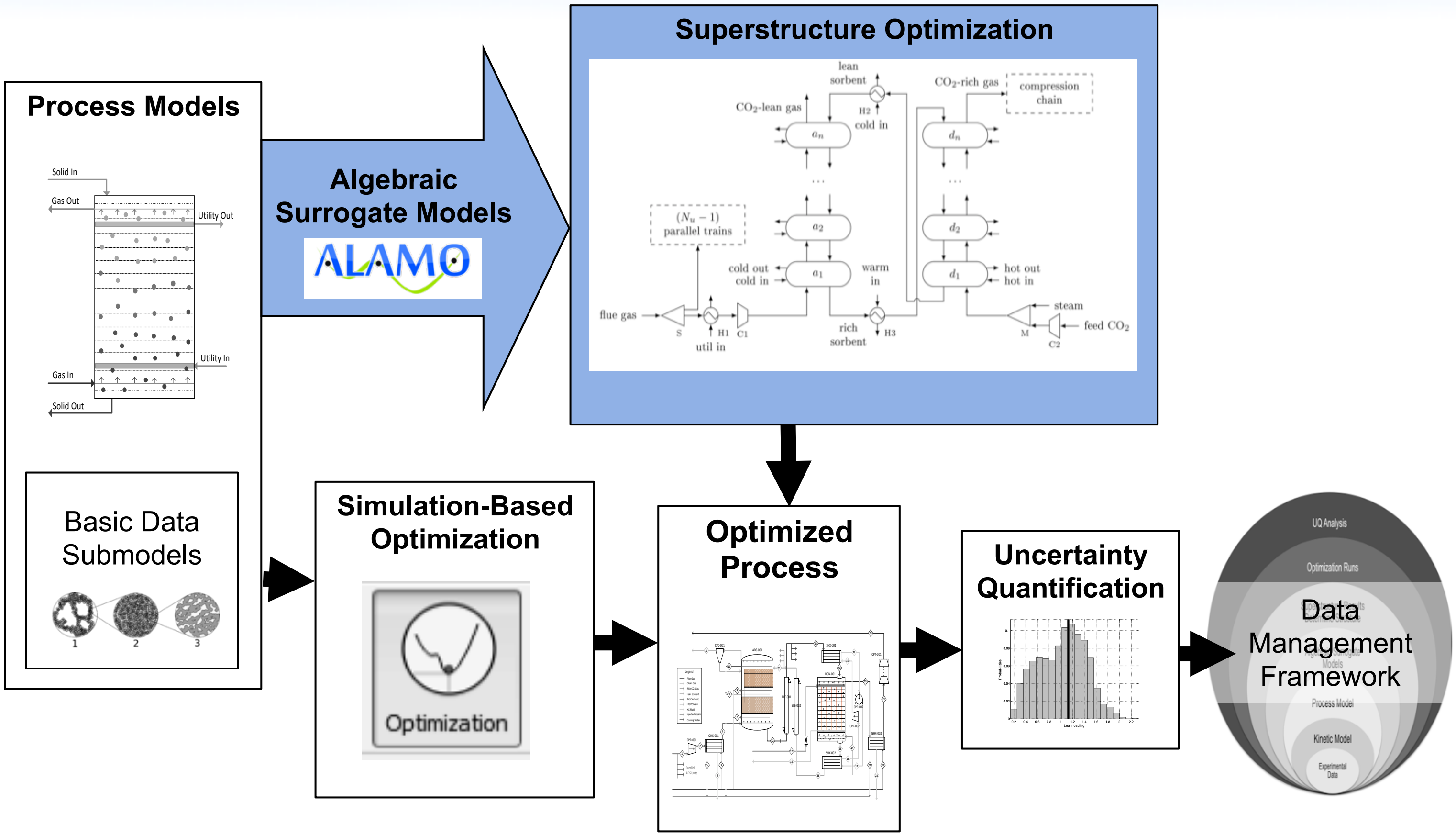
Superstructure & ALAMO



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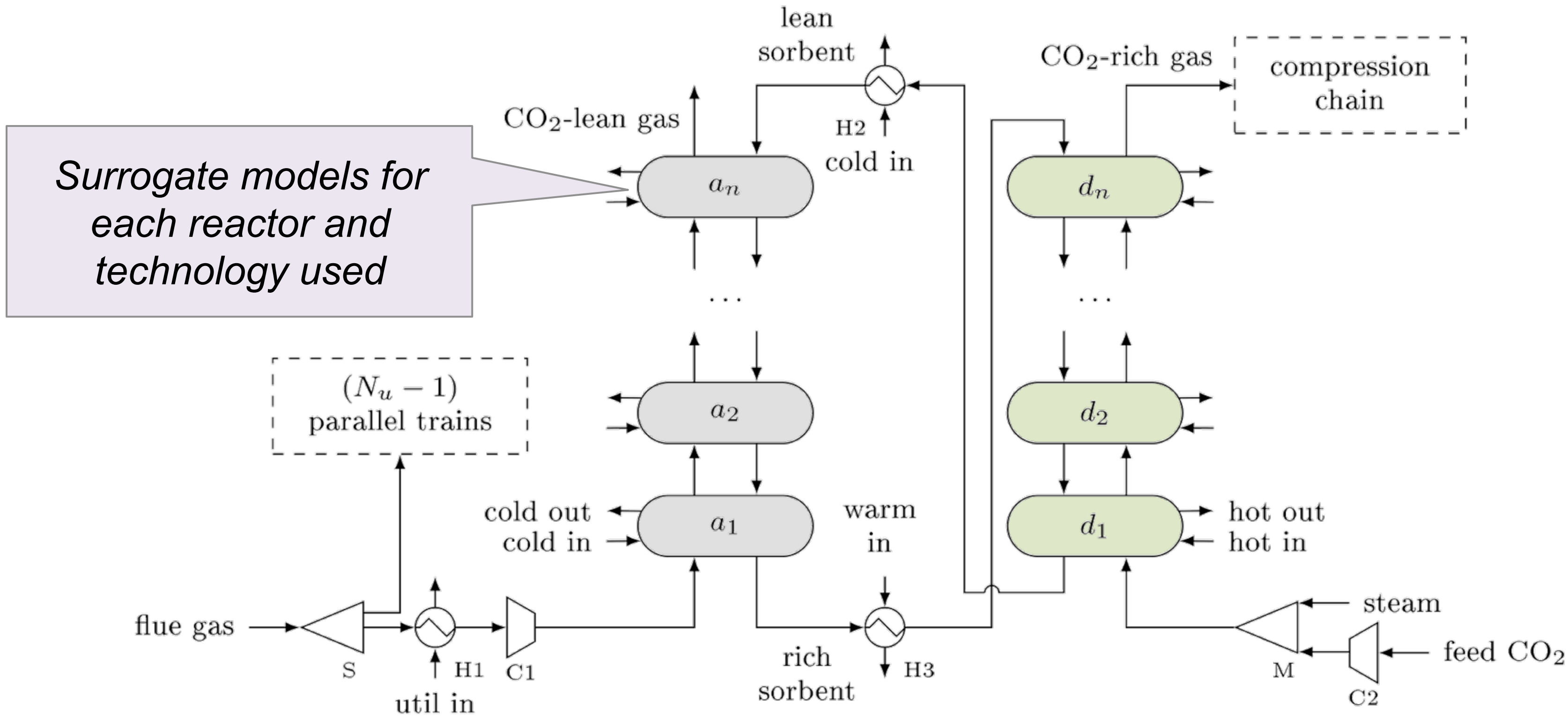
Carbon Capture System Configuration



- 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

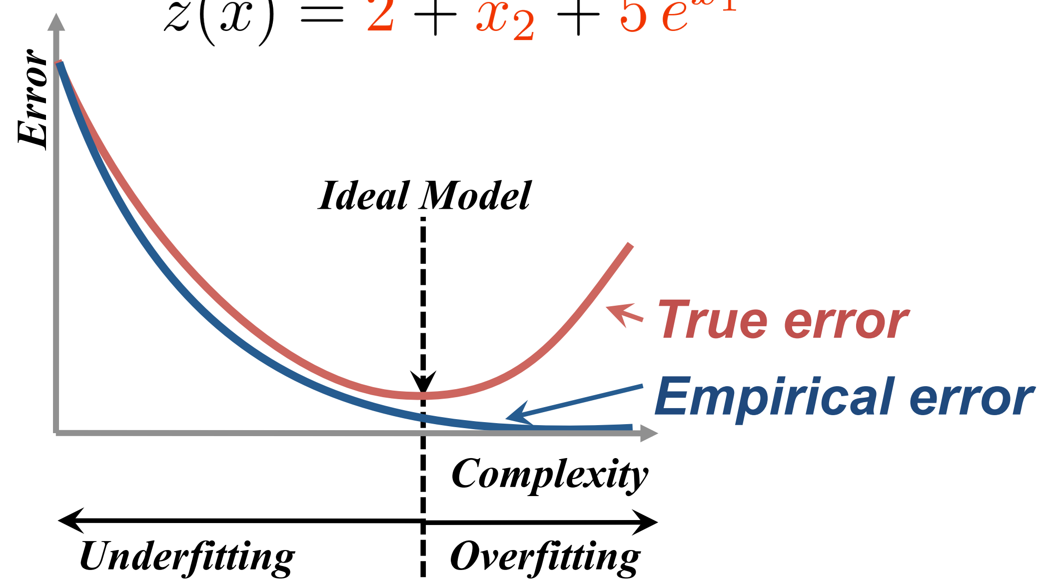
ALAMO: Model Development & Overfitting

- 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

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



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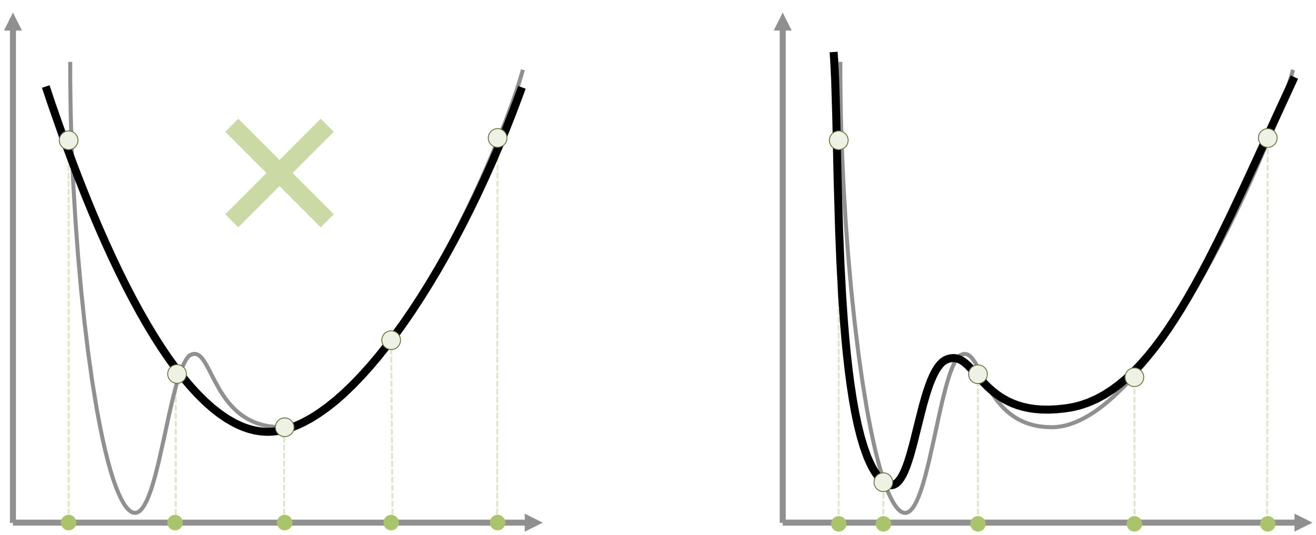
Adaptive Sampling Improves Surrogate Model

- 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***

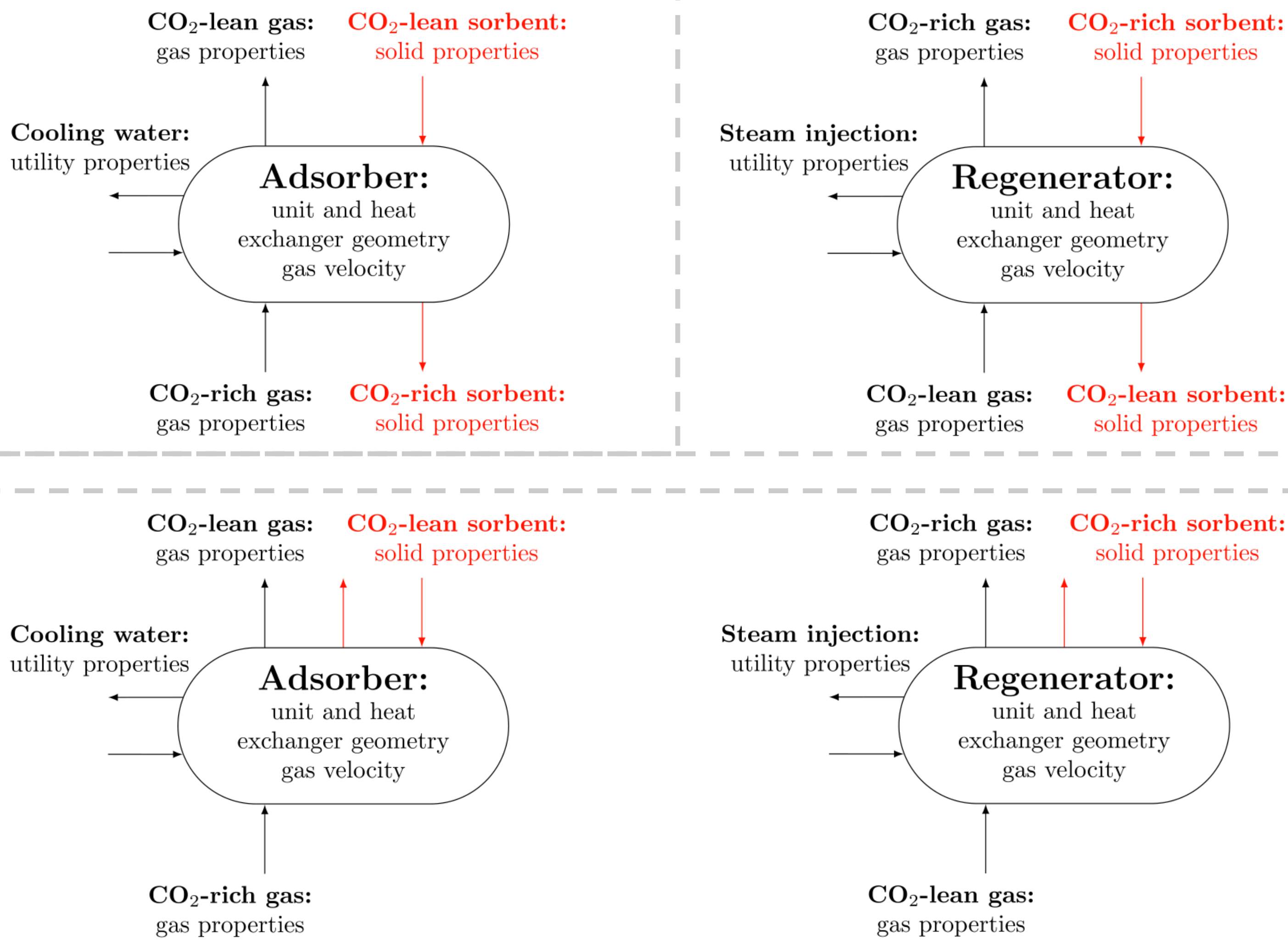
Carbon Capture Reactors

Adsorber

Regenerator

Underflow configuration

Overflow configuration



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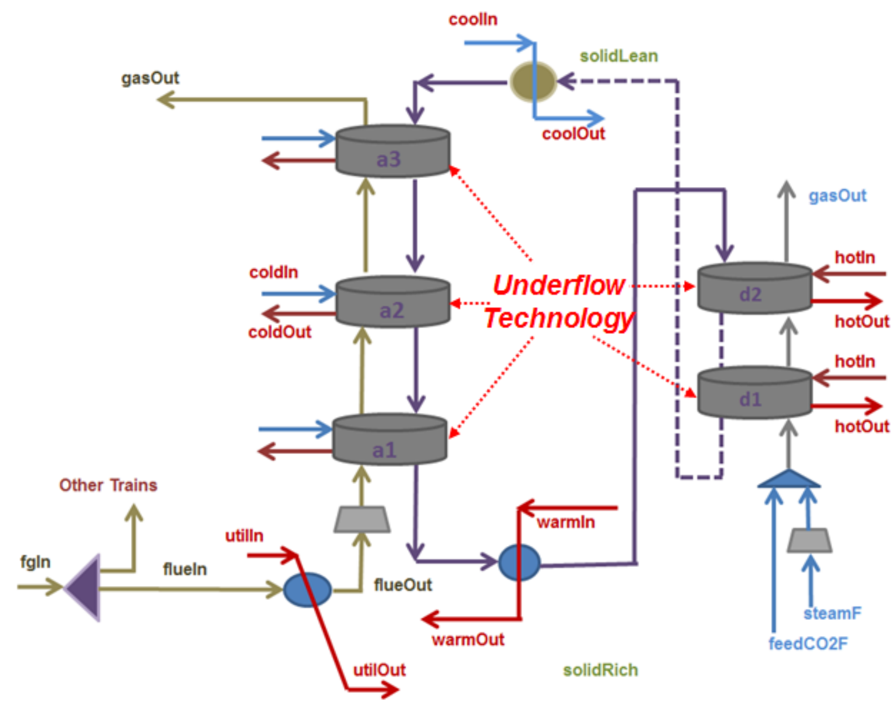
Superstructure Optimization

Mixed-integer nonlinear programming model in GAMS

- *Parameters*
- *Variables*
- *Equations*
  - *Economic modules*
  - *Process modules*
    - *Material balances*
    - *Hydrodynamic/Energy balances*
    - *Reactor surrogate models*
  - *Link between economic modules and process modules*
  - *Binary variable constraints*
  - *Bounds for variables*



Optimal layout

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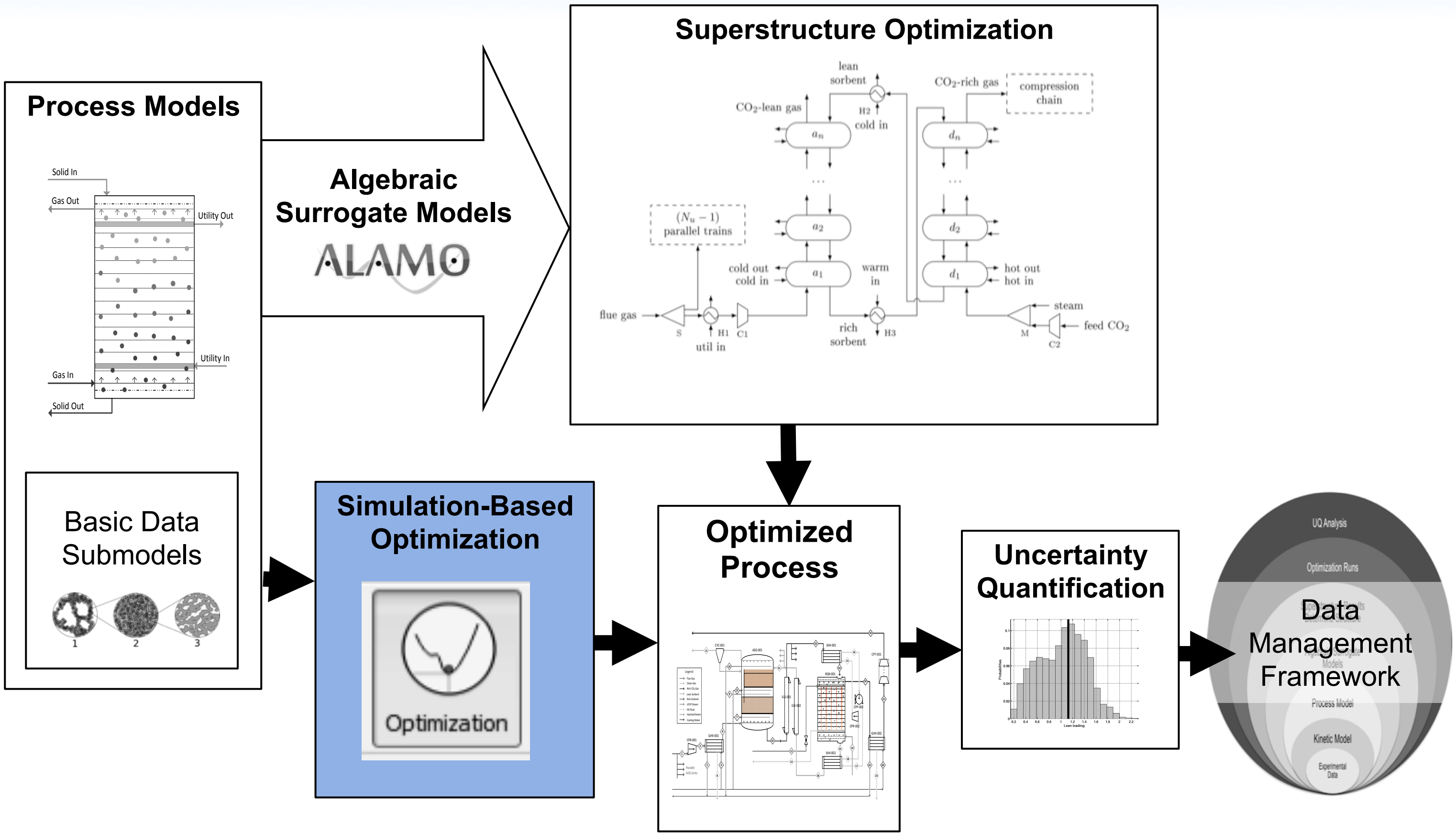
Simulation-Based Optimization and Simultaneous Heat Integration



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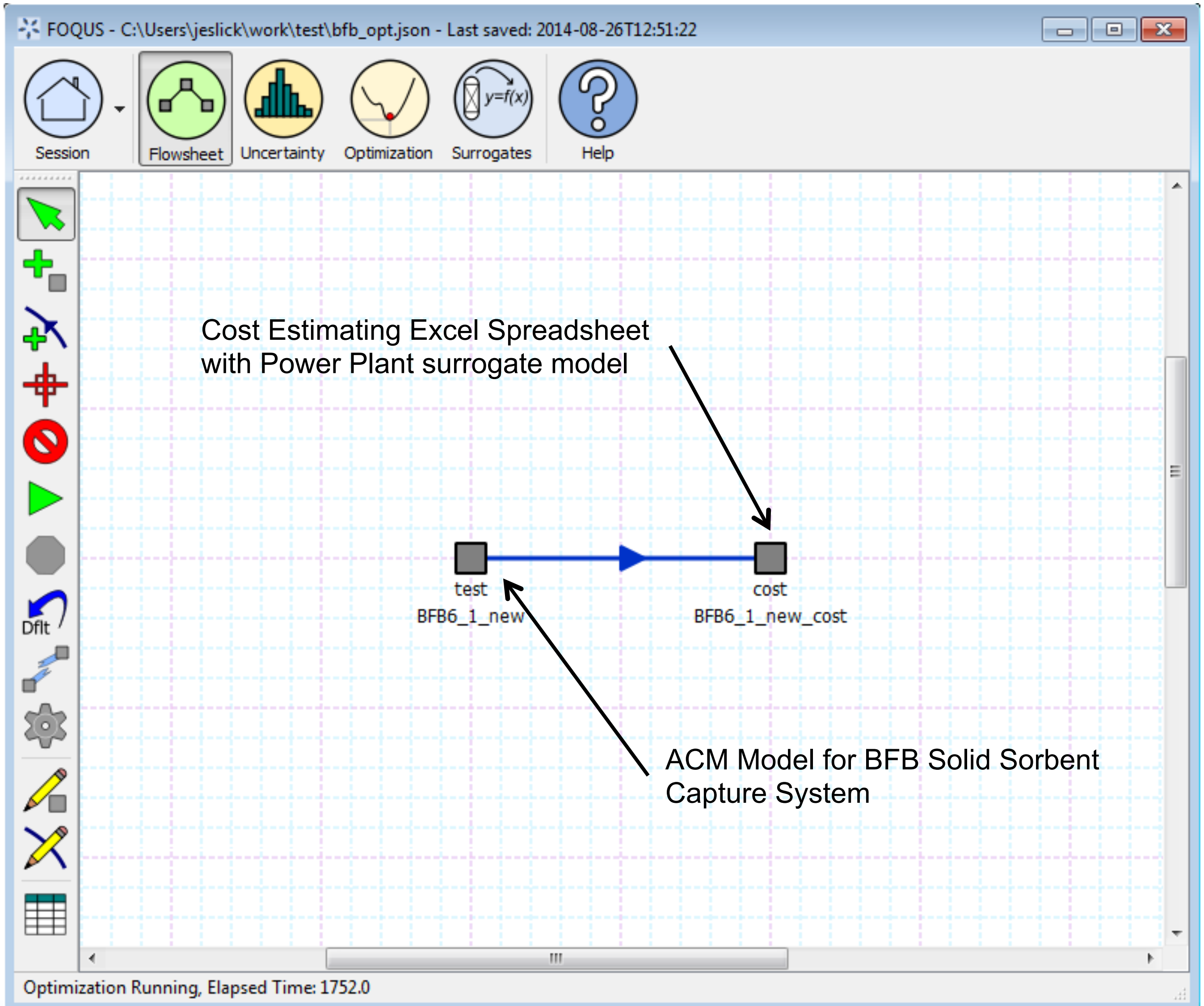
FOQUS Flowsheet



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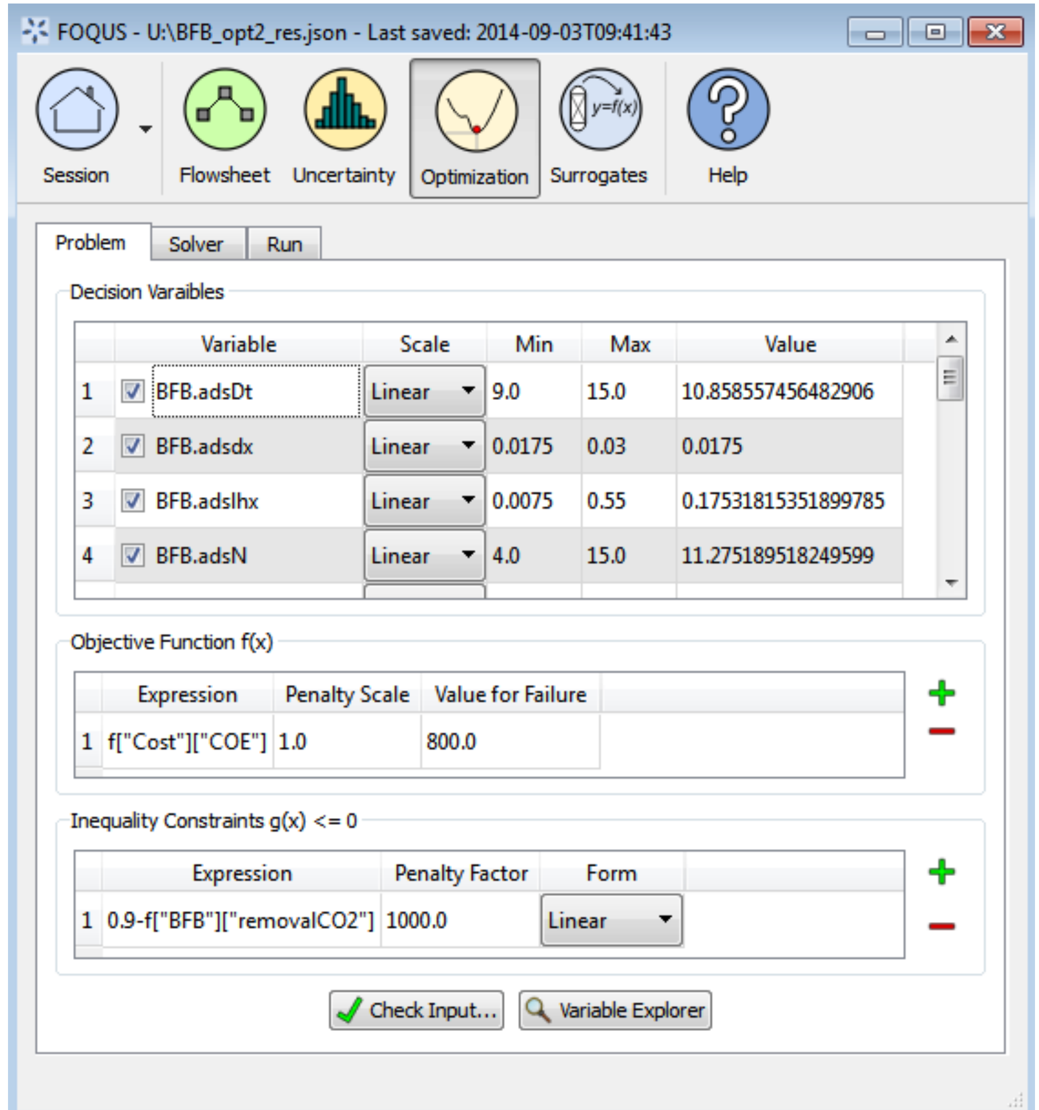
FOQUS Problem Definition

Decision Variables

Objective

Constraints



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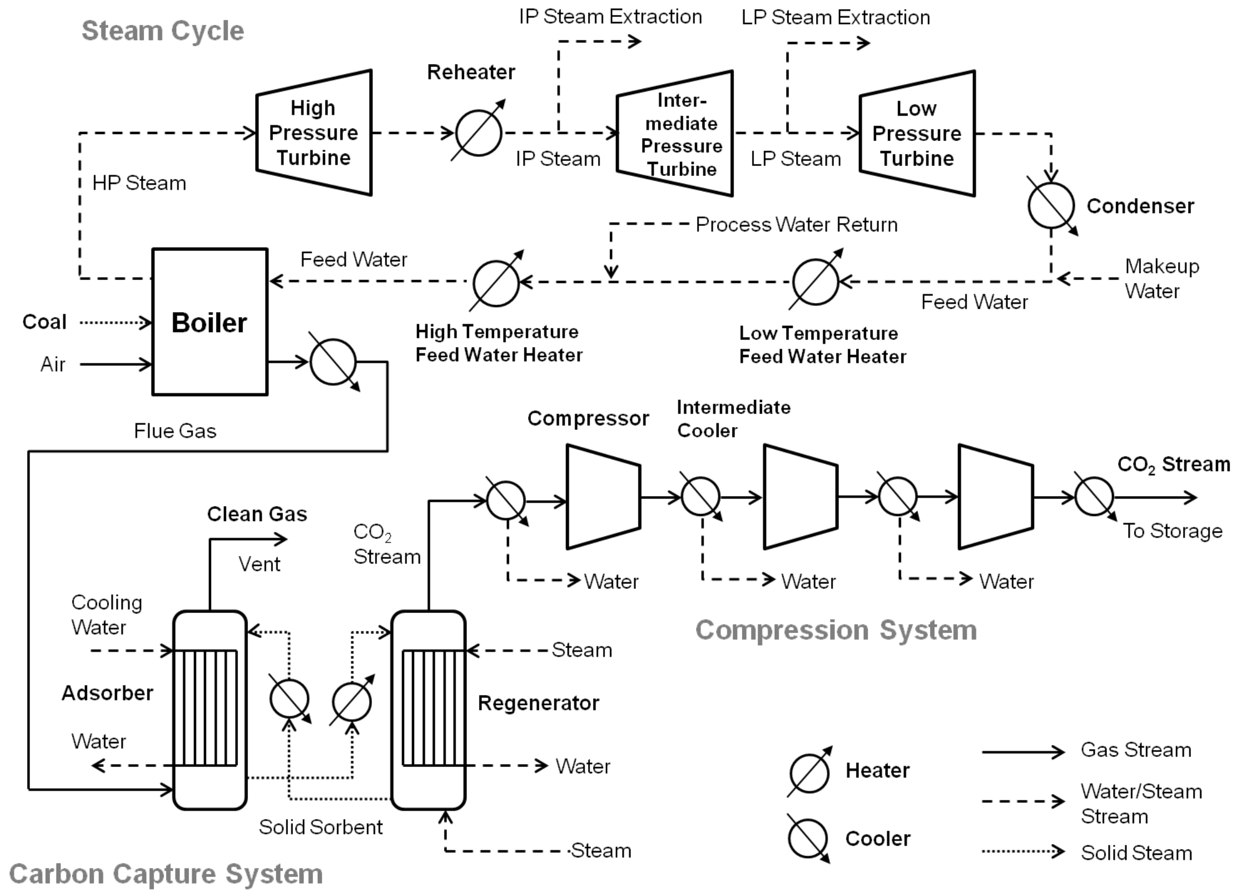
Optimization & Heat Integration



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

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Optimization with Heat Integration

	w/o heat integration	Sequential	Simultaneous
Net power efficiency (%)	31.0	32.7	35.7
Net power output (MW_e)	479.7	505.4	552.4
Electricity consumption [b] (MW_e)	67.0	67.0	80.4
IP steam withdrawn from power cycle (MW_{th})	0	0	0
LP steam withdrawn from power cycle (MW_{th})	336.3	304.5	138.3
Cooling water consumption [b] (MW_{th})	886.8	429.3	445.1
Heat addition to feed water (MW_{th})	0	125.3	164.9

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

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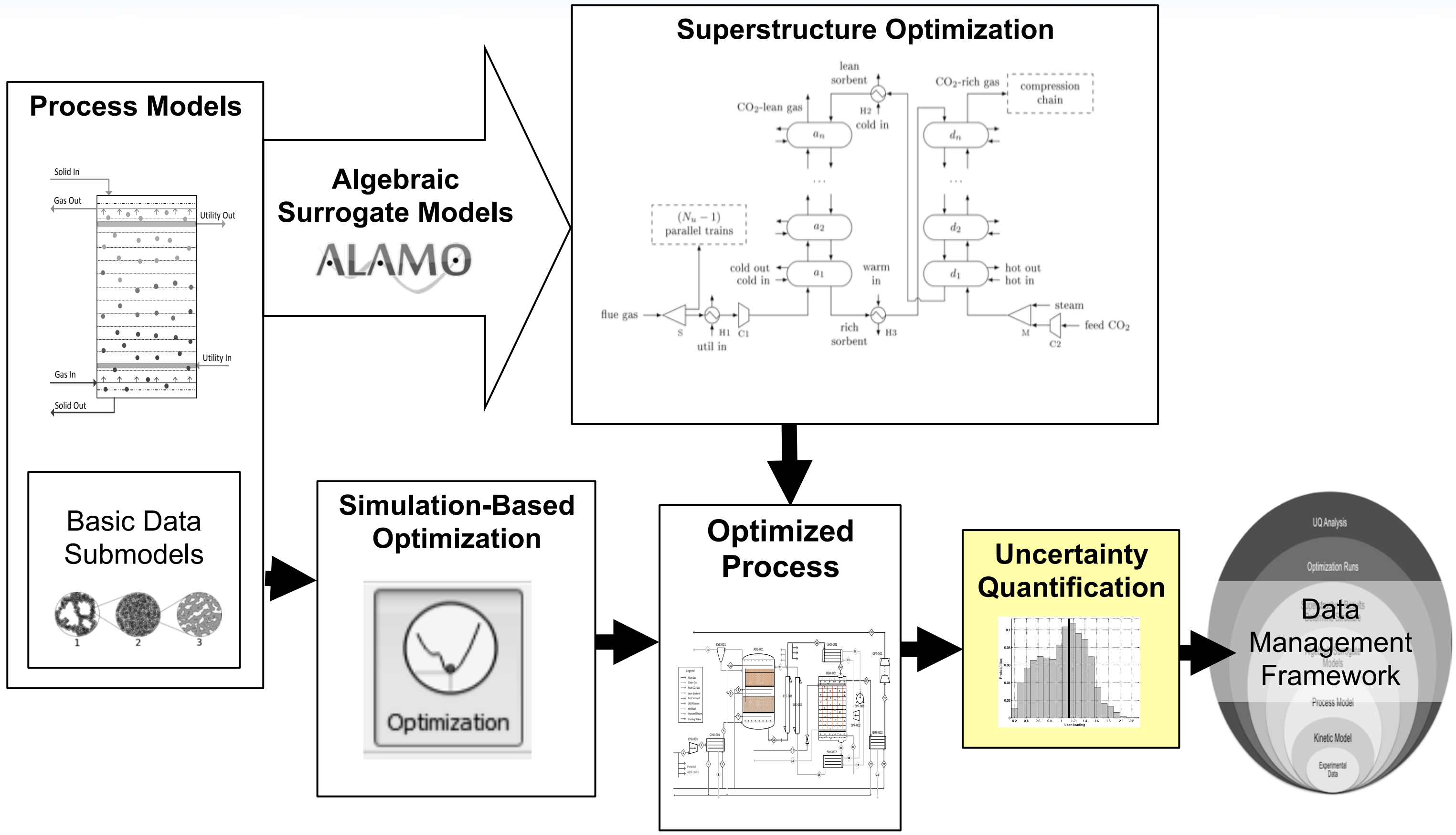
Uncertainty Quantification



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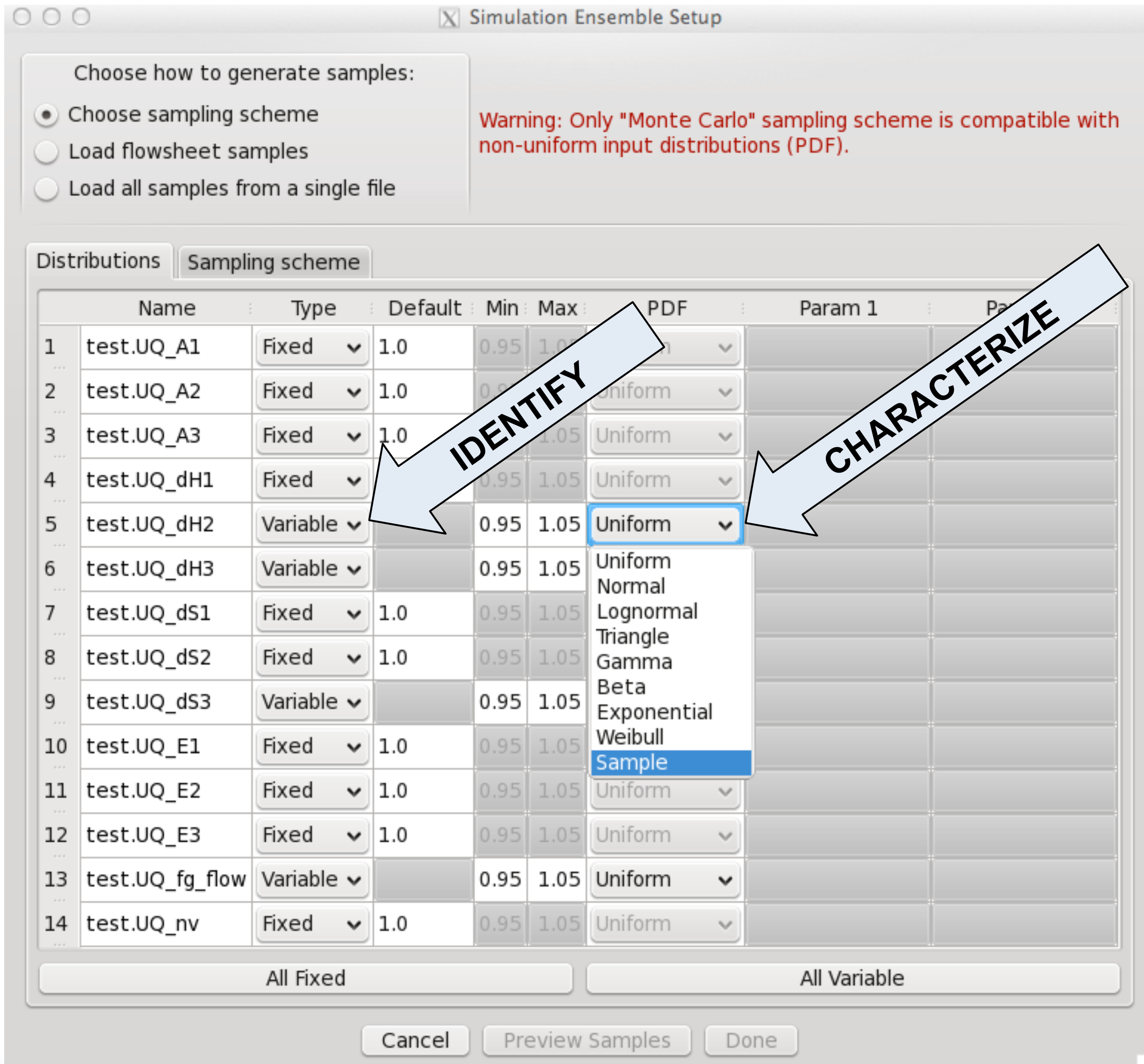
Uncertainty Quantification for Prediction Confidence

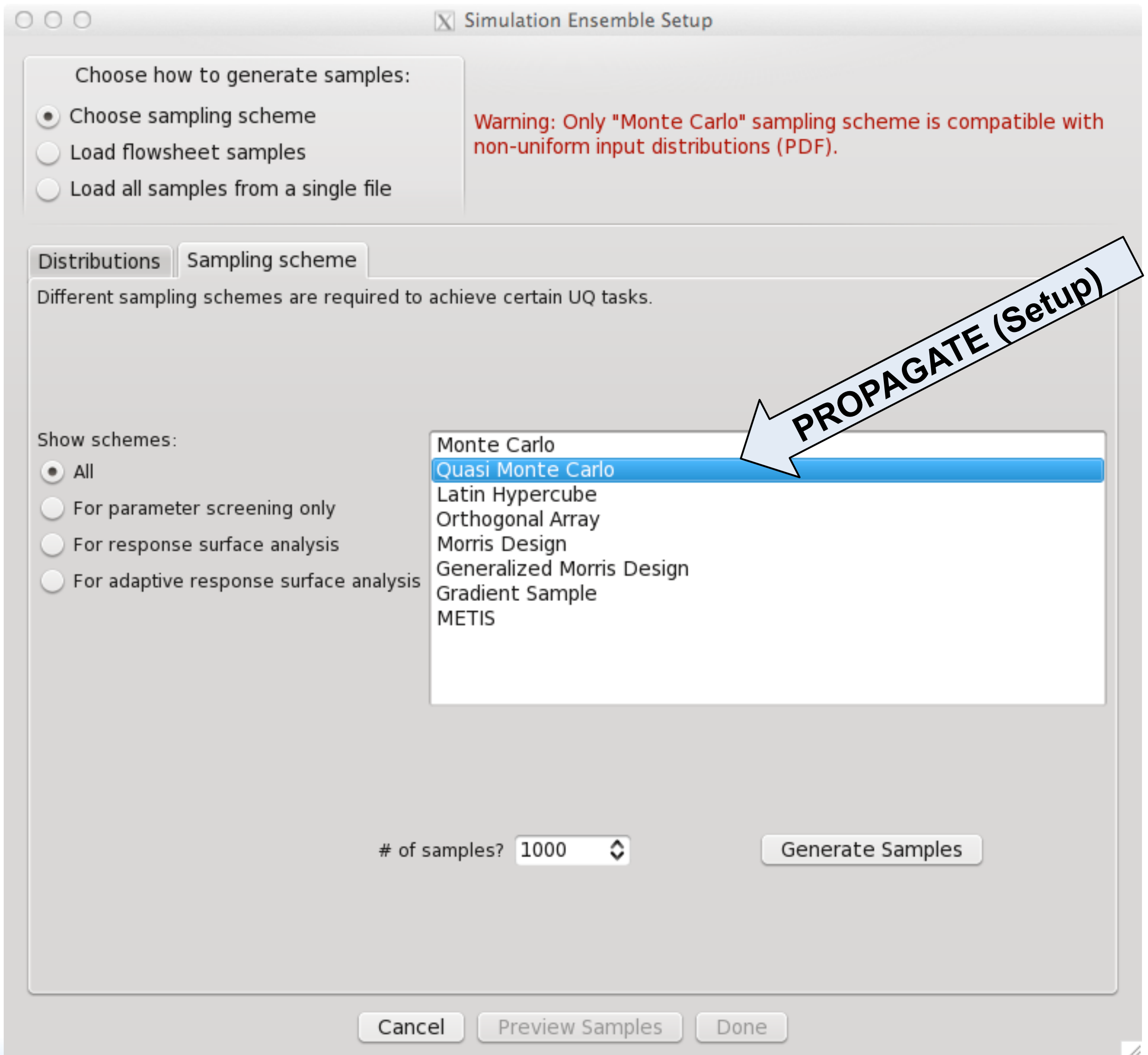
- Now that we have
  - A chemical kinetics model with quantified uncertainty
  - A process model with other sources of uncertainty
  - Surrogates with approximation errors
  - An optimized process based on the above
- UQ questions
  - How do these errors and uncertainties affect our prediction confidence (e.g. operating cost) for the optimized process?
  - Can the optimized system maintain >= 90% CO_2 capture in the presence of these uncertainties?
  - Which sources of uncertainty have the most impact on our prediction uncertainty?
  - What additional experiments need to be performed to give acceptable uncertainty bounds?

CCSI UQ framework is designed to answer these questions

Set up uncertain parameters



Generate simulation ensembles with FOQUS



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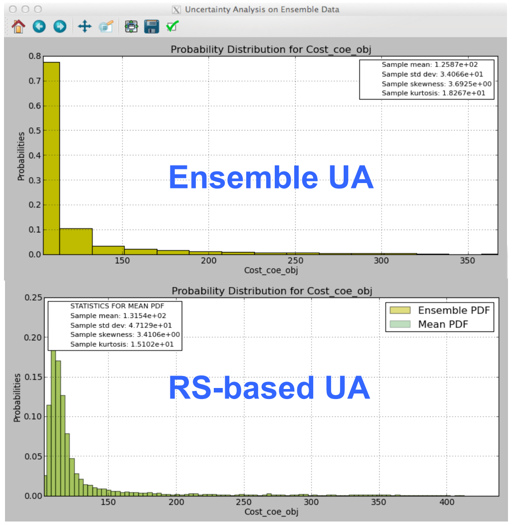
Perform statistical analyses with FOQUS

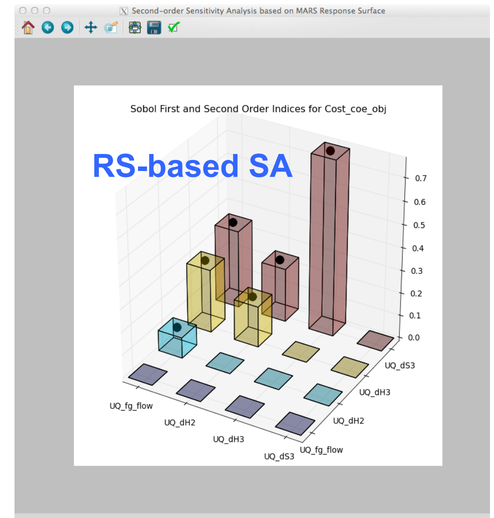


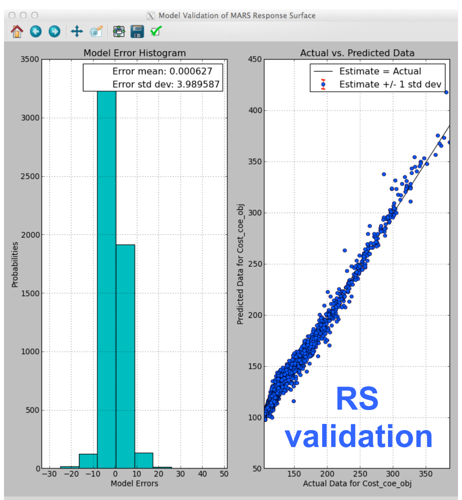
<u>Ensemble Analyses</u>

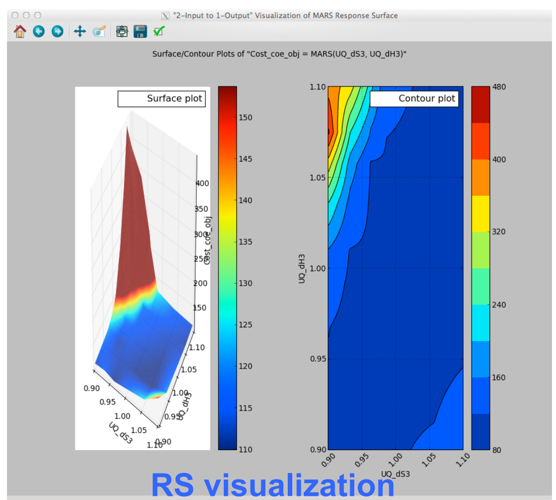
- ➢ Uncertainty analysis
- ➢ Sensitivity analysis
- ➢ Correlation analysis
- ➢ Scatterplots for visualization

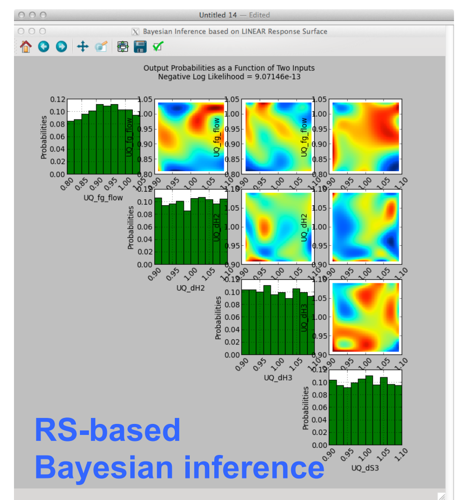
<u>Response Surface (RS) Analyses</u>

- ➢ RS validation
- ➢ RS visualization
- ➢ RS-based uncertainty analysis
- ➢ RS-based sensitivity analysis
- ➢ RS-based Bayesian inference









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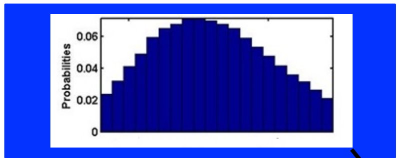
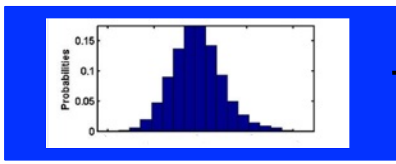
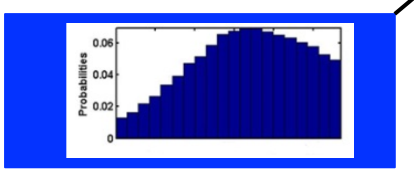
UQ in Solvent System Models



Uncertainty in Properties Models

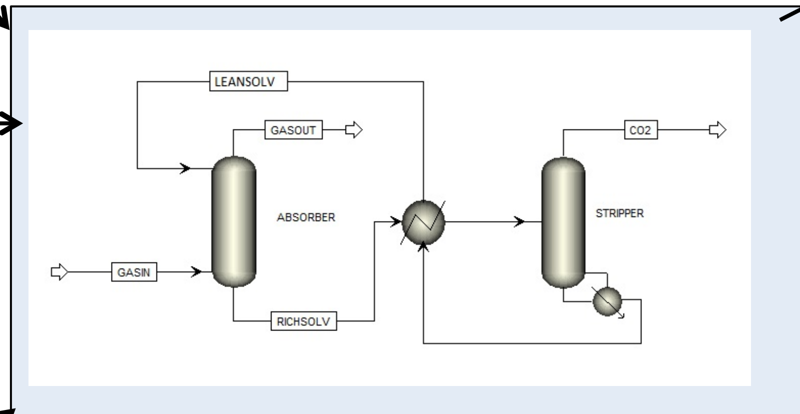


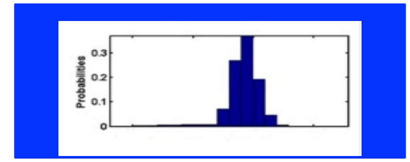
Uncertainty in Hydraulic Models, Mass and Heat Transfer Models



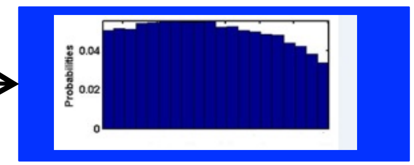
Uncertainty in Kinetic Models

Process Simulation

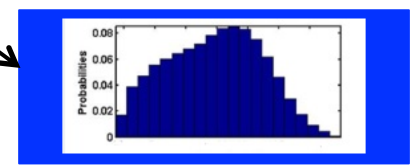




Uncertainty in % CO_2 Capture



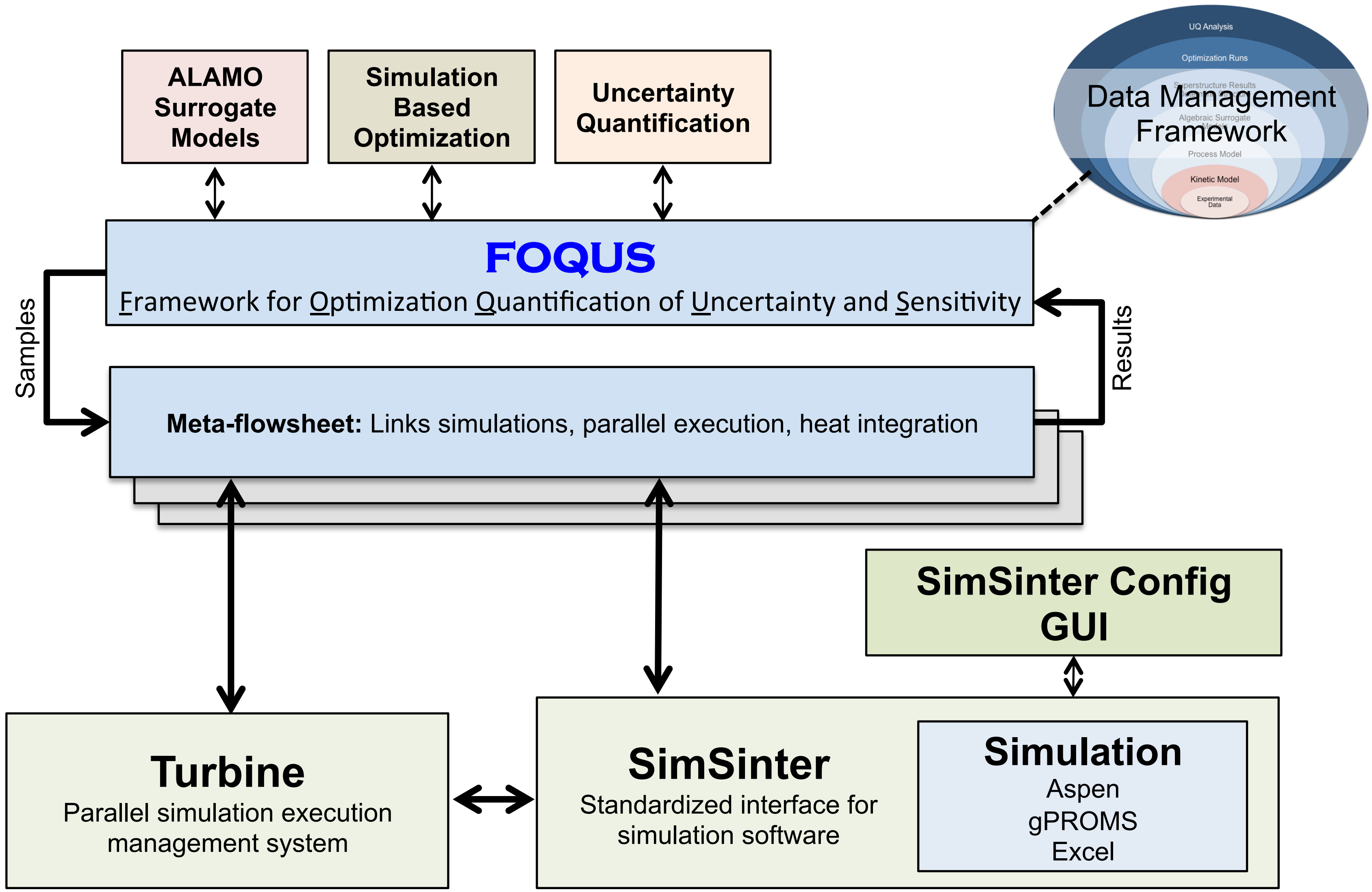
Uncertainty in Energy Requirement



Uncertainty in Estimation of Other Key Variables

Morgan, J. C., D. Bhattacharyya, C. Tong and D. C. Miller (2015). "Uncertainty Quantification of Property Models: Methodology and Its Application to CO2-Loaded Aqueous MEA Solutions1." AIChE Journal. DOI: 10.1002/aic.14762

Framework for Optimization, Quantification of Uncertainty and Sensitivity



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  - UQ: Charles Tong, Brenda Ng, Jeremey Ou
  - Turbine: Josh Boverhof, Deb Agarwal (LBNL)
  - SimSinter: Jim Leek (LLNL), John Eslick (NETL/ORISE, CMU)
- Data Management
  - Tom Epperly (LLNL)
  - Deb Agarwal, You-Wei Cheah (LBNL)

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