

CCSI²

Carbon Capture Simulation for Industry Impact

Solvent Pilot System Test Campaign Guidance

Brenda Ng*, Charles Tong, Lawrence Livermore National Laboratory

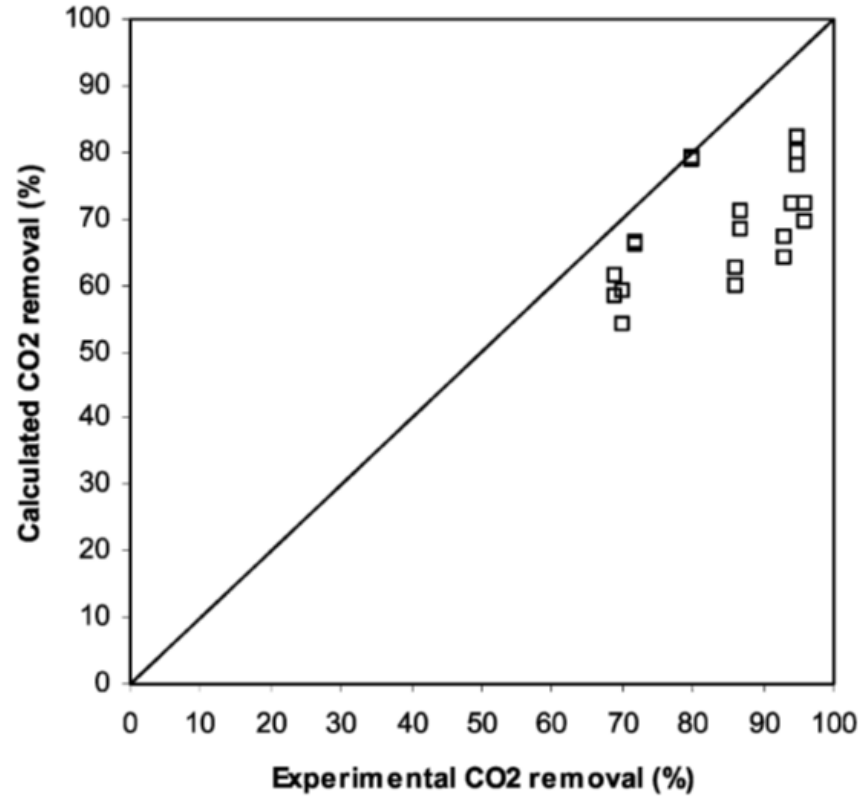
Jim Gattiker*, Christine Anderson-Cook, Los Alamos National Laboratory

Debangsu Bhattacharyya*, Joshua Morgan, West Virginia University



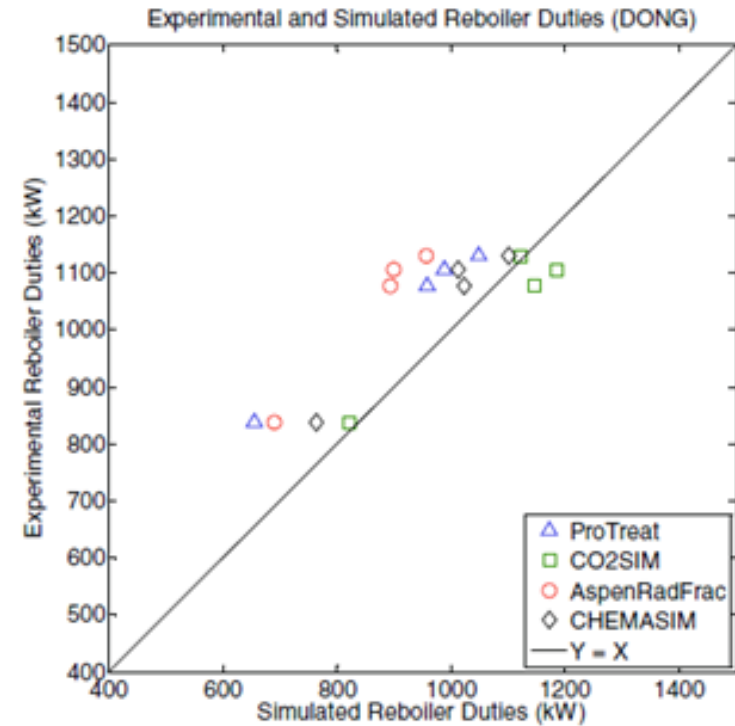
Typical Steady-State DOE

Absorber



Zhang, et al., Rate-Based Process Modeling Study of CO₂ Capture with Aqueous Monoethanolamine Solution, Ind. Eng. Chem Res., 48, 9233-9246, 2009

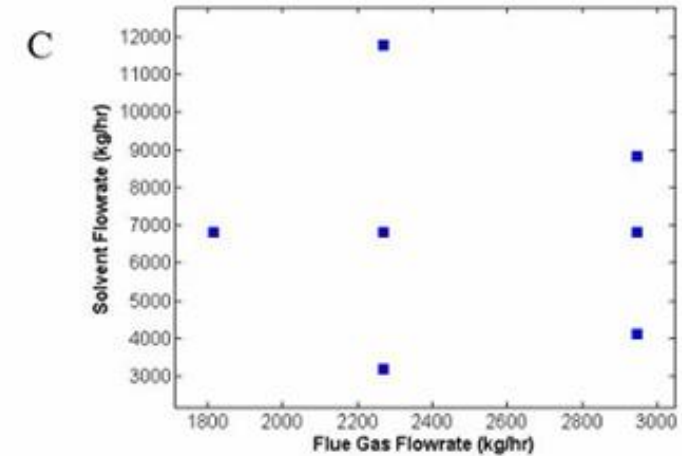
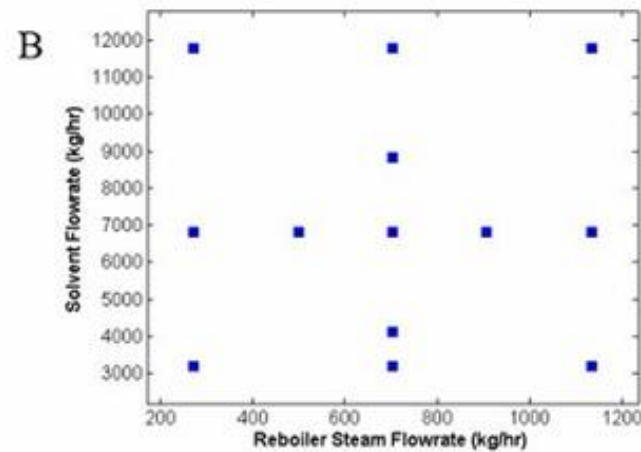
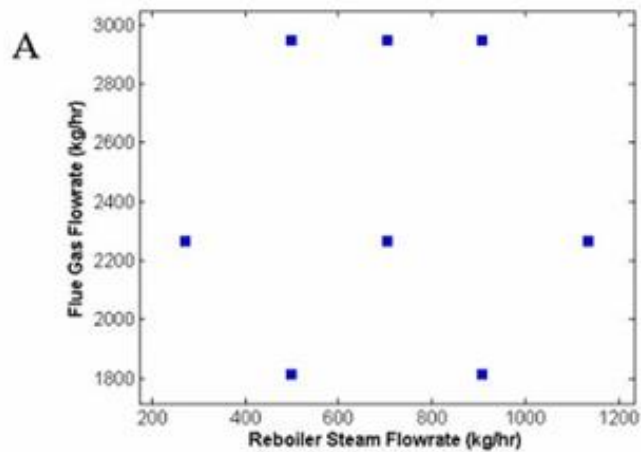
Regenerator



Luo et al., "Comparison and validation of simulation codes against sixteen sets of data from four different pilot plants", Energy Procedia, 1249-1256, 2009

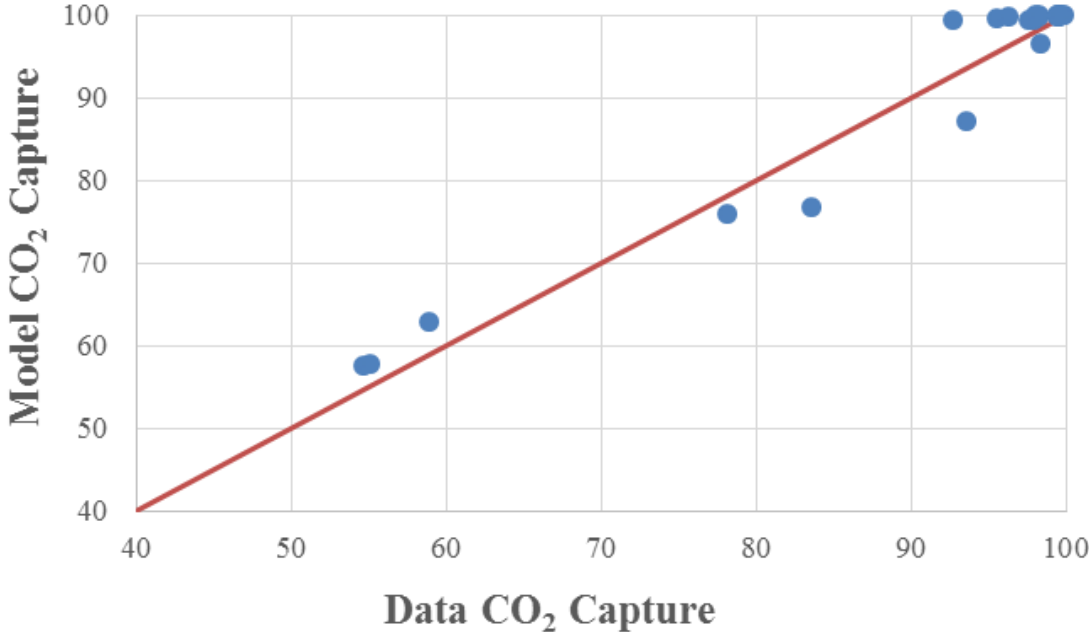
CCSI DOE for National Carbon Capture Center

Operating Conditions	Range
Solvent Flow (lb/hr)	7,000-26,000
Inlet Flue Gas (lb/hr)	5,000-6,500
Reboiler Steam Flow (lb/hr)	600-2,500
Inlet FG CO ₂ vol%	9-11%
# of beds	1-3
Intercooler	no - yes

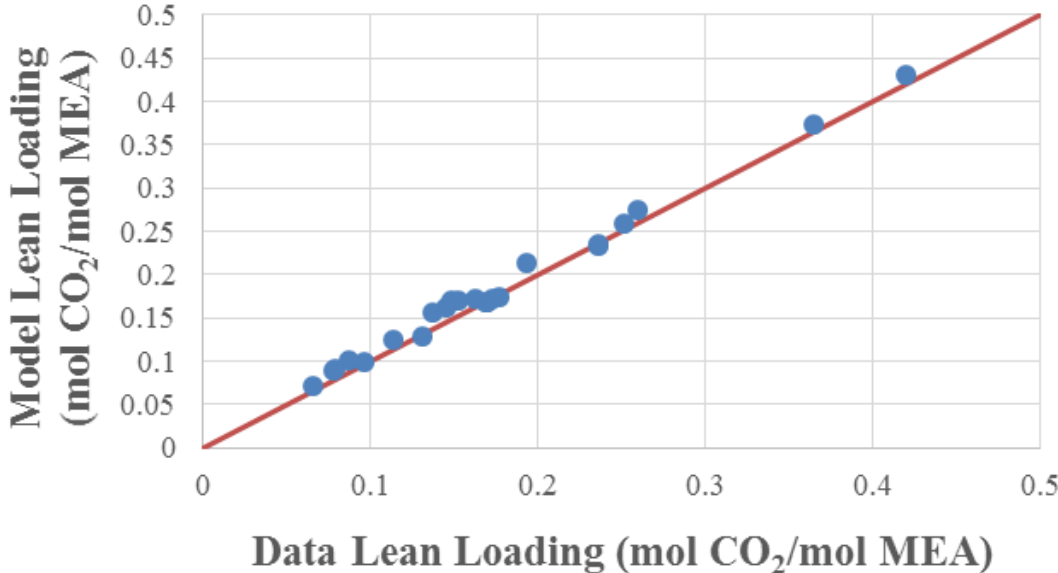


Results from 2014 CCSI DOE and Comparison with CCSI Model

Absorber



Regenerator



Motivation and Goals

Motivations

- Collecting a strategic sample of data can:
 - Help reach required precision or understanding faster
 - Maximize learning with a fixed set of resources or minimize required resources for a given learning objective

Goal

- Our goal is to develop a predictive model that can be used for cost-optimal plant design and operation
- To satisfy this goal, our objective for DOE is:
 - G-optimality – minimizing the worst prediction variance in the design space (minimizing the largest uncertainty value for input combinations)
 - For variables: carbon capture (and lean loading)

Issues

What was missing in the previous DOE?

- Mainly designed using a space-filling approach without considering the output space
- When designed considering the output space, feedback from the experimental data are not leveraged to update the DOE

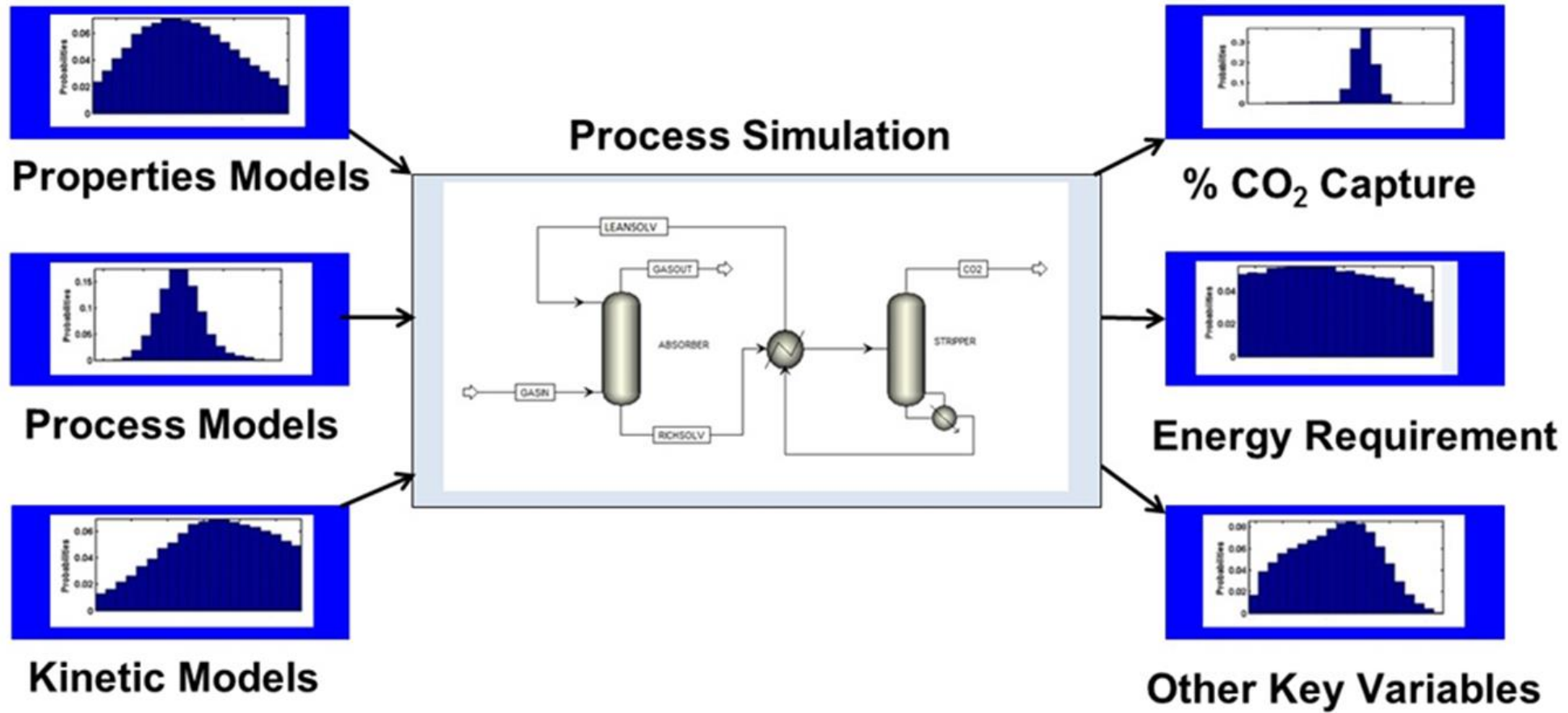
How to solve these issues?

- Develop DOE by taking into consideration the output space by using a preliminary process model
- Use a sequential approach to improve DOE as experimental data are obtained

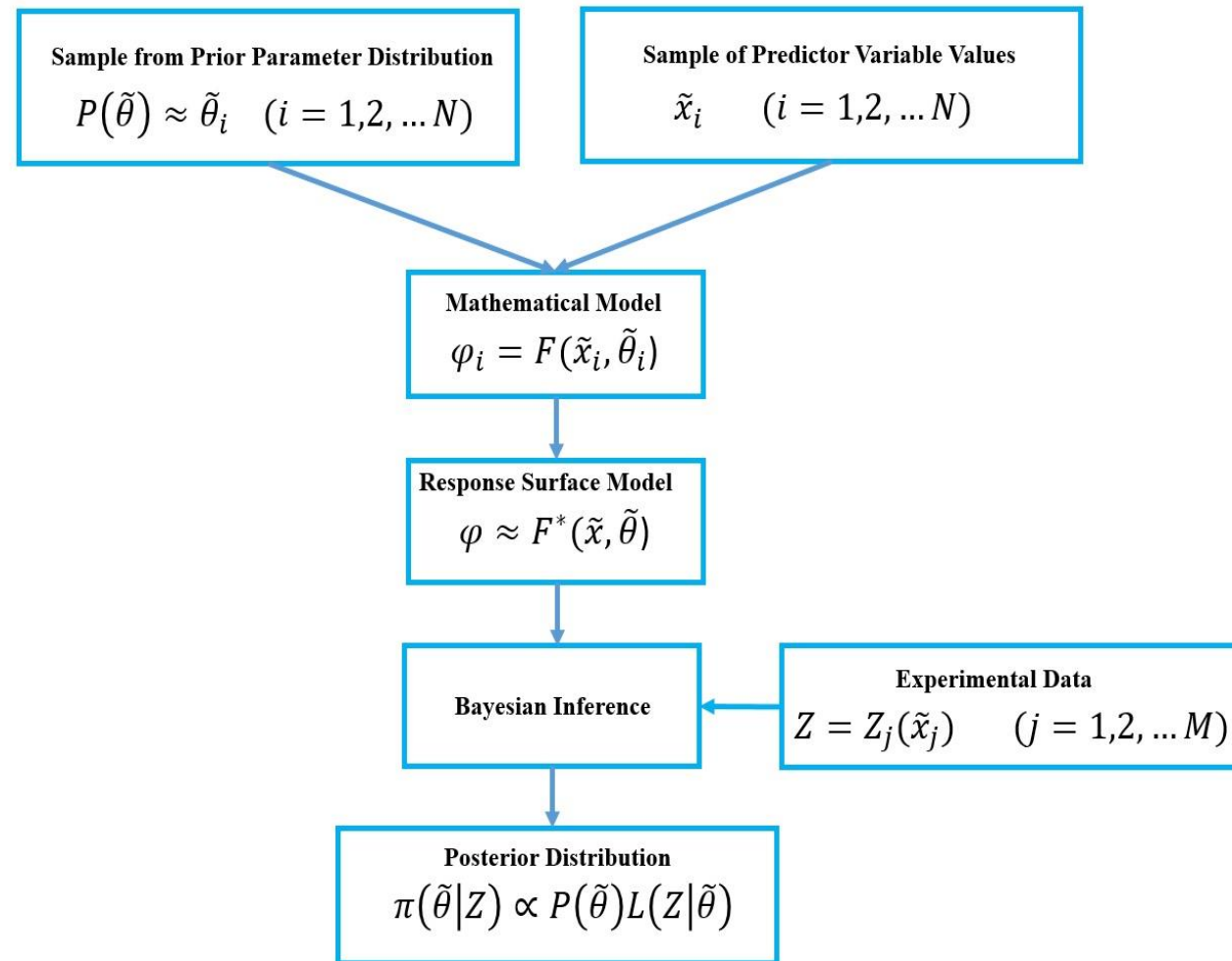
Other issues?

- There are uncertainties in the measurements, process model and its parameters

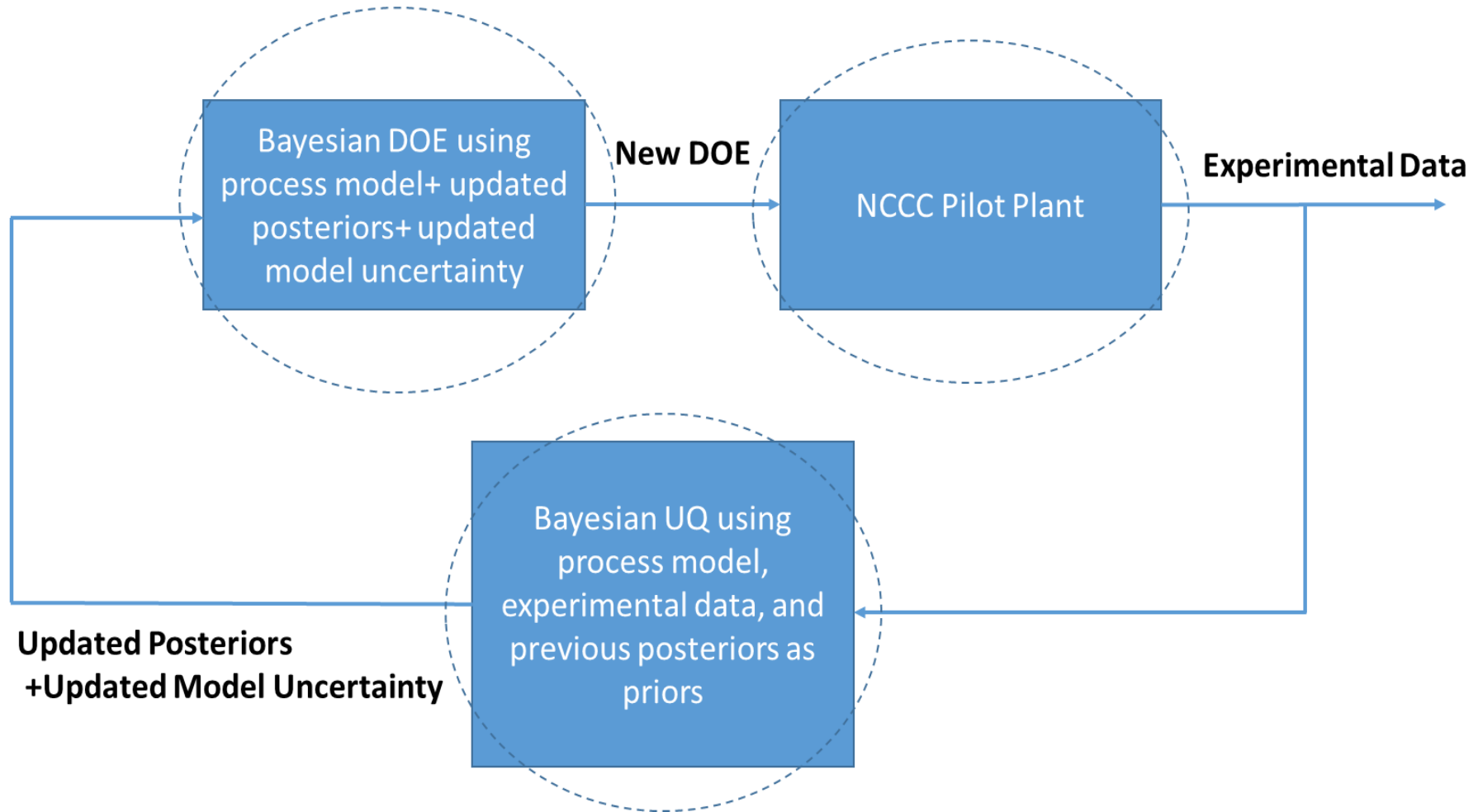
CCSI² Approach to Uncertainty Quantification

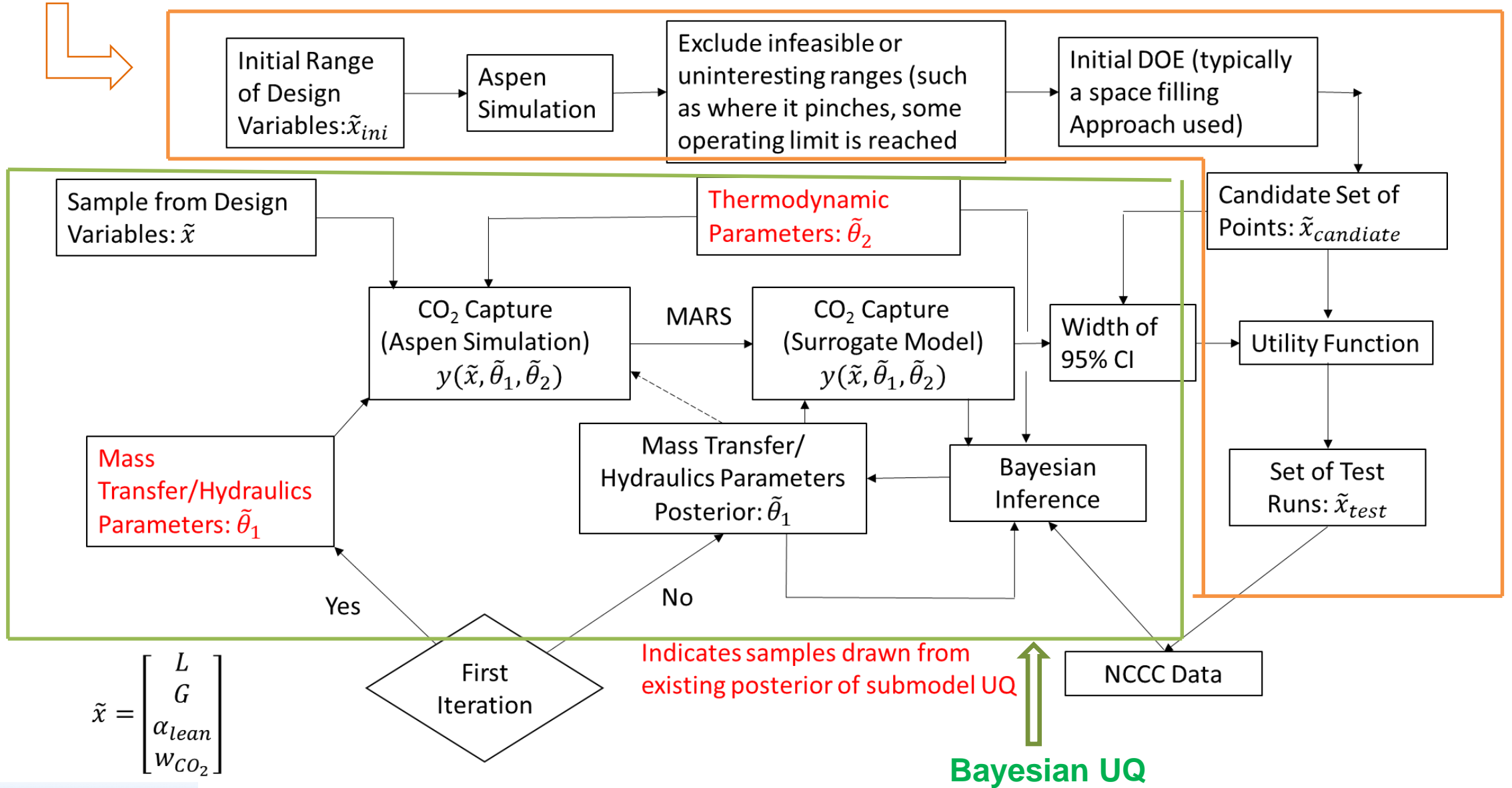


Bayesian Uncertainty Quantification Approach



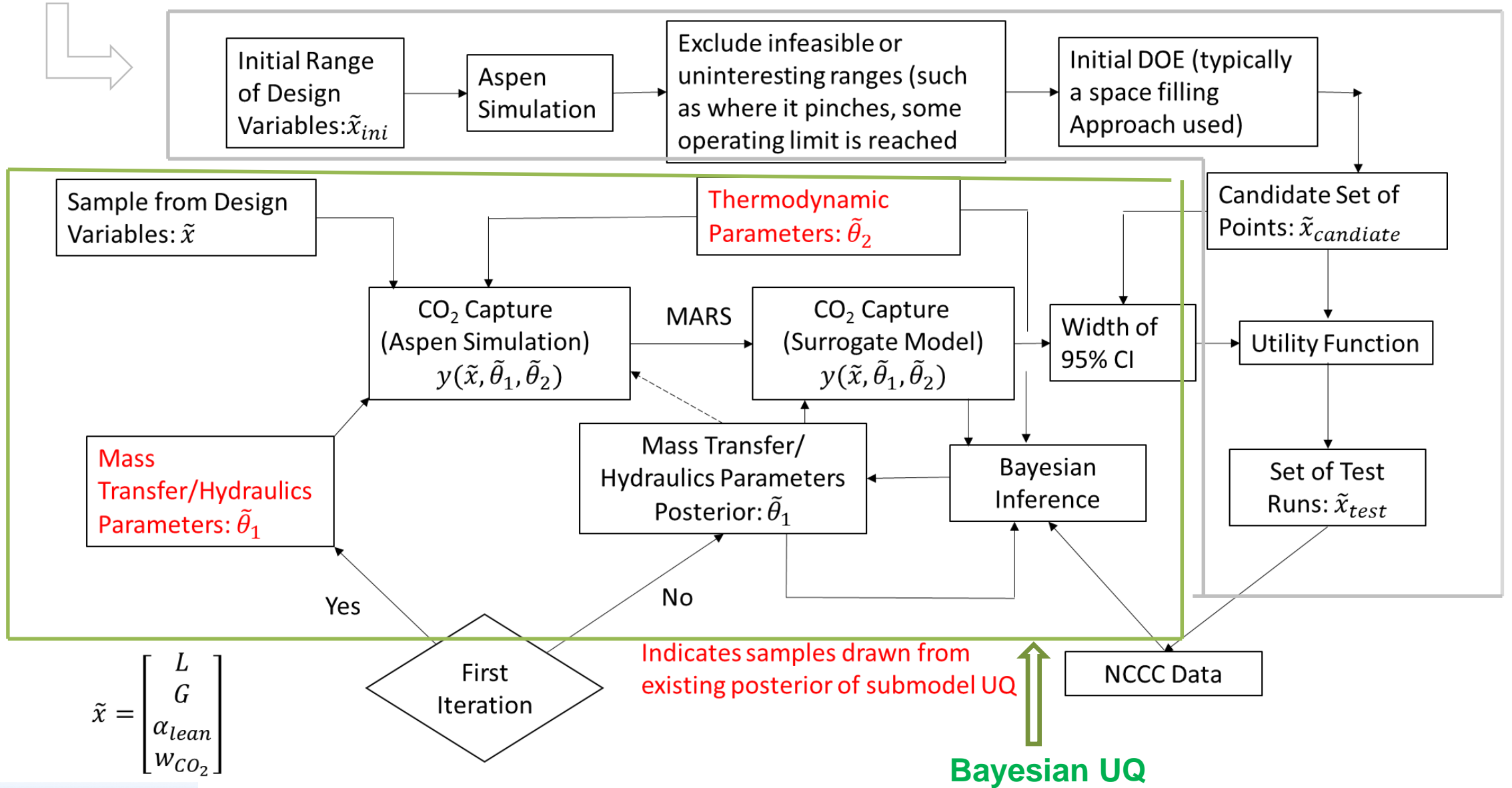
Overall Approach to Design of Experiments: Bayesian Sequential Design of Experiments



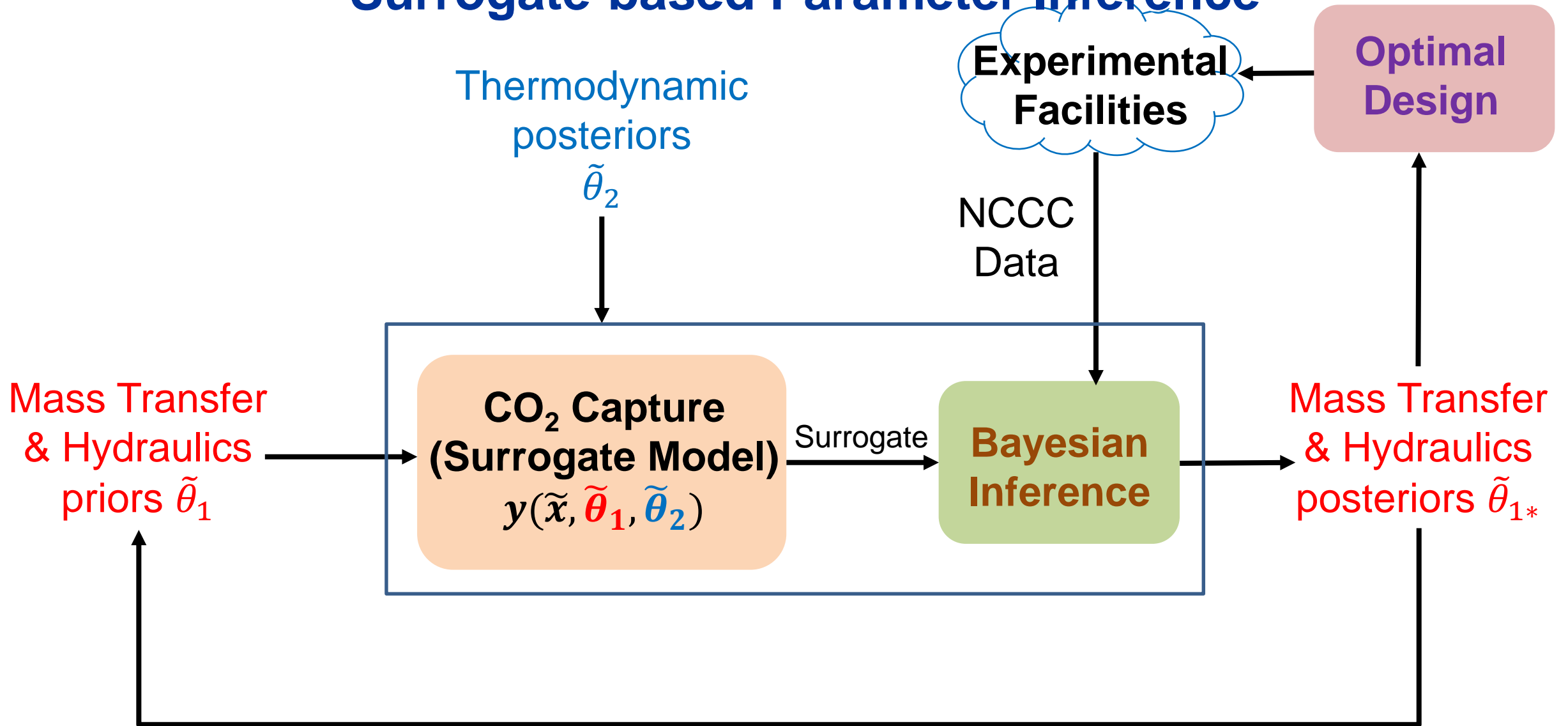


$$\tilde{x} = \begin{bmatrix} L \\ G \\ \alpha_{lean} \\ w_{CO_2} \end{bmatrix}$$

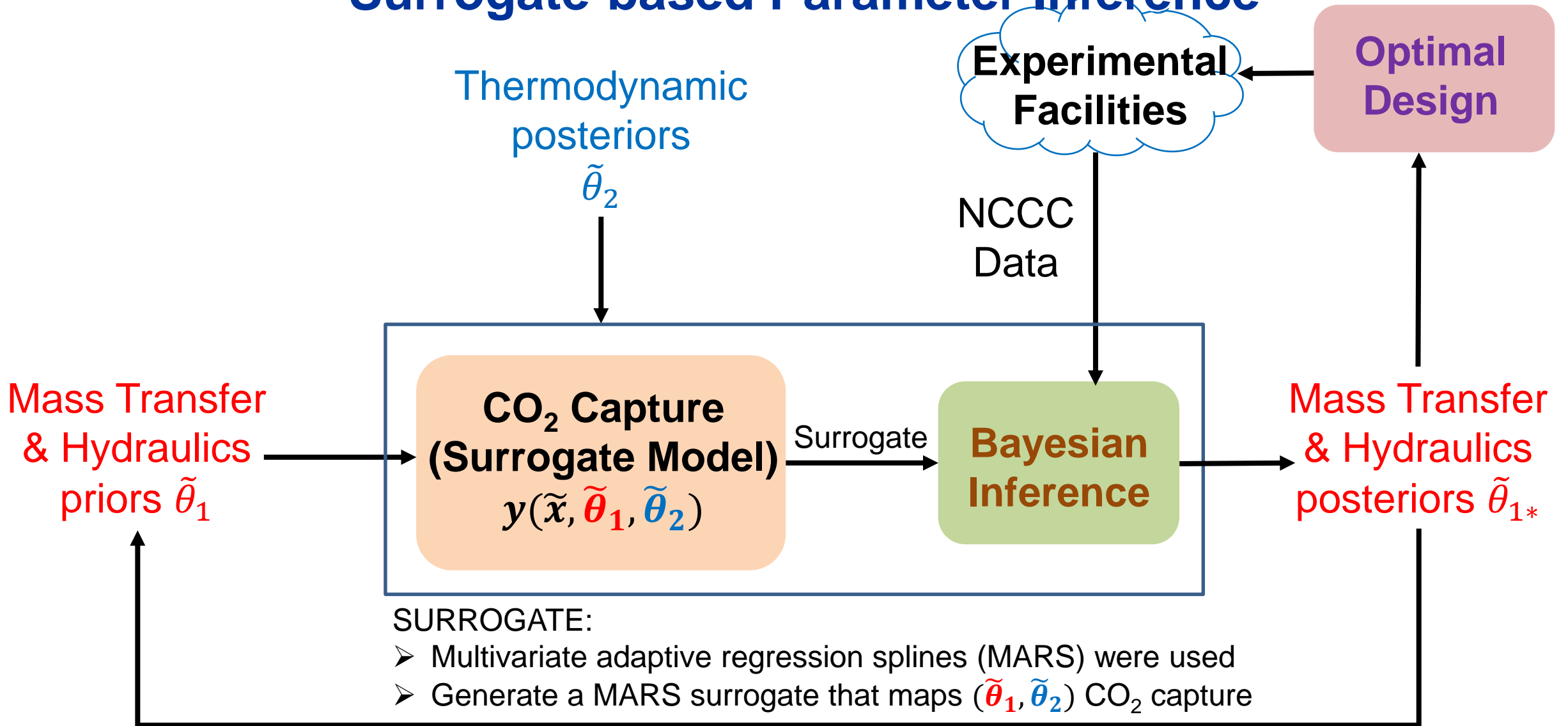
Methodology



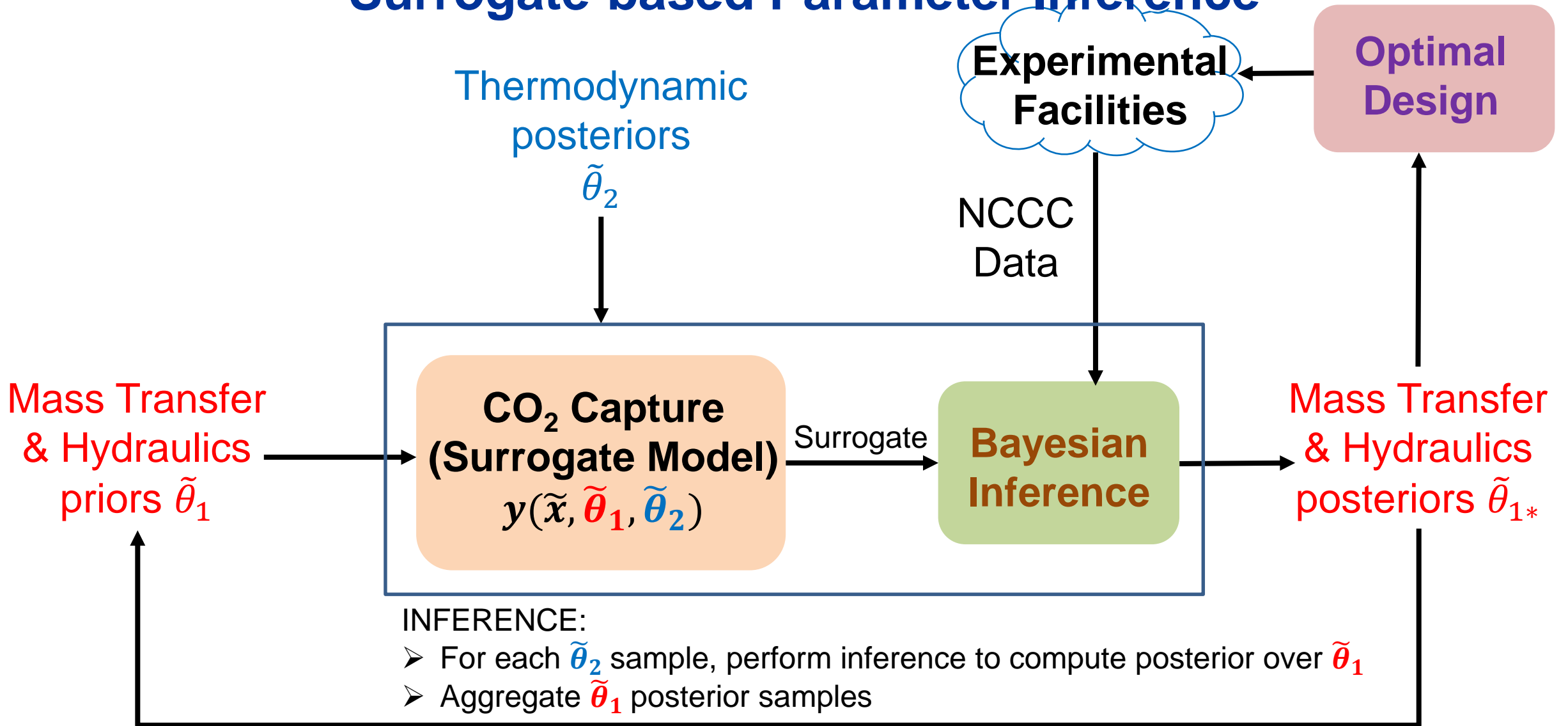
Surrogate-based Parameter Inference



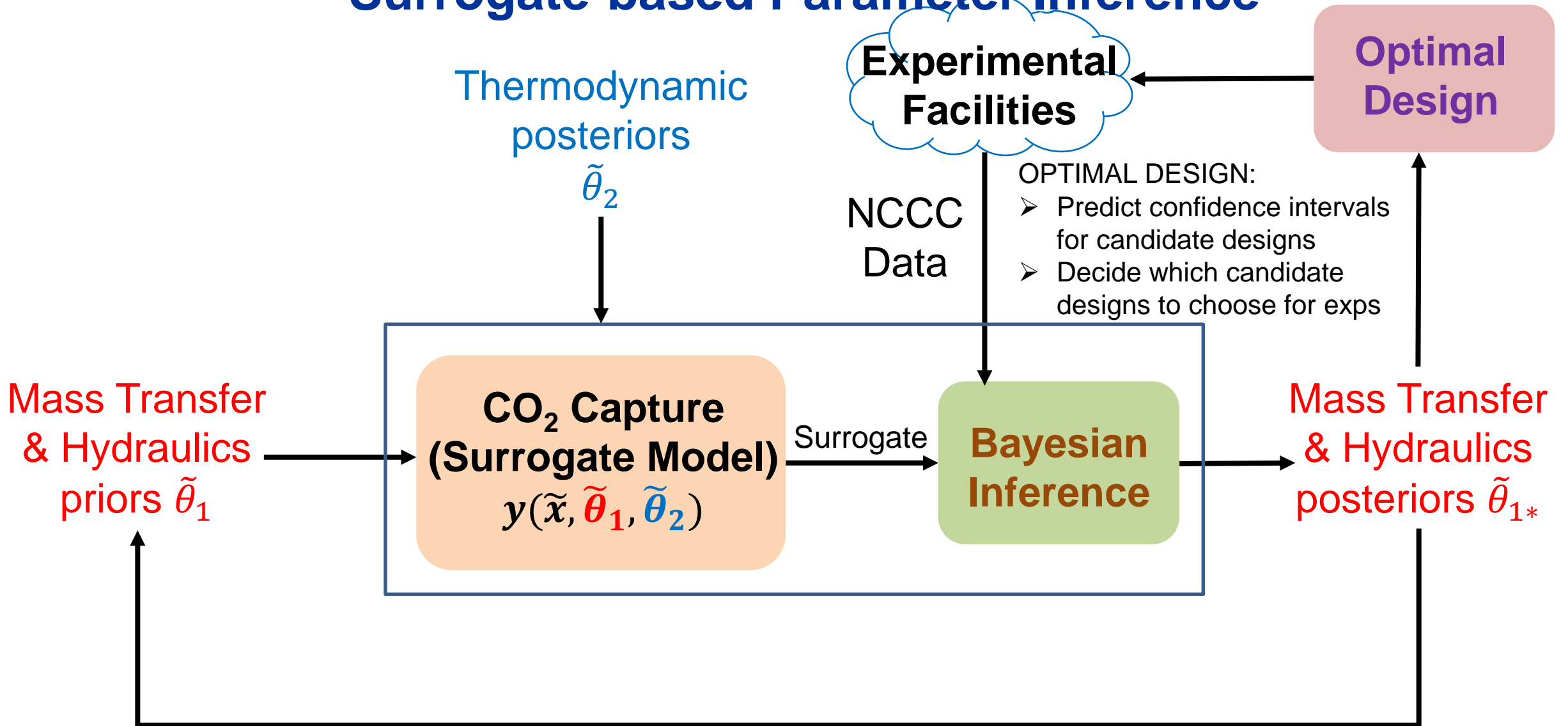
Surrogate-based Parameter Inference



Surrogate-based Parameter Inference



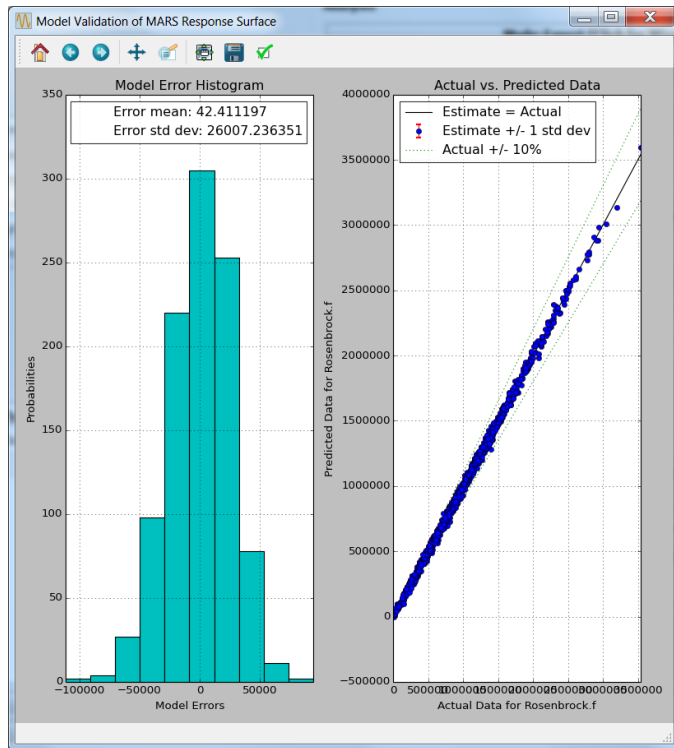
Surrogate-based Parameter Inference



Surrogate Support

UQ

- Train and validate surrogates
- Perform surrogate-based analyses



The screenshot shows the 'Analysis' window in the software. The 'Mode' is set to 'Expert (Click for Wizard Mode)'. The 'Select Output under Analysis' is 'Rosenbrock.f'. Under 'Qualitative Parameter Selection', the 'Choose Parameter Selection Method' is 'MARS Ranking' and there is a 'Compute input importance' button. The 'Ensemble Data Analysis' section has 'Choose UQ Analysis' set to 'Uncertainty Analysis' and an 'Analyze' button. The 'Response Surface (RS) Based Analysis' section is highlighted with a red box and includes: 'Select RS:' set to 'MARS ->' and 'MARS'; 'Legendre Polynomial Order:' set to 1; 'MARS Number of basis functions:' set to 100; 'MARS Degree of interaction:' set to 6; and a 'Browse...' button for the 'User Regression File'. Below this, there is a 'Validate:' section with a 'Use test set for output Rosenbrock.f' checkbox, a 'Browse...' button, and a 'Validate' button. The 'Number of Cross-Validation Groups' is set to 10, and there is a 'Save RS interpolation code to file...' button. The 'Visualize RS:' section has three 'None selected' dropdowns and a 'Visualize' button. There are also 'Upper Threshold:' and 'Lower Threshold:' checkboxes. The 'Choose UQ Analysis:' dropdown is open, showing options: 'Sensitivity Analysis ->', 'Uncertainty Analysis ->', 'Sensitivity Analysis ->', and 'Point Evaluation'. Below this is a table with columns 'PDF Param1', 'PDF Param2', and 'Mi'. The table contains two rows: '1 Rosenbrock.x1 Uniform -1' and '2 Rosenbrock.x2 Uniform -1'. At the bottom, there is a 'Bayesian Inference' section with an 'Infer...' button.

Bayesian Inference

UQ

- Import experimental data on observed variables
- Specify prior distribution on input parameters
- Apply surrogate to perform inference
- Save sample of posterior distribution

Bayesian Inference of Ensemble UQ_Ensemble

Output Settings:

Observed?	Output Name	Response Surface	(cont...)
<input type="checkbox"/>	graph.error		
<input checked="" type="checkbox"/>	Rosenbrock.f	Polynomial ->	Linear

Input Settings:

Input Name	Type	Display?	Fixed Value	PDF
1 Rosenbrock.x1	Variable	<input checked="" type="checkbox"/>	4	Uniform
2 Rosenbrock.x2	Variable	<input checked="" type="checkbox"/>	5	Uniform
3 Rosenbrock.x3	Variable	<input checked="" type="checkbox"/>	4	Uniform
4 Rosenbrock.x4	Variable	<input checked="" type="checkbox"/>	5	Uniform
5 Rosenbrock.x5	Variable	<input checked="" type="checkbox"/>	4	Uniform
6 Rosenbrock.x6	Variable	<input checked="" type="checkbox"/>	4	Uniform

Observations:

Number of experiments: 1

Load Observations File... Save Observations File...

	Rosenbrock.f Mean	Rosenbrock.f Std Dev
Experiment 1	1.02171e+06	620380

Save Posterior Input Samples to File: utPostSample Browse...

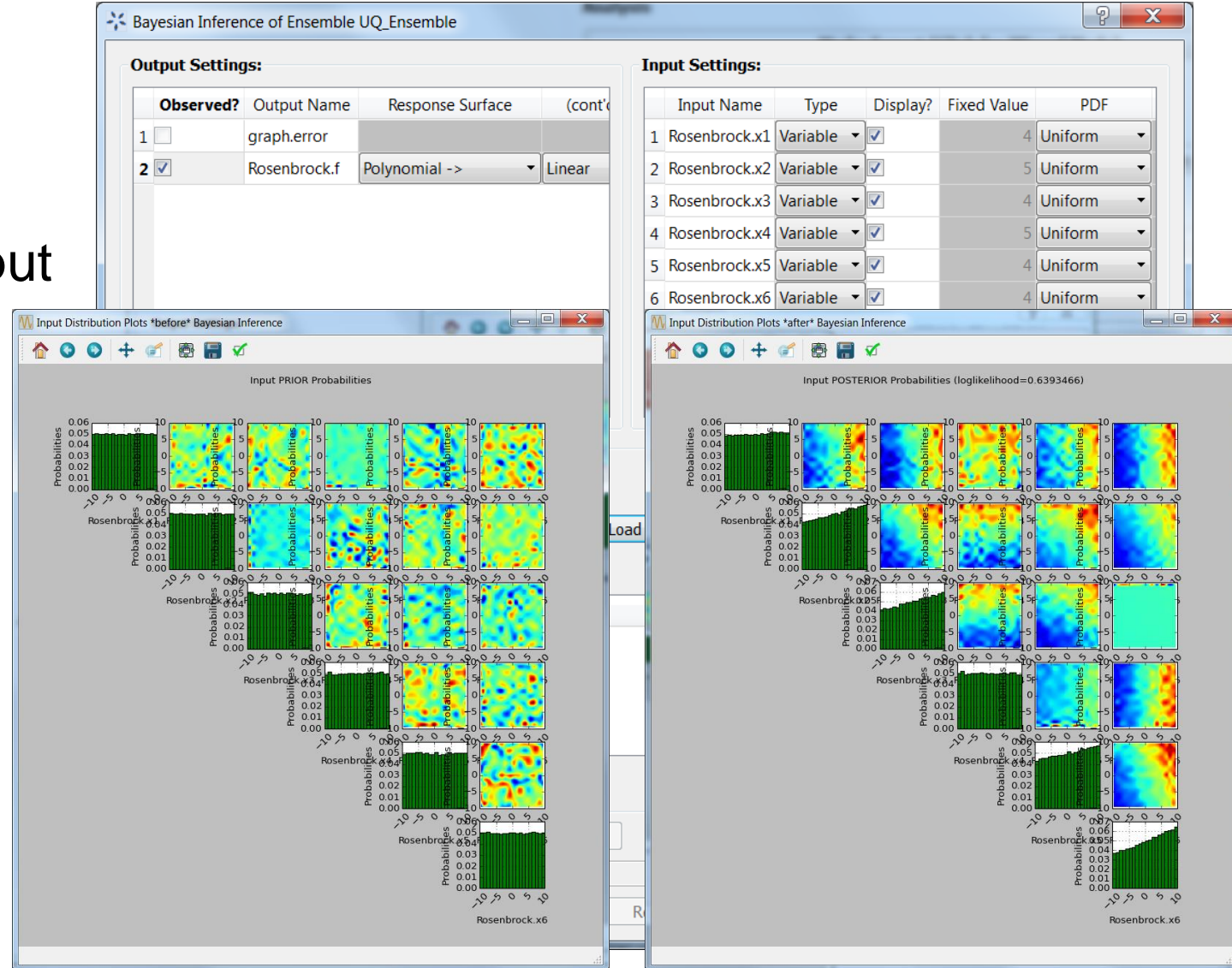
Use Discrepancy Save Discrepancy Input Samples to File: Browse...

Infer Replot Close

Bayesian Inference

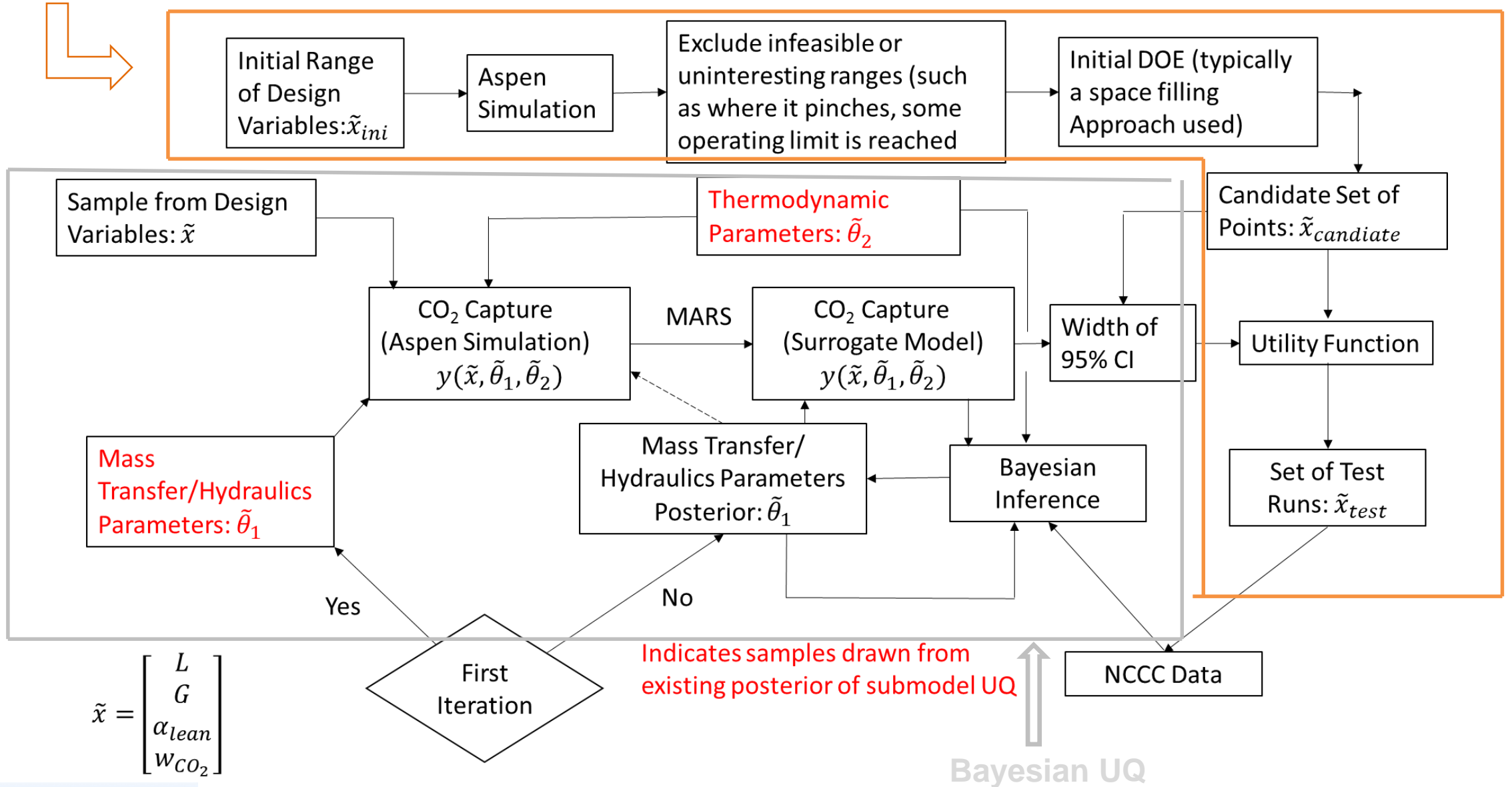
UQ

- Import experimental data on observed variables
- Specify prior distribution on input parameters
- Apply surrogate to perform inference
- Save sample of posterior distribution



Bayesian DOE

Methodology



Goals for Designed Experiments

- Be efficient about learning from:
 - Historical data
 - System model
 - Expert knowledge and judgement in the domain
 - Experiments
- Characterize Carbon Capture systems and models
- Accelerate technology development

NCCC Experimental Design, First step:

Design: the settings of experimental conditions.

Define the settings of interest for experimentation

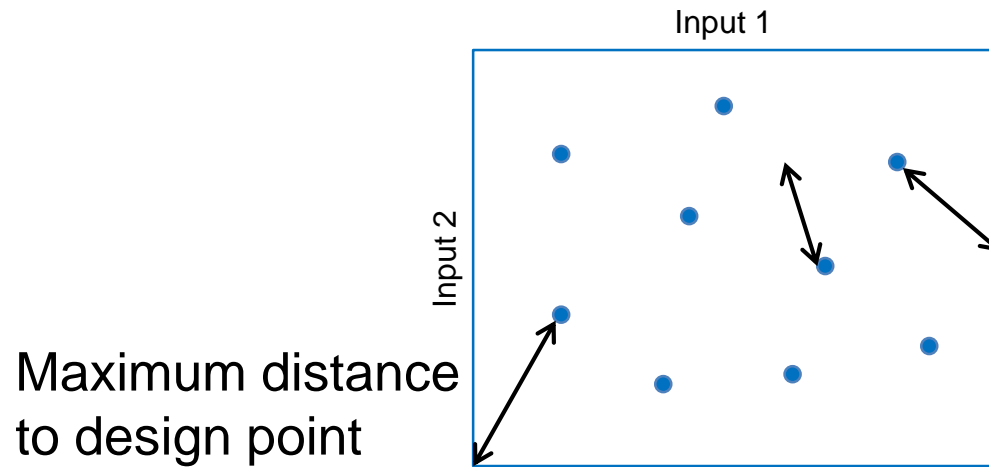
- Flue Gas Flowrate, G in [1000-3000] kg/hr;
- CO₂ weight fraction, w in [0.125-0.175], i.e. (8.4-11.7 mol% CO₂);
- Lean solvent loading, l_{ldg} in [0.1-0.3] and;
- Lean solvent flowrate L in [3000-12000] kg/hr

Explore constraints, dependencies, experimental realities.

Designing NCCC Experiments

Initial goal is *exploration* of the input space

- Criterion used was “minimax” = minimize the largest distance from any point in the input space to a design point



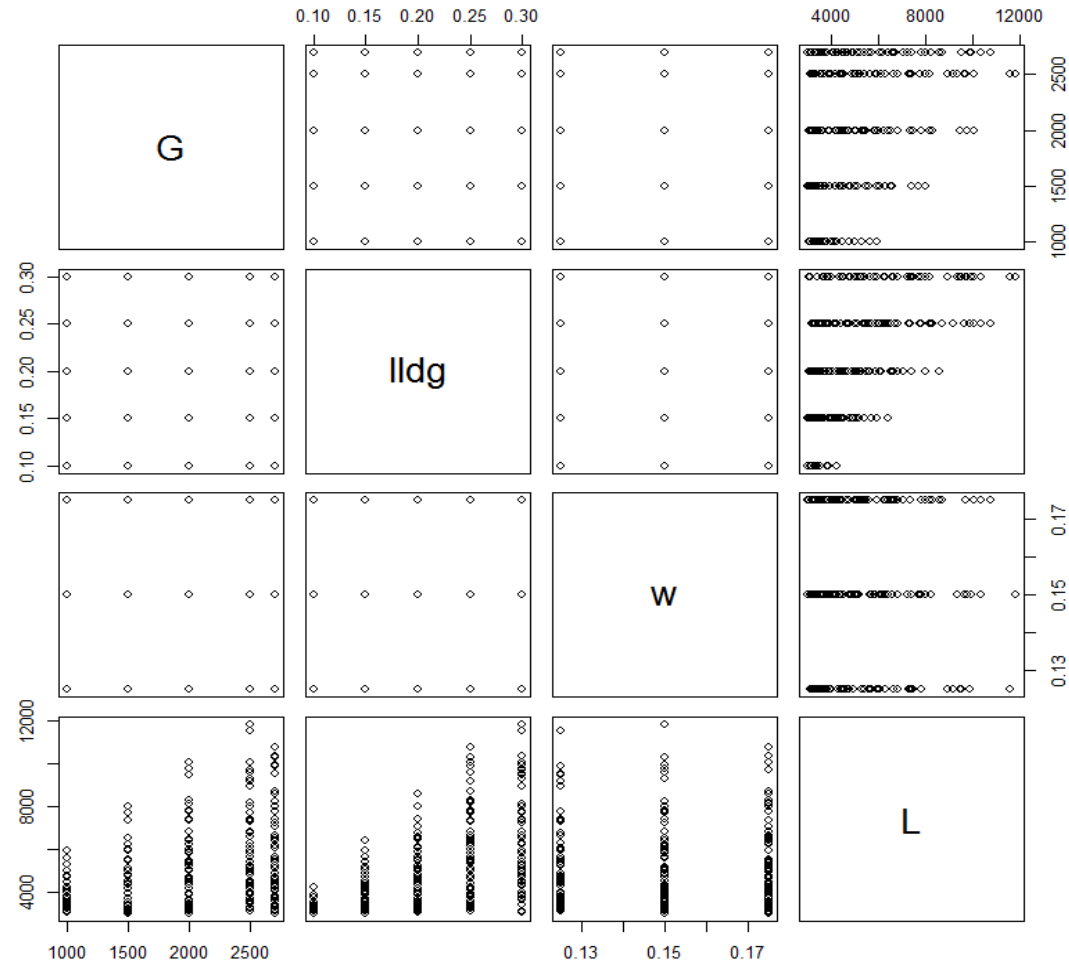
- Design points

Candidate input combinations

For NCCC experiment:

- 5 levels of G
- 5 levels of Ildg
- 3 levels of w
- 5 levels of L for each combination of G, Ildg and w

Balance richness of potential experiments against the computation of model evaluation

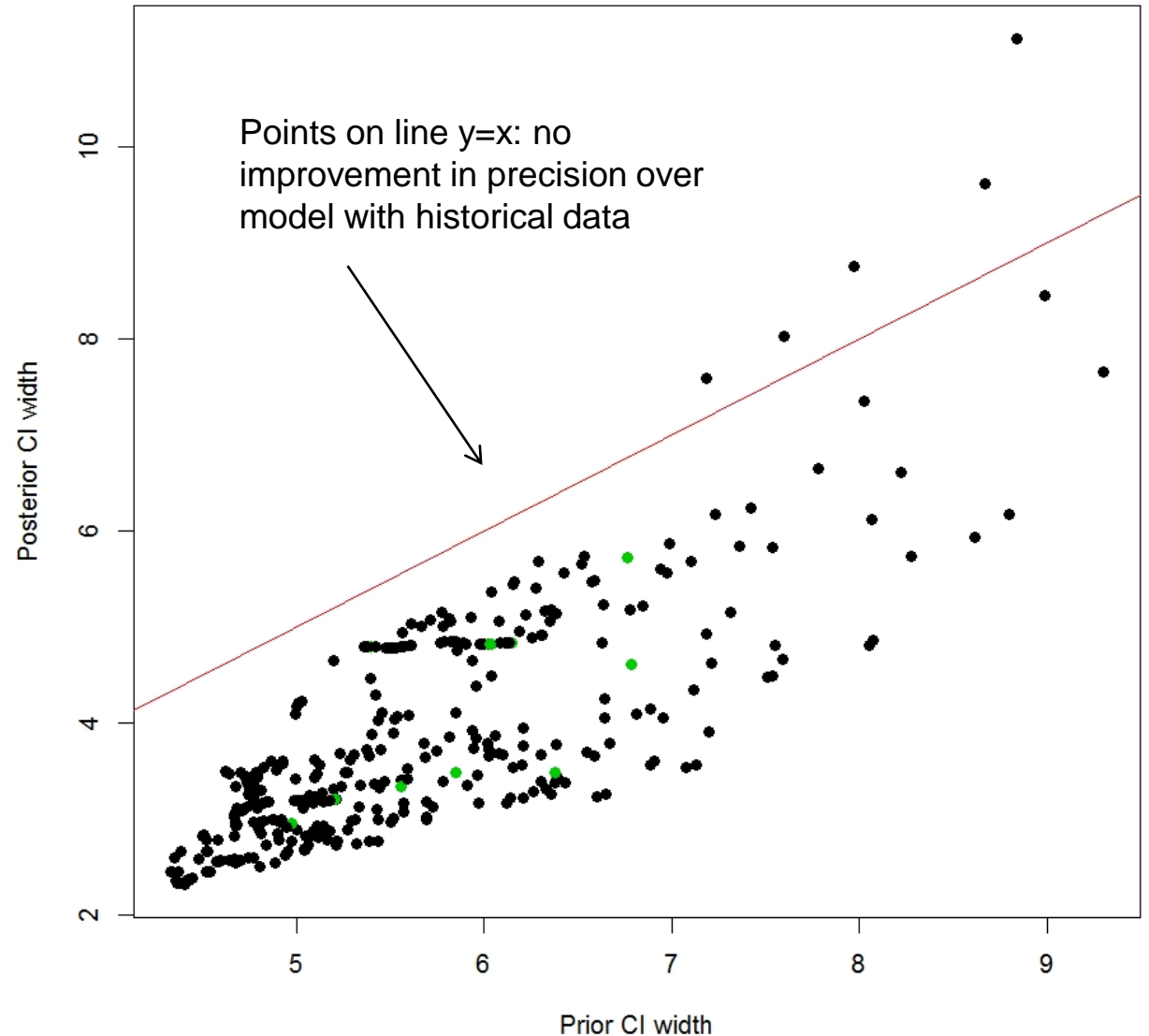
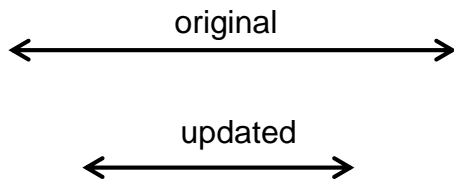


Update the System Model with Experimental Data

With the new data from the first batch, the model of the process was updated and the focus shifted

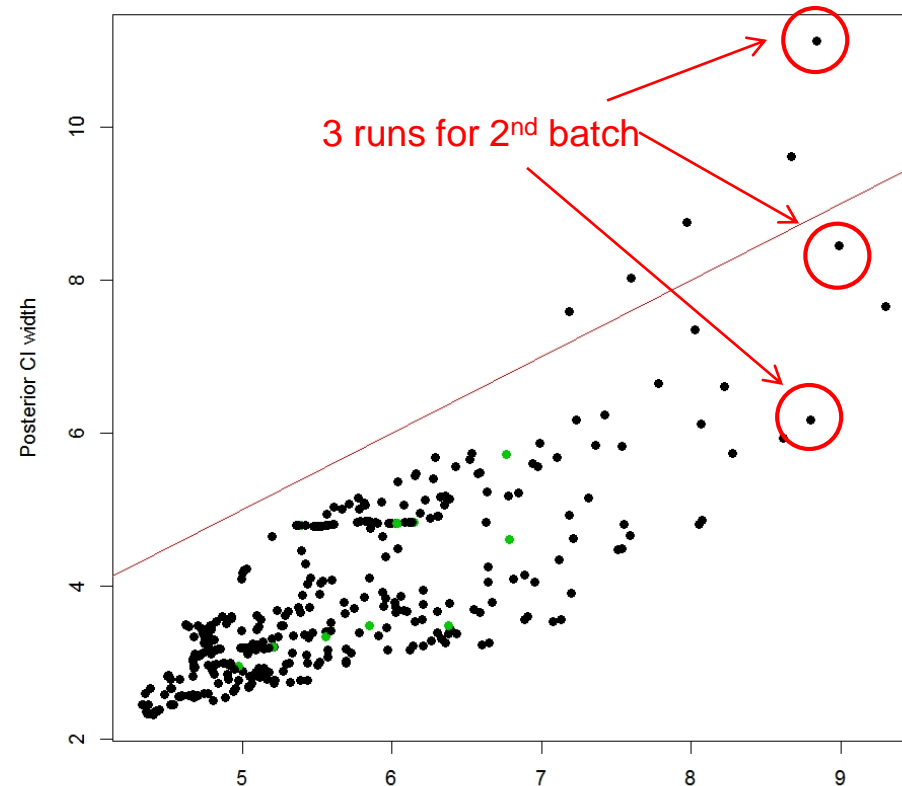
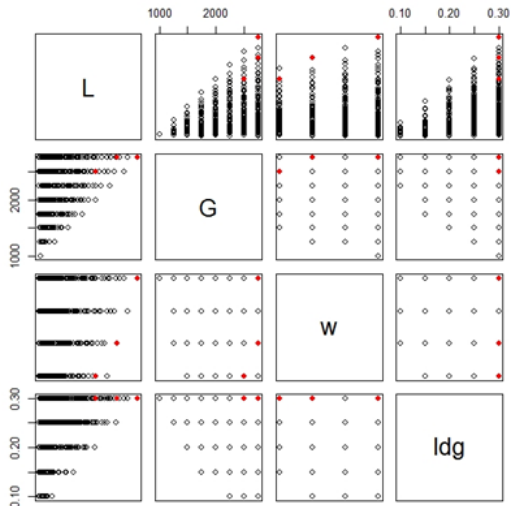
- From: exploration of the design space and clarifying regions of exclusion
- To: improving the precision of prediction for new observations

Points below line: improvement in precision (here many of CI widths are reduced by ~40%)



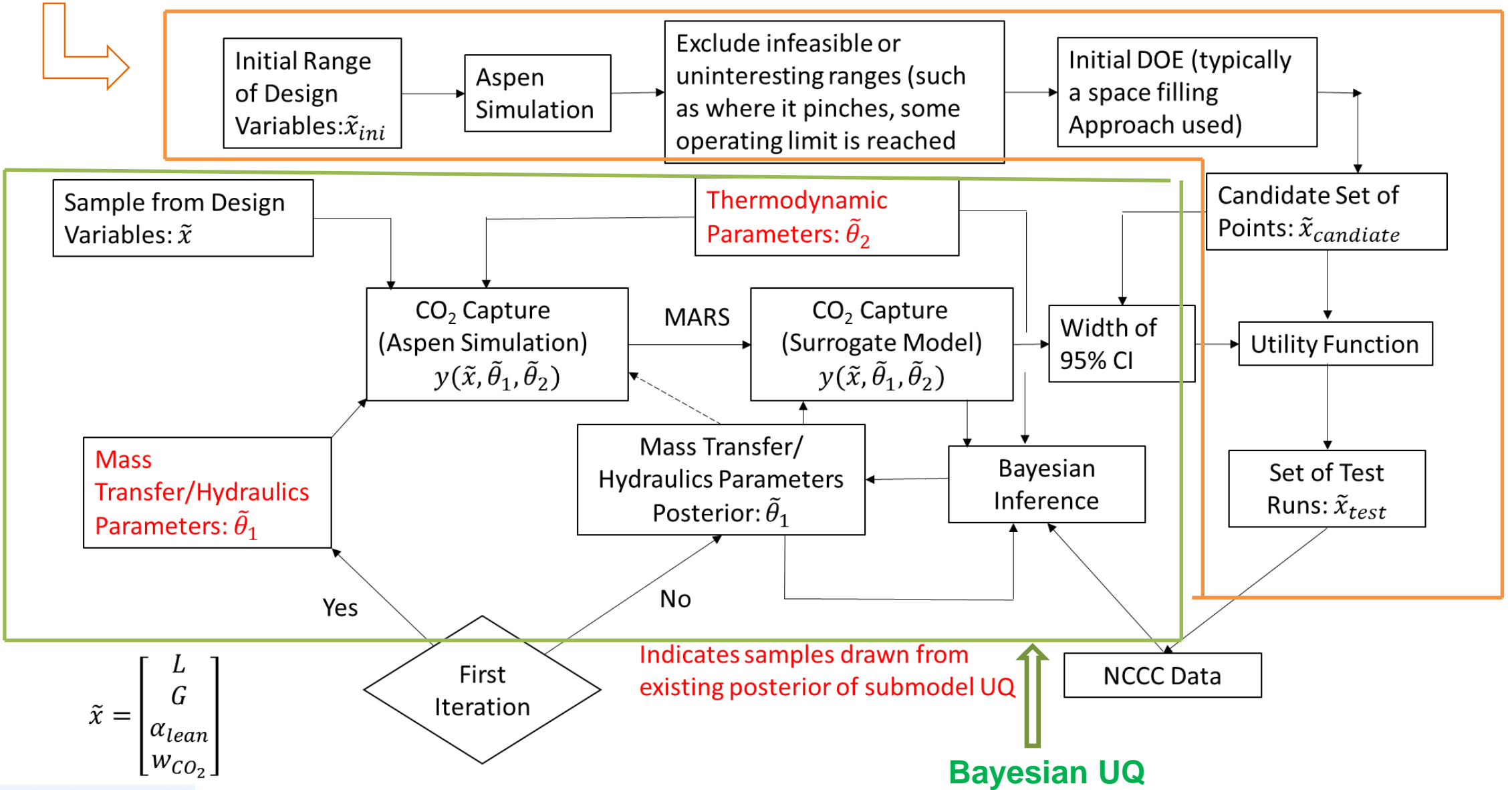
Generate Next Set of Experiments

- With newly updated model, identify the best candidate input combinations to be used as the next batch
- 3 additional runs
- Locations selected based on G-optimality (improving the worst prediction in the input space), while not putting the new runs too close together (space-filling tendency).



L	G	w	ldg
7971	2500	0.1250	0.3
9881	2750	0.1417	0.3
1675	2750	0.1750	0.3

Implementation of Methodology for NCCC DOE



Process Surrogate Model (MARS)

$$\hat{y} = \hat{y}(\tilde{x}, \tilde{\theta}_1, \tilde{\theta}_2) \quad y \text{ is CO}_2 \text{ capture percentage}$$

Parameters of fixed uncertainty
(thermodynamic model): $\tilde{\theta}_1$

Parameters for which uncertainty is
updated (mass transfer + hydraulics): $\tilde{\theta}_2$

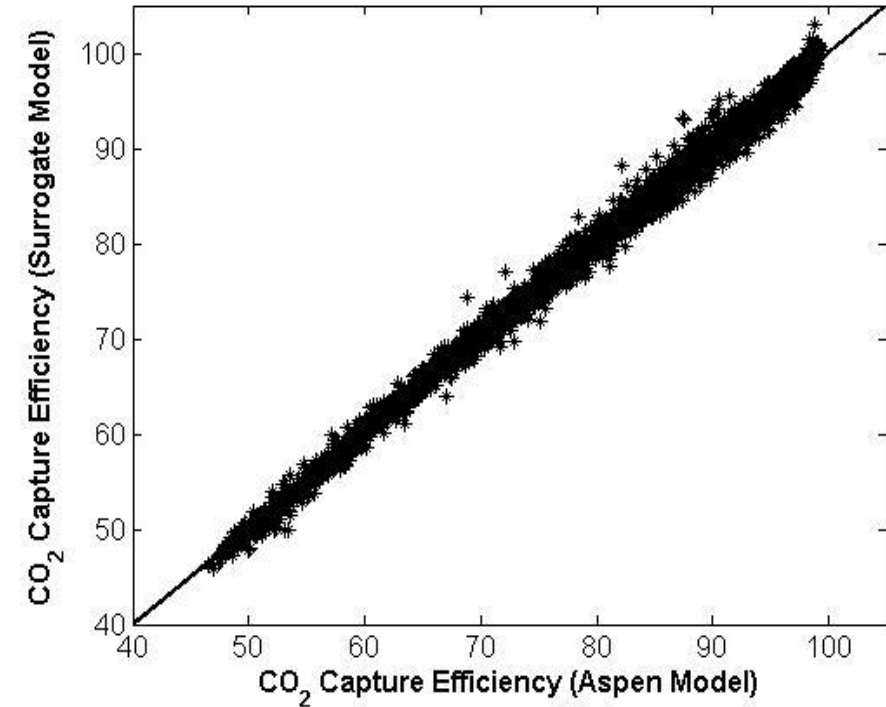
$$\tilde{x} = \begin{Bmatrix} L \\ G \\ \alpha_{lean} \\ w_{CO_2} \end{Bmatrix}$$

$$3000 \leq L \leq 13000 \text{ kg/hr}$$

$$1000 \leq G \leq 3000 \text{ kg/hr}$$

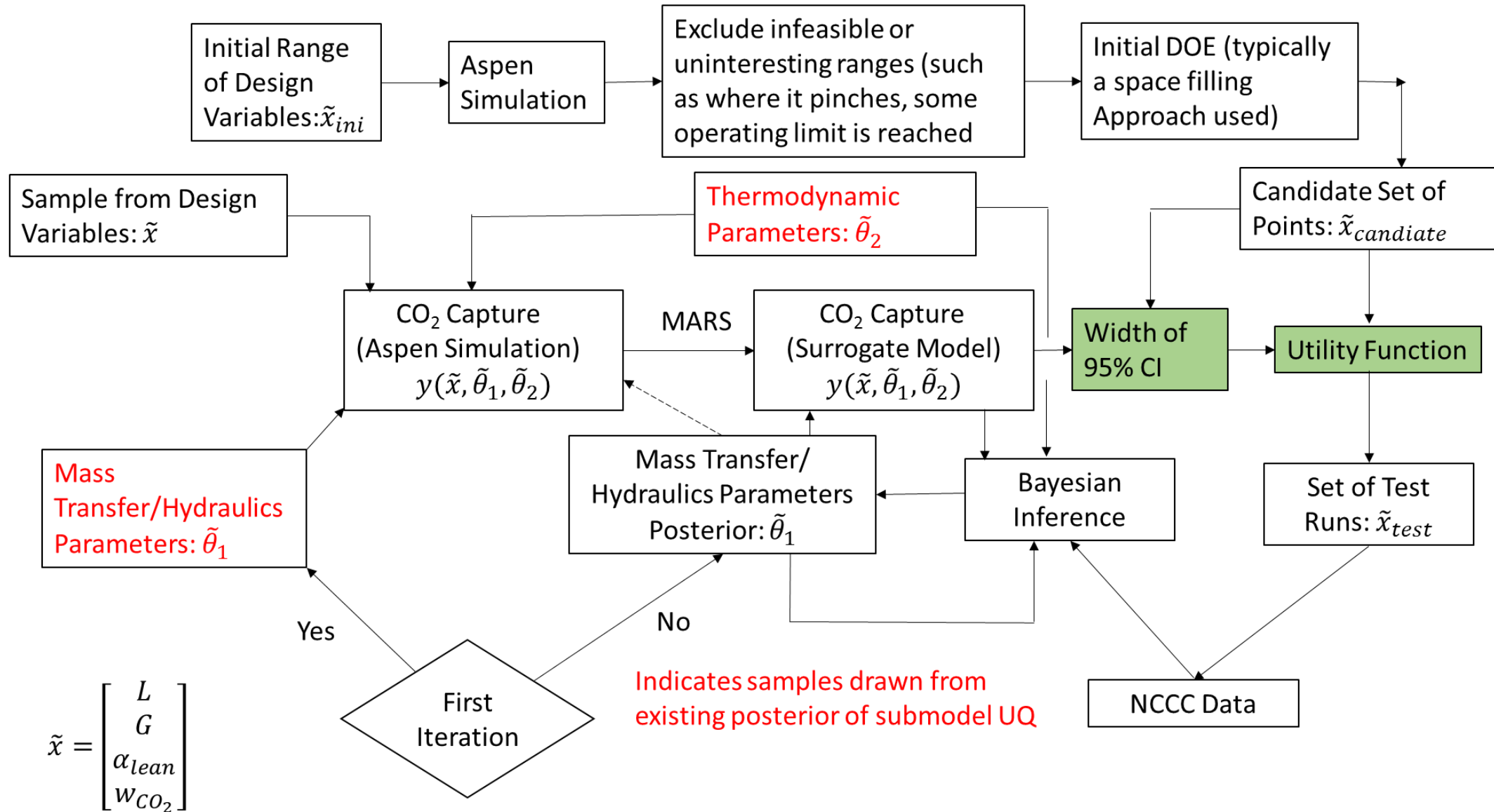
$$0.1 \leq \alpha_{lean} \leq 0.35 \text{ mol CO}_2/\text{MEA}$$

$$0.1 \leq w_{CO_2} \leq 0.175$$



Ranges for lean loading and CO₂ weight fraction modified to accommodate all experimental data

Utility Function

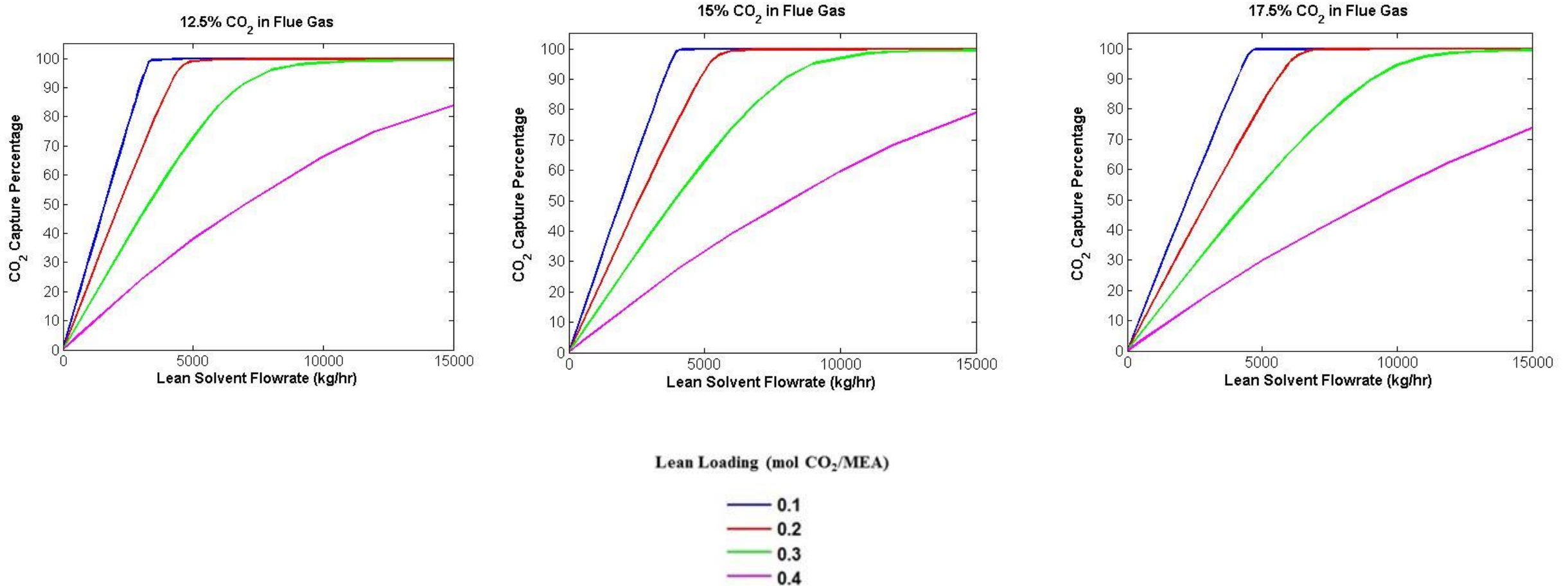


$$\tilde{x} = \begin{bmatrix} L \\ G \\ \alpha_{lean} \\ w_{CO_2} \end{bmatrix}$$

Indicates samples drawn from existing posterior of submodel UQ

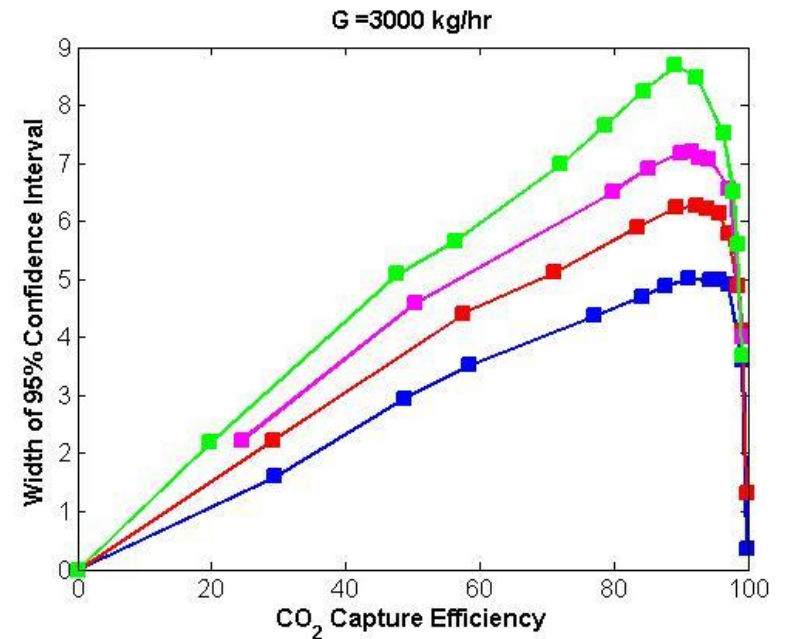
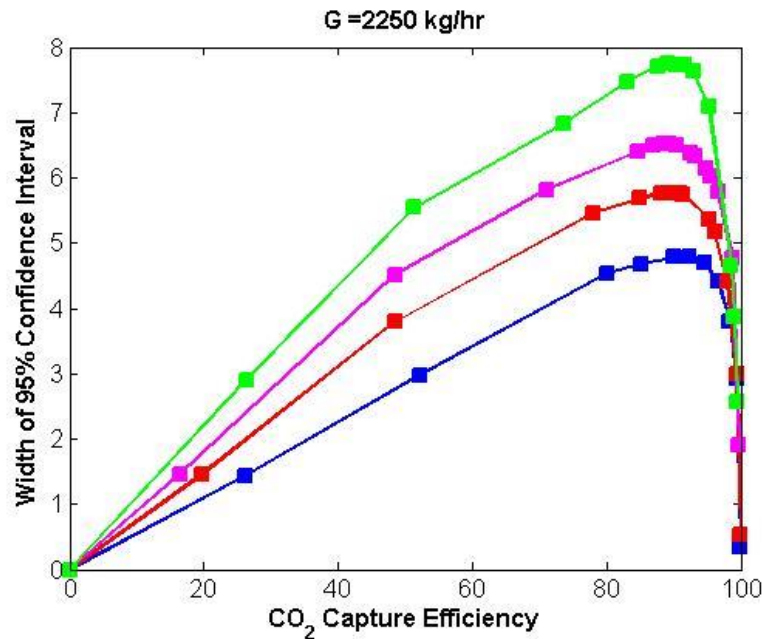
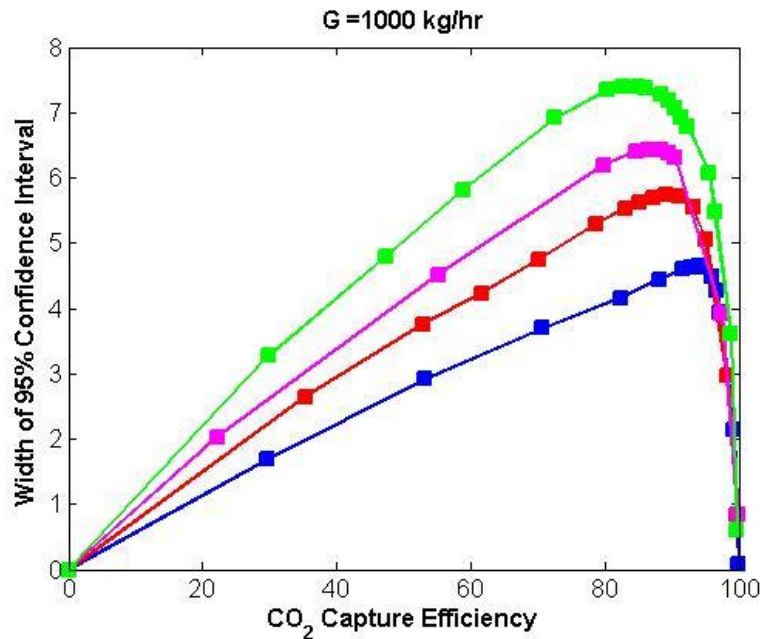
Absorber Model Performance

$G = 2250 \text{ kg/hr}$



Width of 95% Confidence Intervals

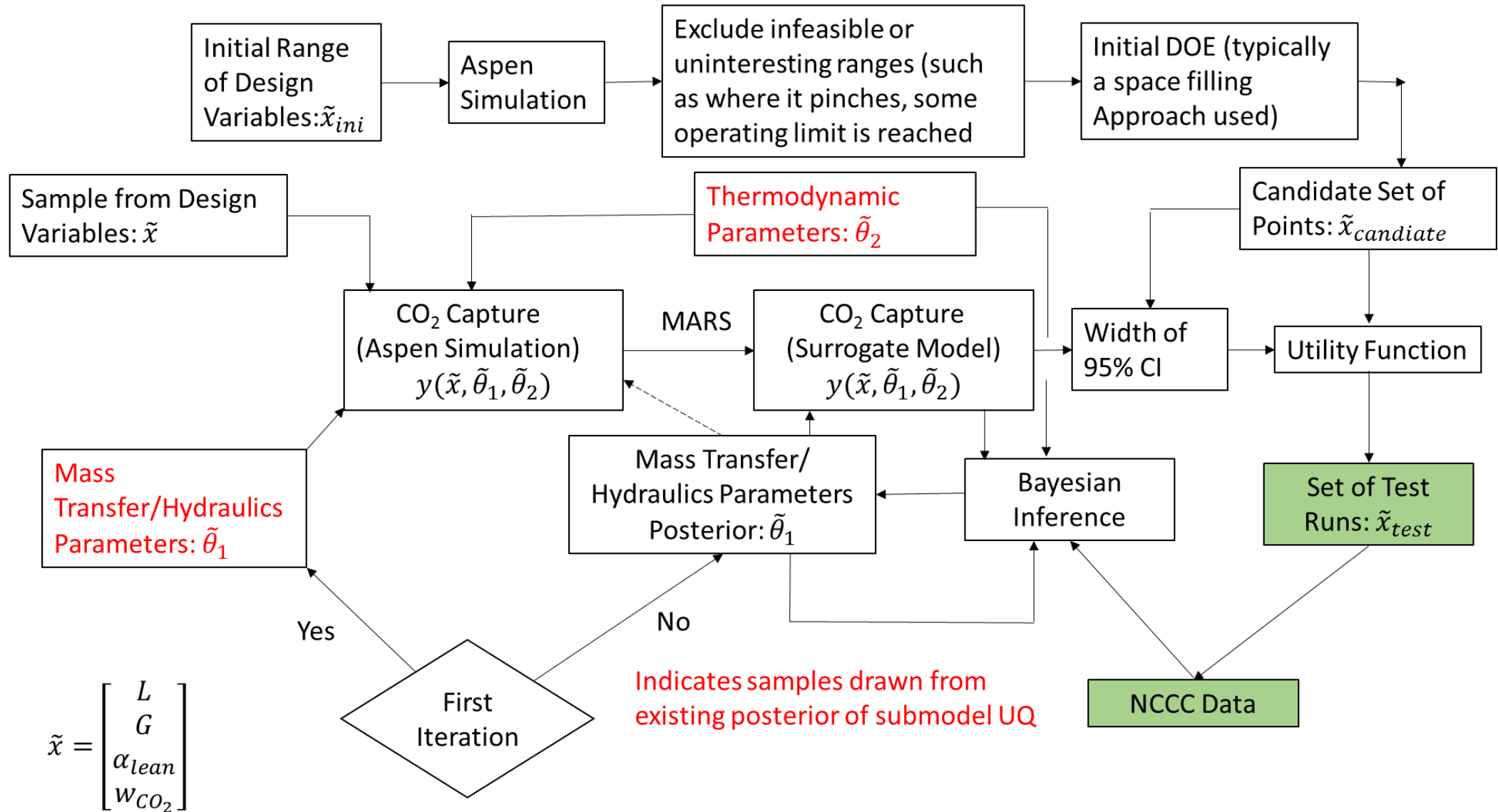
15 wt% MEA



Lean Loading (mol CO₂/MEA)

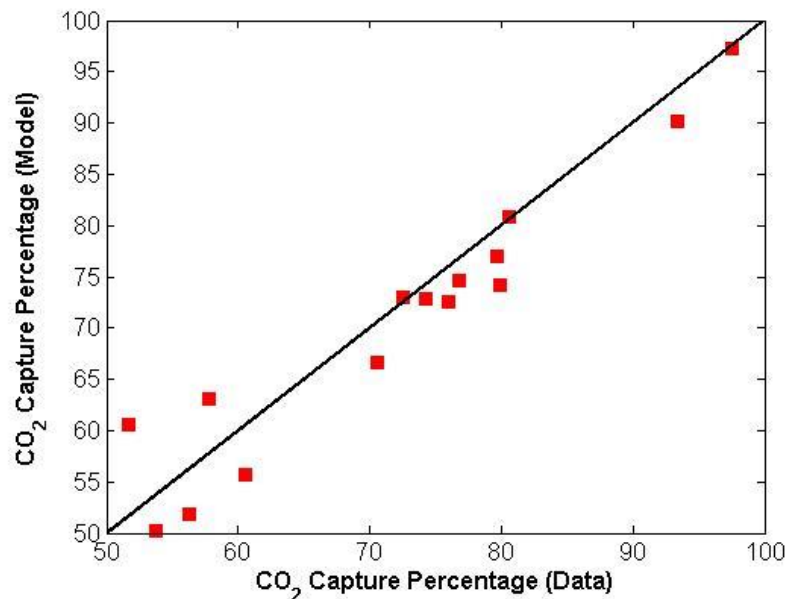
- 0.10
- 0.20
- 0.25
- 0.30

Implementation of Test Runs at NCCC

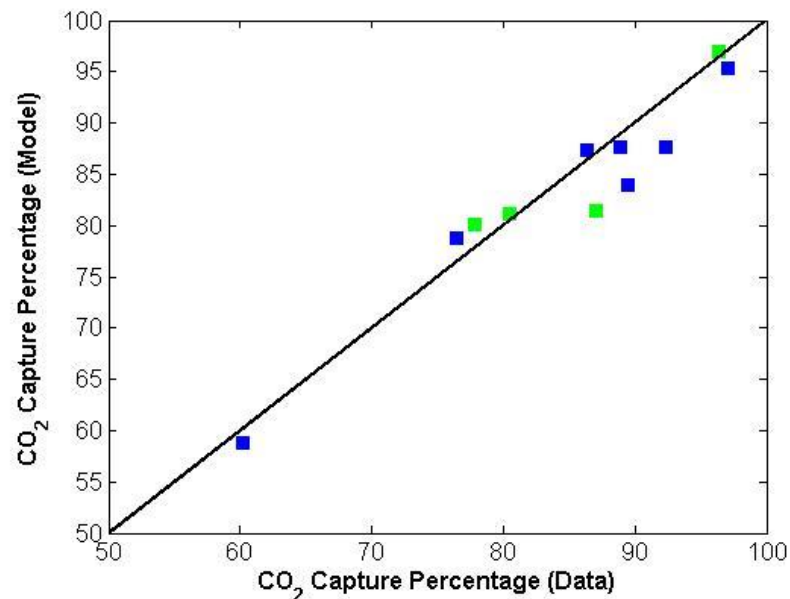


Absorber Performance – Parity Plots

Three Beds (With Intercooling)



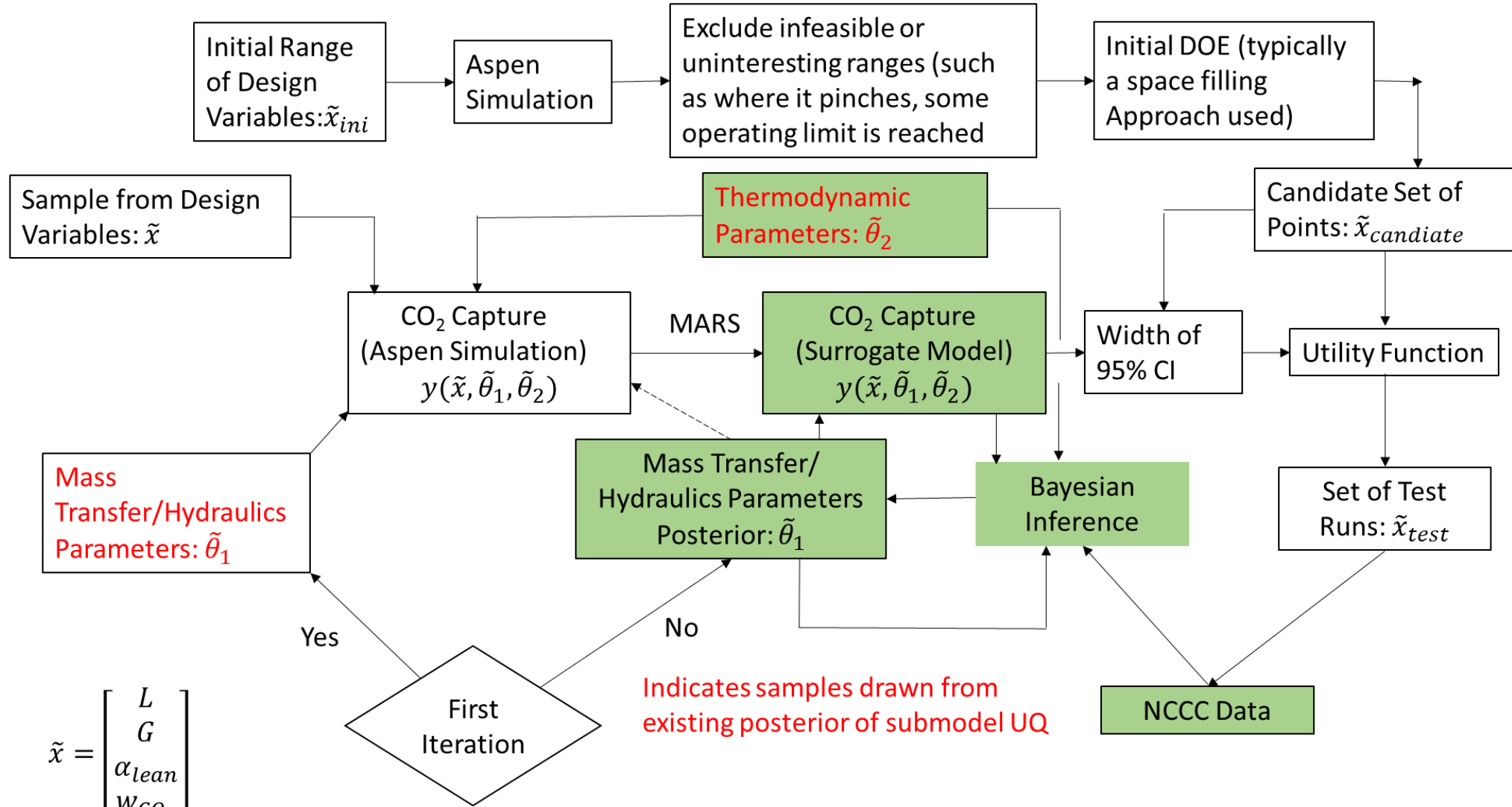
One or Two Beds (Without Intercooling)



Beds/Intercoolers	Percent Error
3 (2)	5.28 ± 4.42 %
2 (0)	2.75 ± 2.86 %
1 (0)	3.00 ± 1.94 %

■ One Bed Cases
■ Two Bed Cases

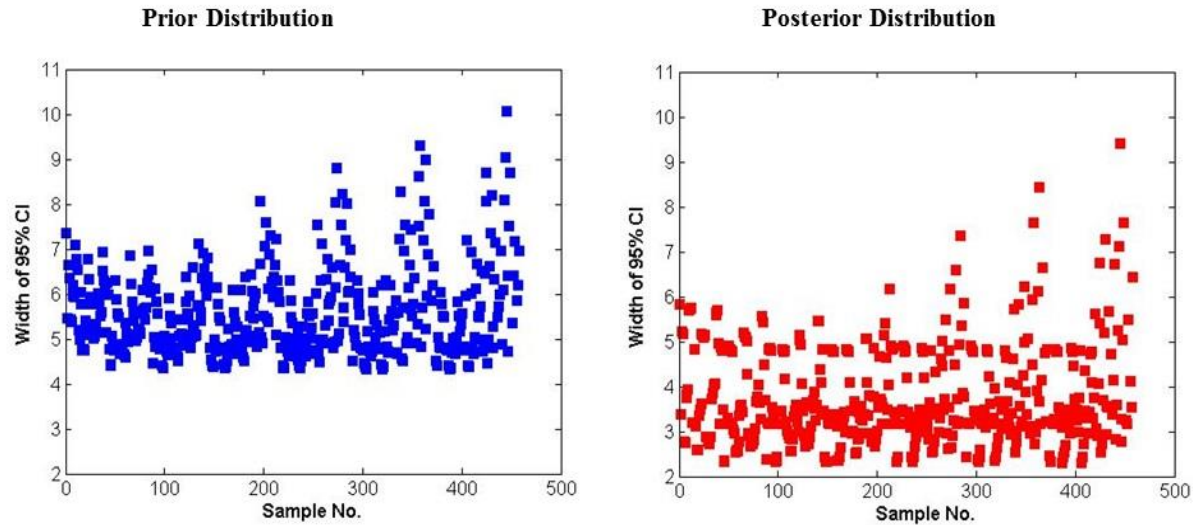
Learning from the Experimental Data: Updating Quantified Uncertainty



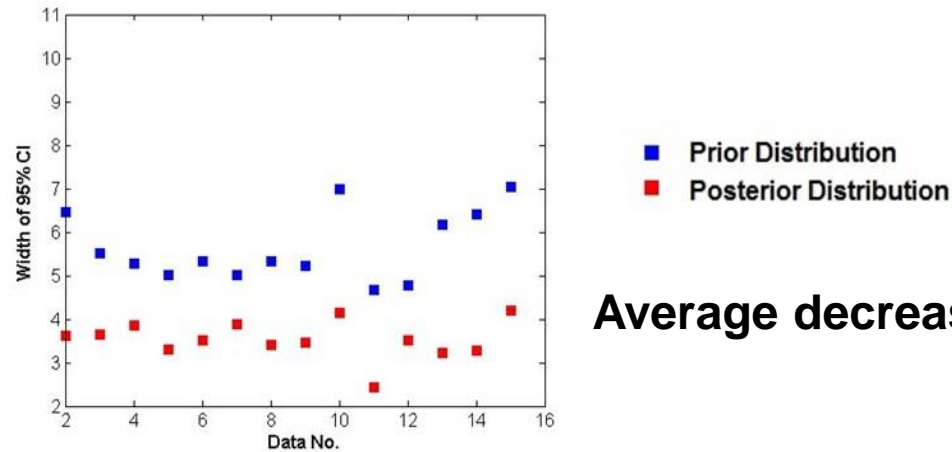
$$\tilde{x} = \begin{bmatrix} L \\ G \\ \alpha_{lean} \\ w_{CO_2} \end{bmatrix}$$

Effect of Bayesian Inference on CI Width (1st Iteration)

Candidate Points



Points with Experimental Data



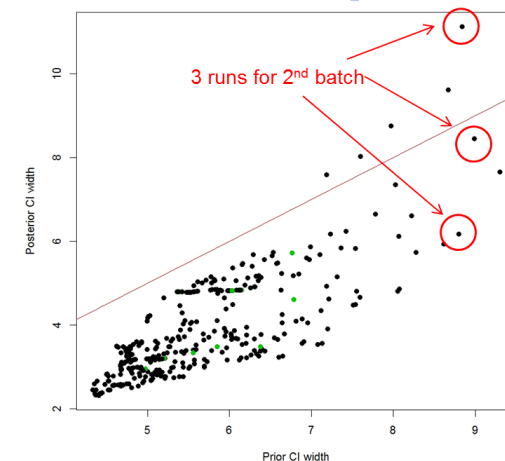
Average decrease in CI width (% CO₂ Capture):

1.79

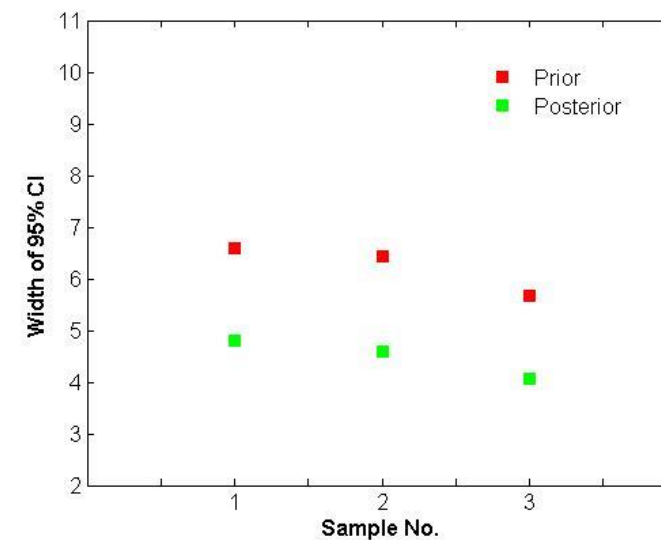
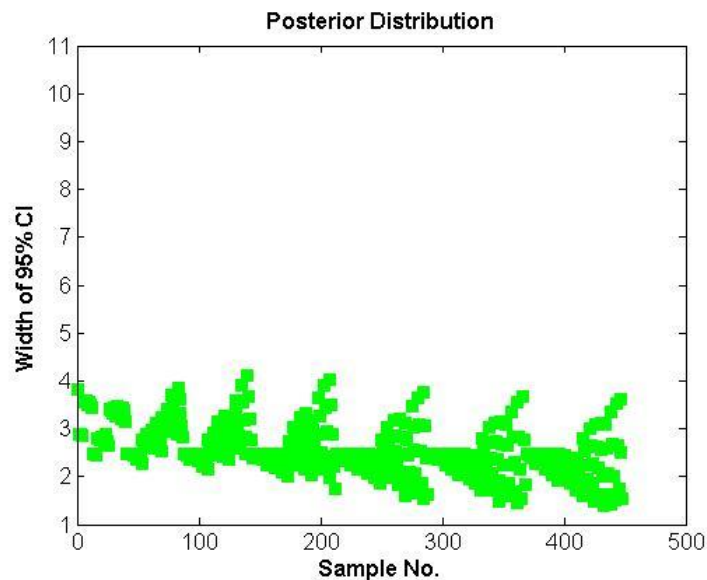
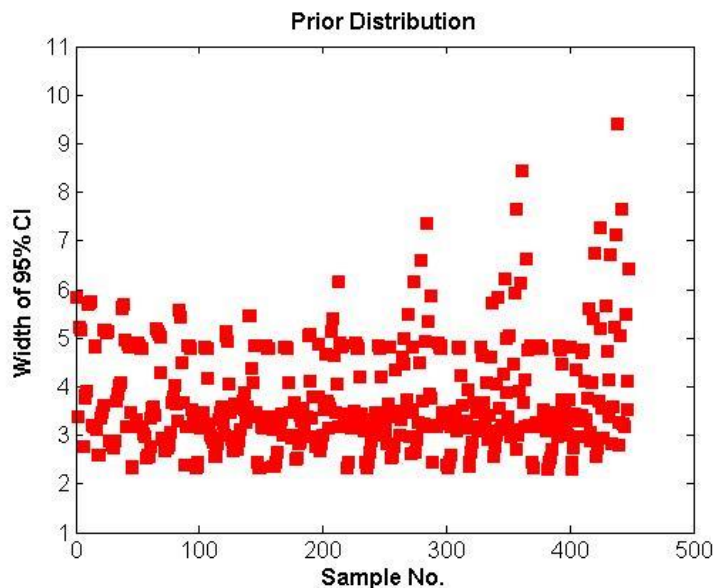
Effect of Bayesian Inference on CI Width (2nd Iteration)

Test Cases

Case No.	L (kg/hr)	G (kg/hr)	α_{lean}	w_{CO_2}	CO ₂ Capture
1	7959	2497	0.3	0.118	96.1
2	9871	2746	0.3	0.133	97.7
3	11412	2748	0.3	0.162	94.9



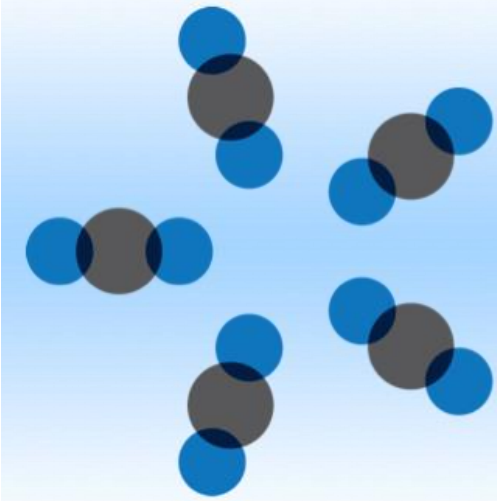
Update in CI Width



Average decrease in CI width (% CO₂ Capture): 1.23

Conclusions

- Accelerated learning through optimal DOE
- Process model uncertainty has been shown to decrease as process level data are incorporated into a Bayesian inference methodology
 - Two iterations performed in this work
- Methodology would provide quantitative measure of diminishing return (i.e. reduced learning) as optimal experimental data are collected



CCSI²

Carbon Capture Simulation for Industry Impact

For more information

<https://www.acceleratecarboncapture.org/>

Debangsu Bhattacharyya, Ph.D.

debangsu.bhattacharyya@mail.wvu.edu

Jim Gattiker, Ph.D.

gatt@lanl.gov

Brenda Ng, Ph.D.

ng30@llnl.gov

