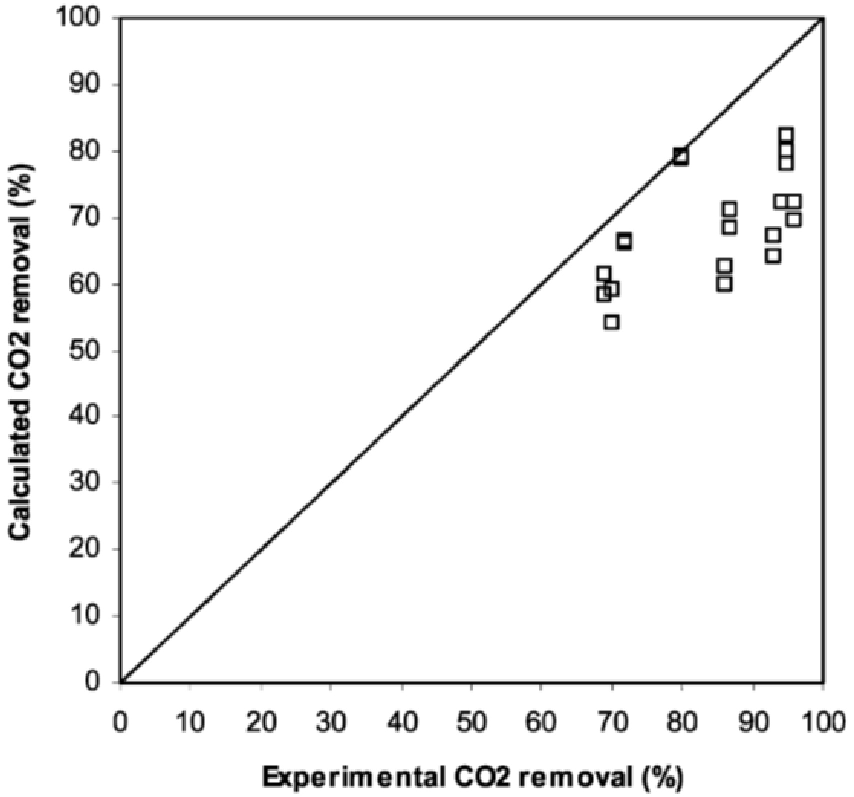
Solvent Pilot System Test Campaign Guidance

Brenda Ng*, Charles Tong, Lawrence Livermore National Laboratory
Jim Gattiker*, Christine Anderson-Cook, Los Alamos National Laboratory
Debangsu Bhattacharyya*, Joshua Morgan, West Virginia University

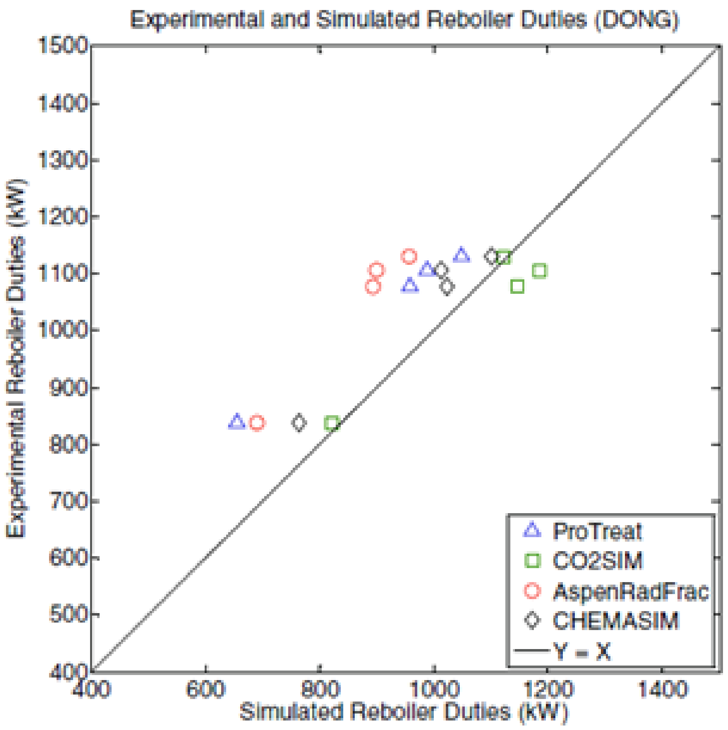
Typical Steady-State DOE

Absorber



Zhang, et al., Rate-Based Process Modeling Study of CO_2 Capture with Aqueous Monoethanolamine Solution, Ind. Eng. Chem Res., 48, 9233-9246, 2009

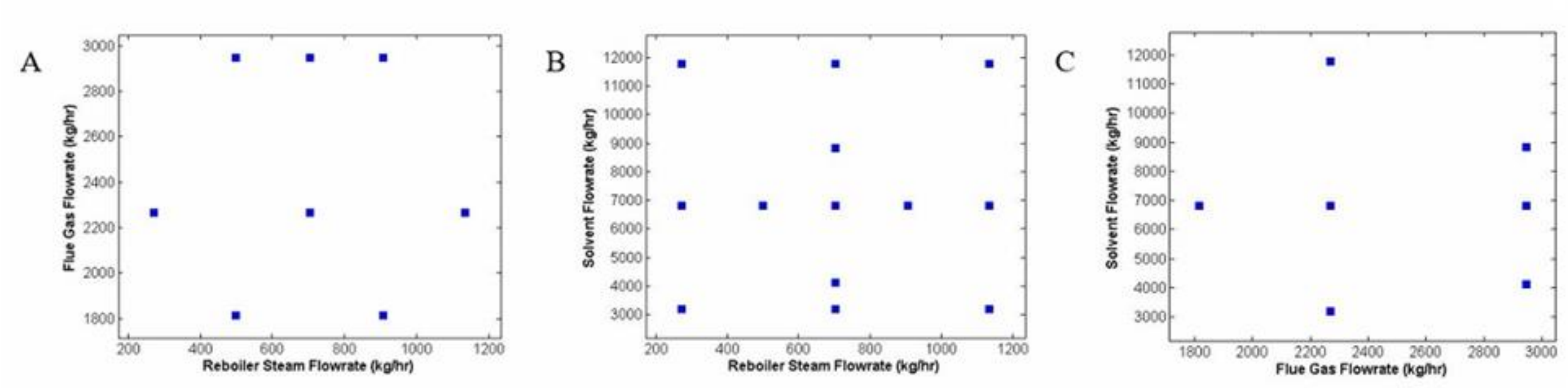
Regenerator



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

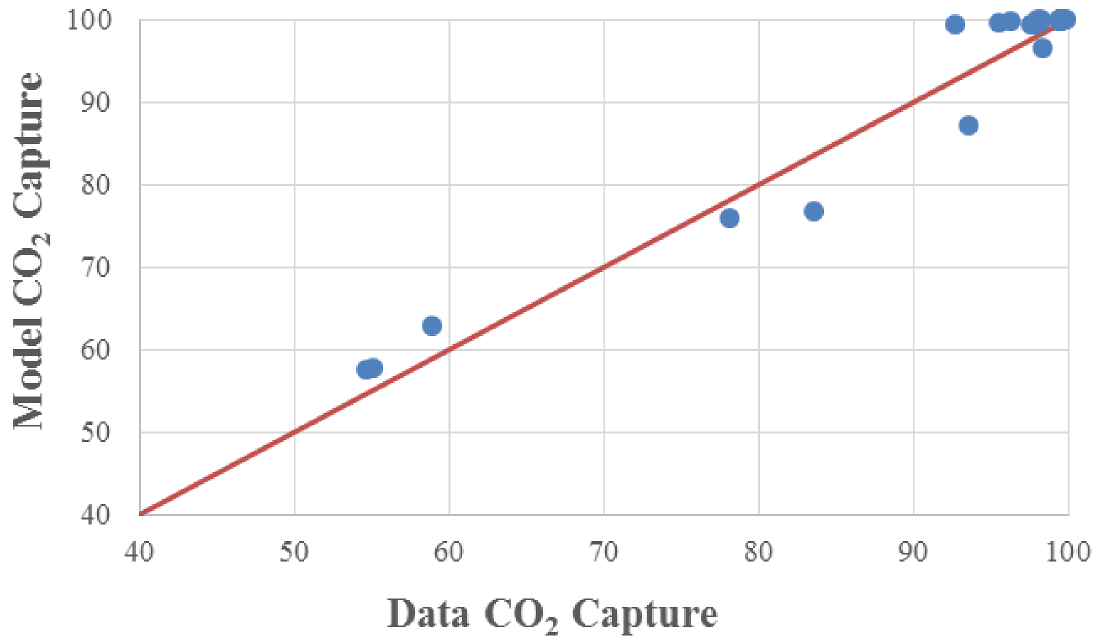
Operating Conditions	Range
Solvent Flow (lb/hr)	7,000-26,000
Inlet Flue Gas (lb/hr)	5,000-6,500
Reboiler Steam Flow (lb/hr)	600-2,500
Inlet FG CO_2 vol%	9-11%
# of beds	1-3
Intercooler	no - yes



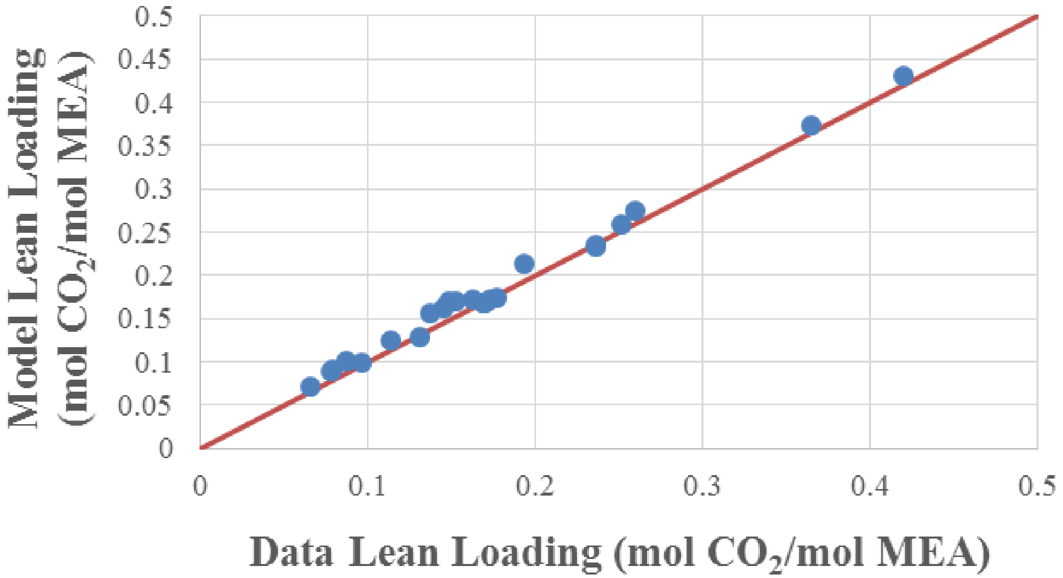
CCSI² Carbon Capture Simulation for Industry Impact
NATIONAL ENERGY TECHNOLOGY LABORATORY
BERKELEY LAB
Lawrence Livermore National Laboratory
Los Alamos NATIONAL LABORATORY EST. 1943
Pacific Northwest NATIONAL LABORATORY
U.S. DEPARTMENT OF ENERGY

Results from 2014 CCSI DOE and Comparison with CCSI Model

Absorber



Regenerator



CCSI[2] Carbon Capture Simulation for Industry Impact
NATIONAL ENERGY TECHNOLOGY LABORATORY
BERKELEY LAB
Lawrence Livermore National Laboratory
Los Alamos NATIONAL LABORATORY EST. 1943
Pacific Northwest NATIONAL LABORATORY
U.S. DEPARTMENT OF ENERGY

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

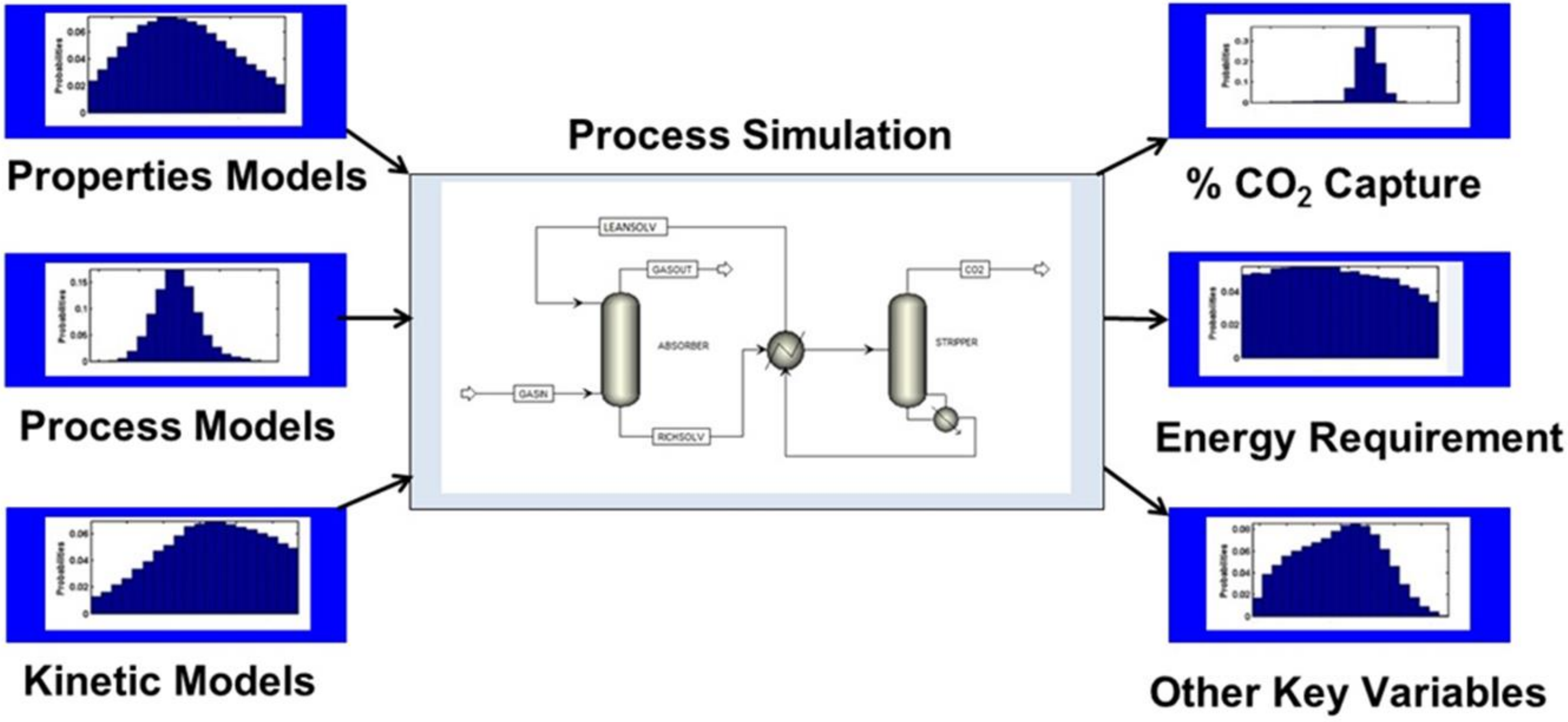
How to solve these issues?

- 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

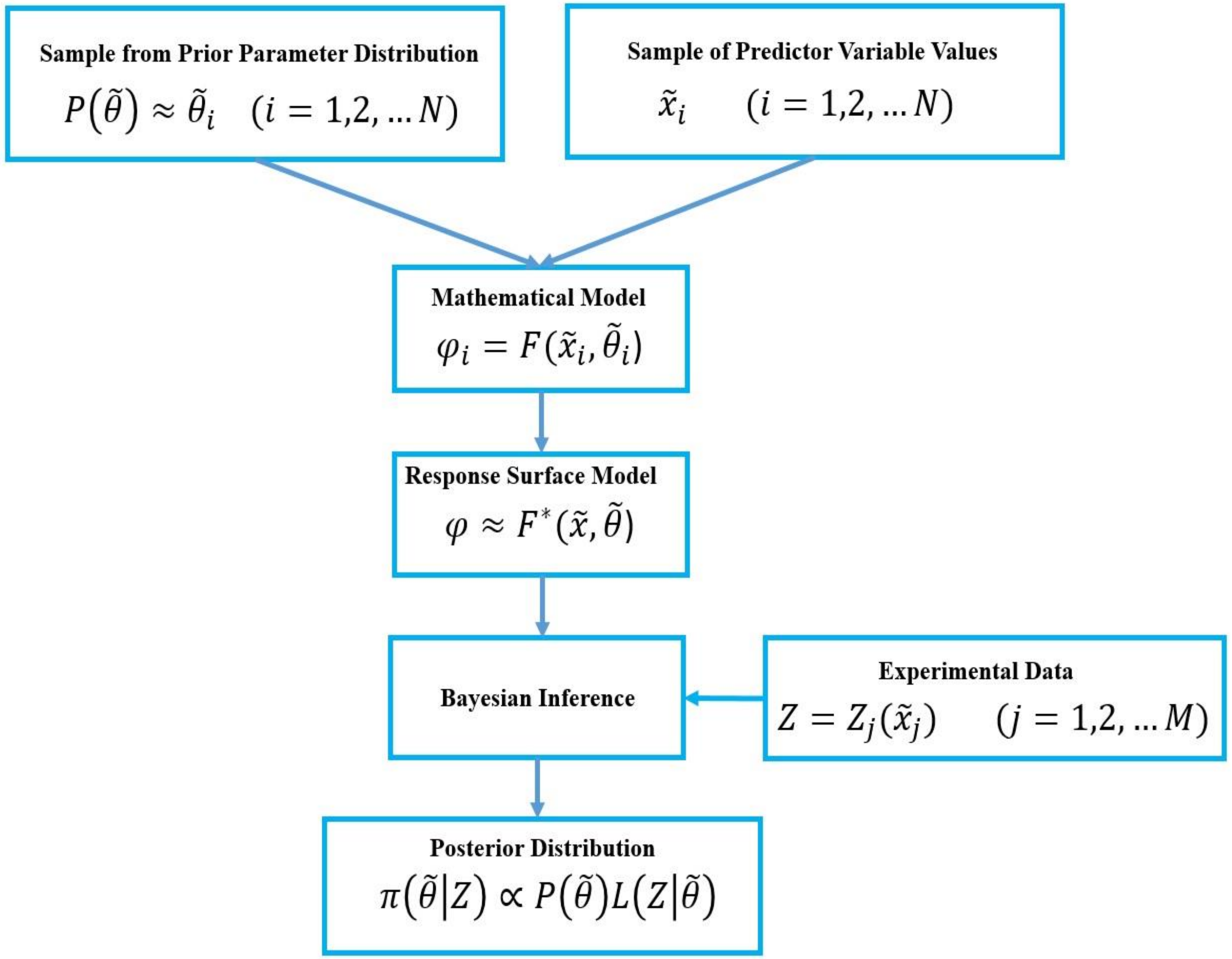
Other issues?

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

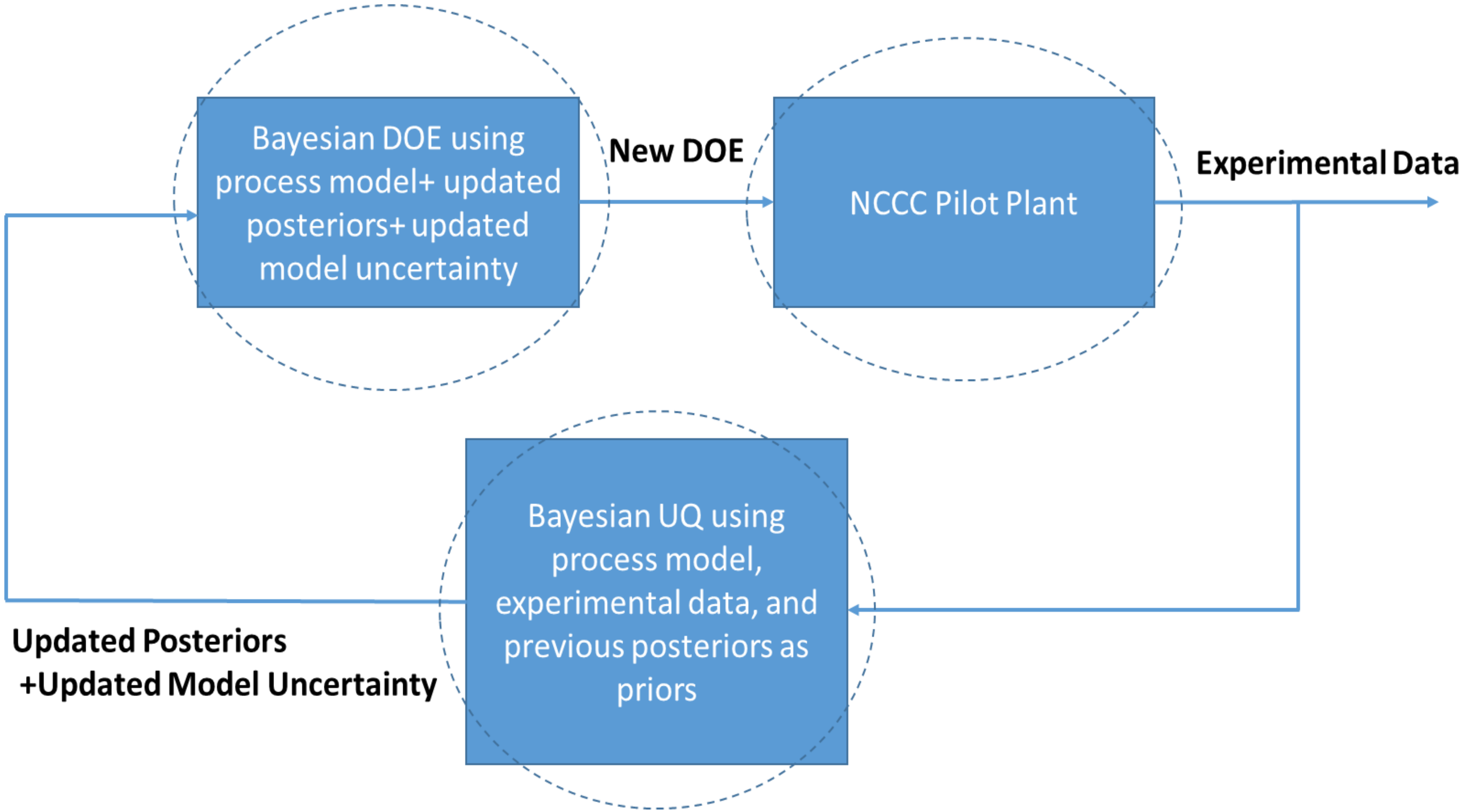
CCSI^2 Approach to Uncertainty Quantification



Bayesian Uncertainty Quantification Approach

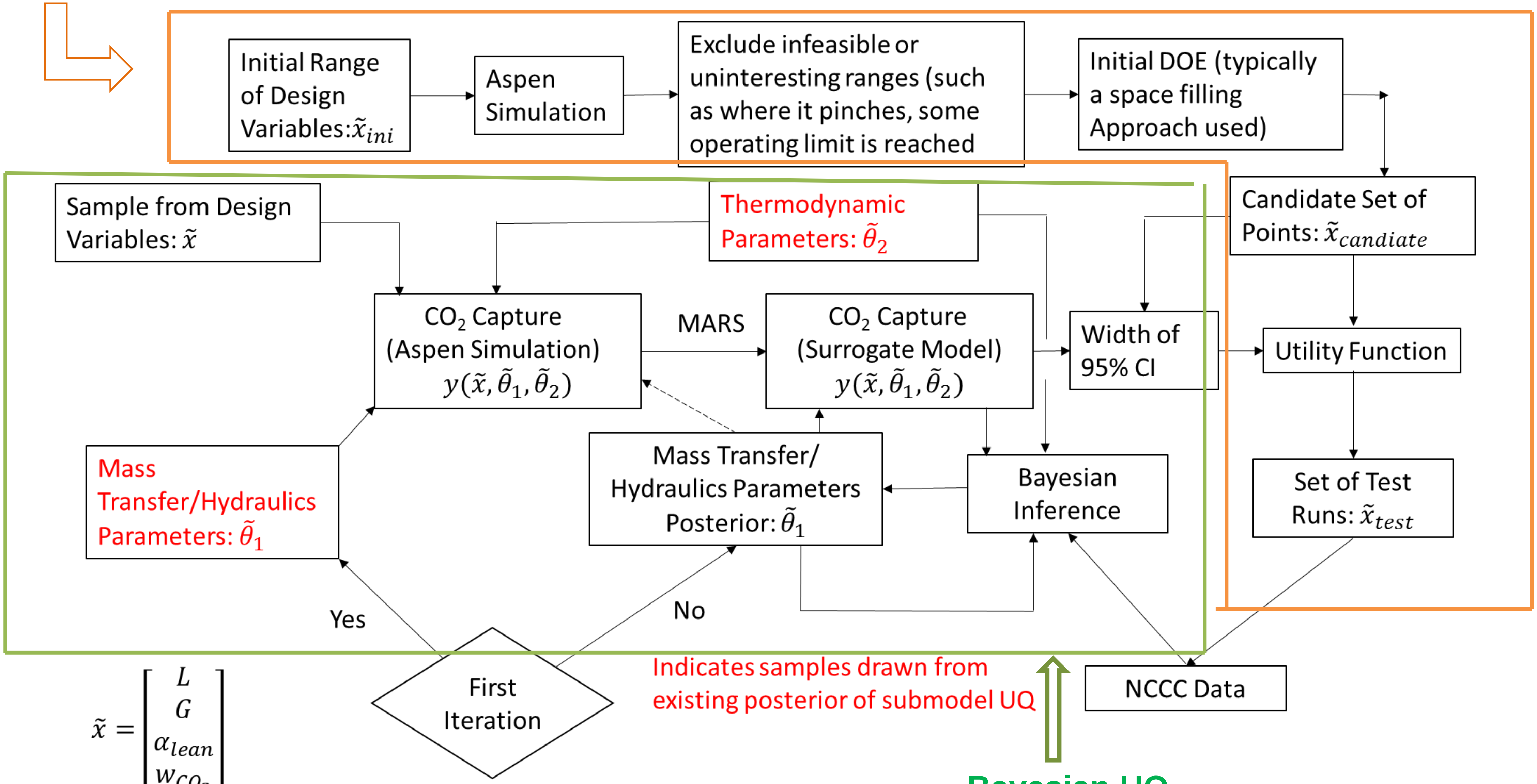


Overall Approach to Design of Experiments: Bayesian Sequential Design of Experiments



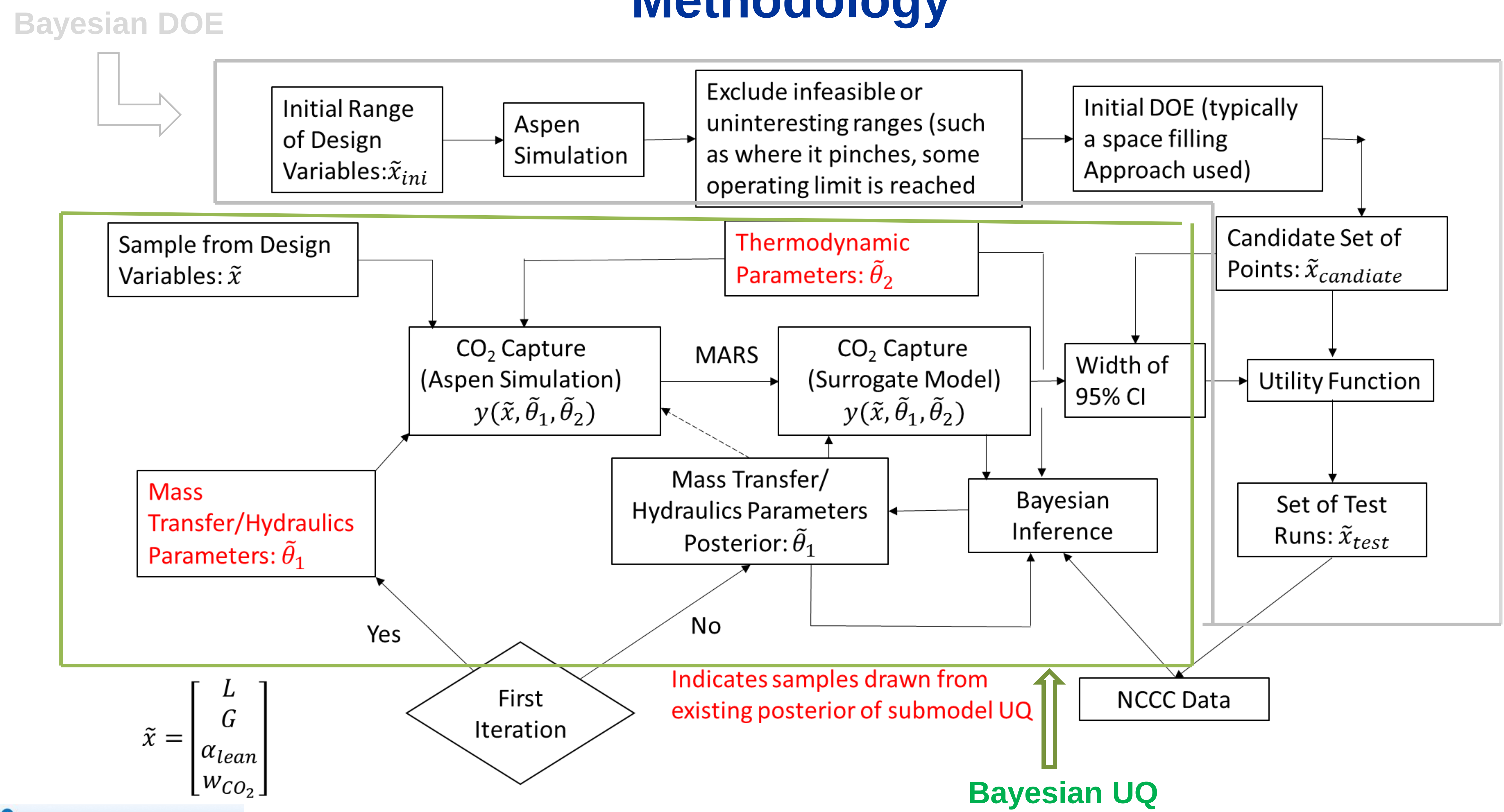
Methodology

Bayesian DOE

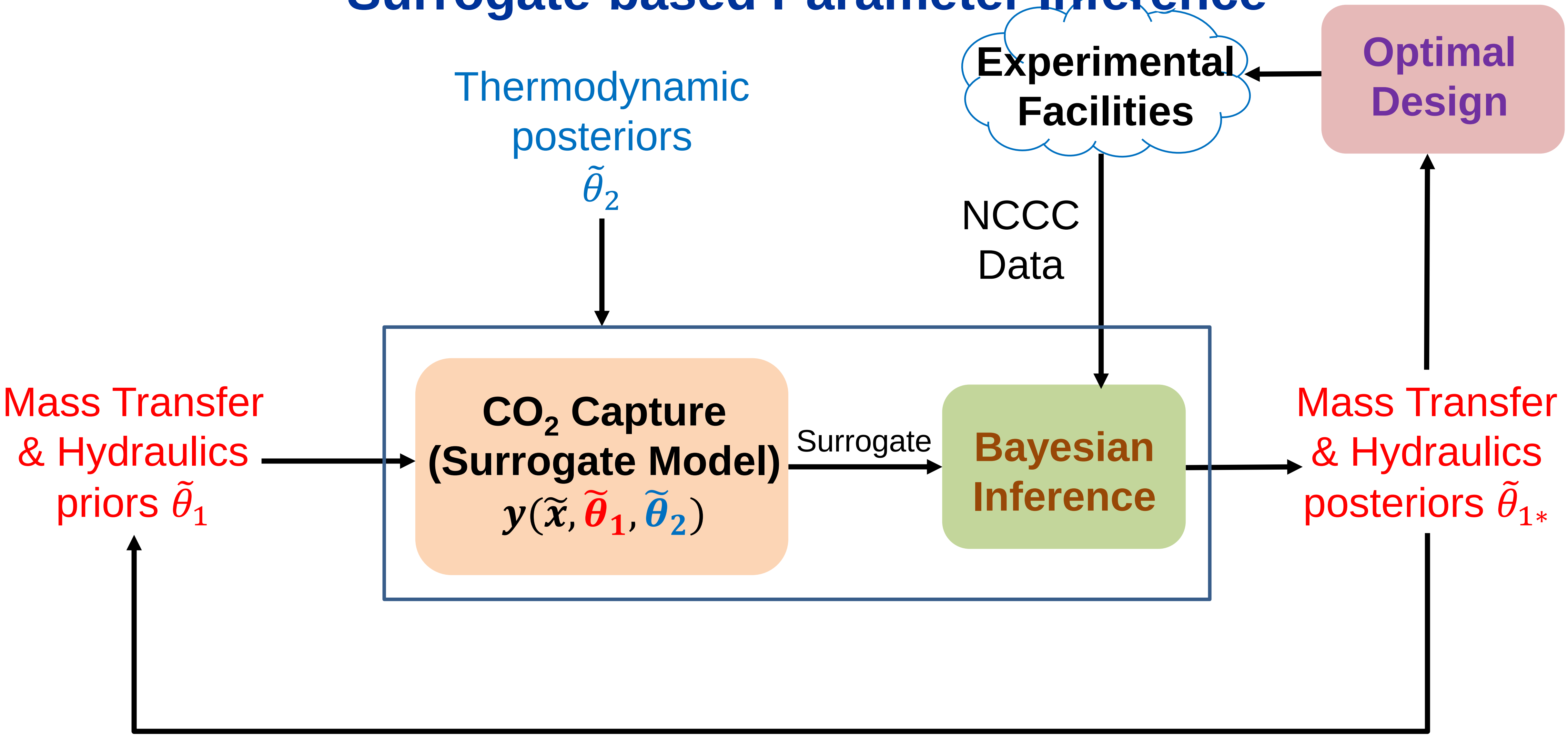


Bayesian UQ

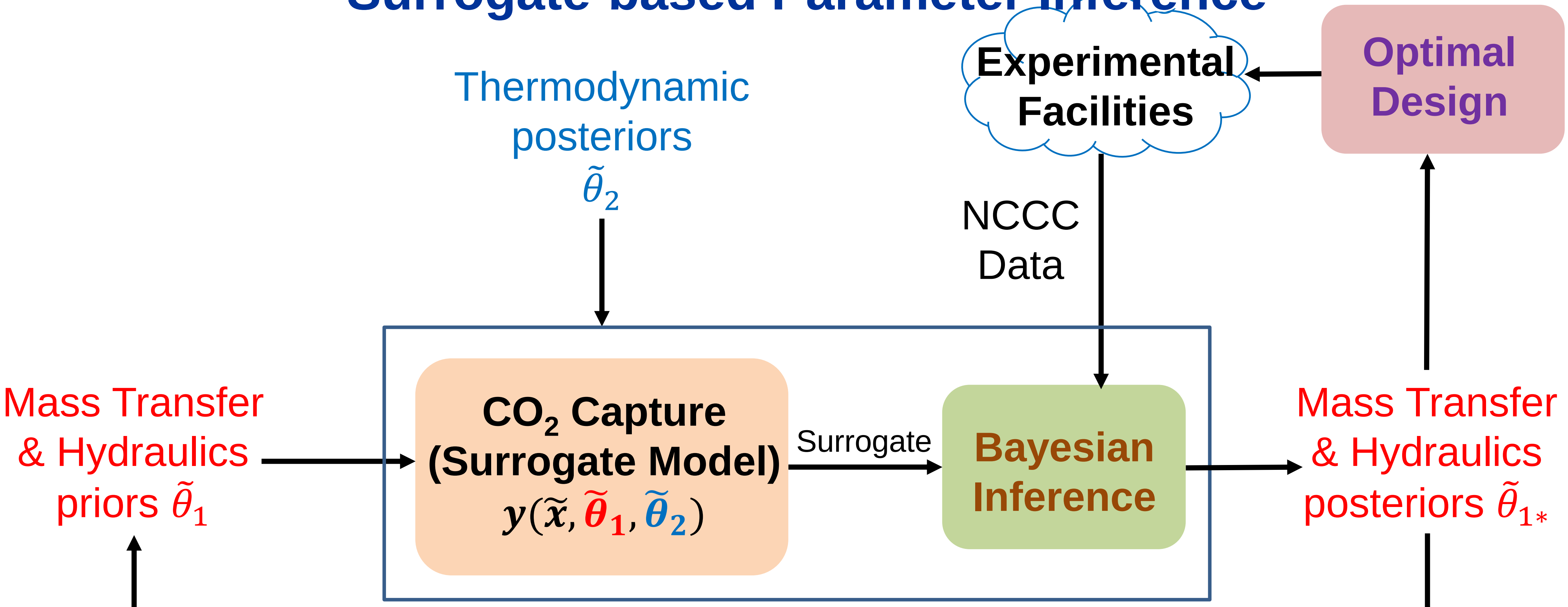
Methodology



Surrogate-based Parameter Inference



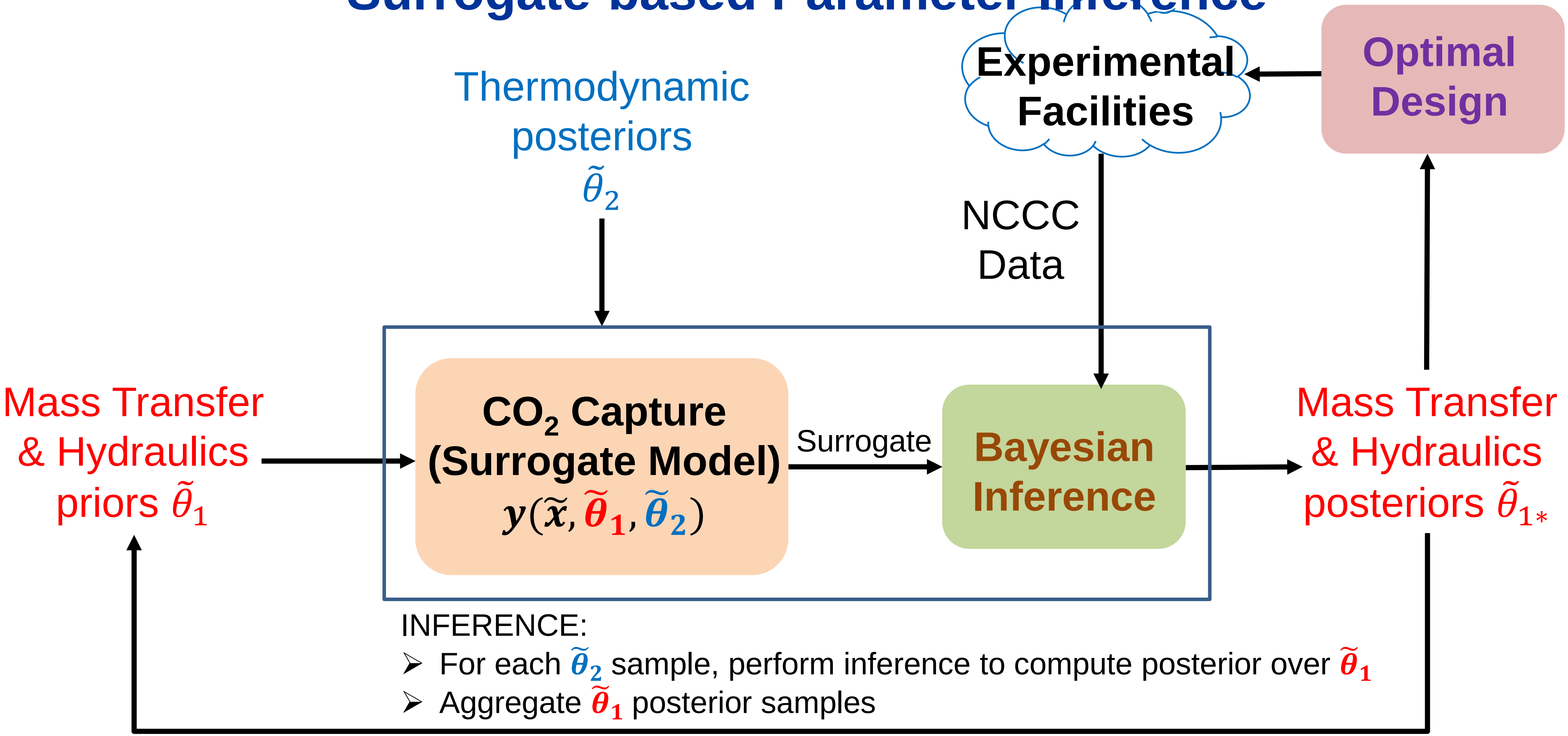
Surrogate-based Parameter Inference



SURROGATE:

- Multivariate adaptive regression splines (MARS) were used
- Generate a MARS surrogate that maps $(\tilde{\boldsymbol{\theta}}_1, \tilde{\boldsymbol{\theta}}_2)$ CO_2 capture

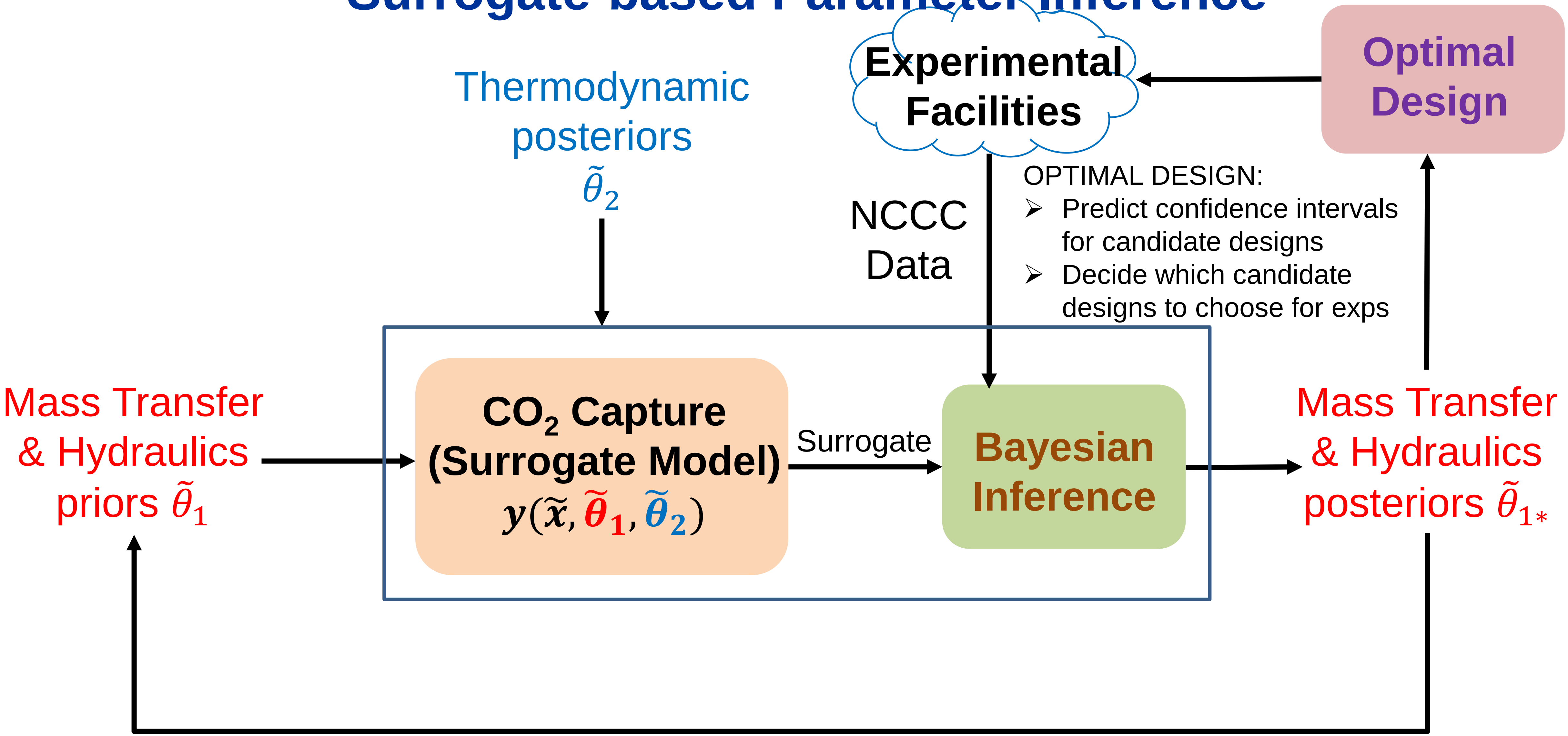
Surrogate-based Parameter Inference



INFERENCE:

- For each $\tilde{\boldsymbol{\theta}}_2$ sample, perform inference to compute posterior over $\tilde{\boldsymbol{\theta}}_1$
- Aggregate $\tilde{\boldsymbol{\theta}}_1$ posterior samples

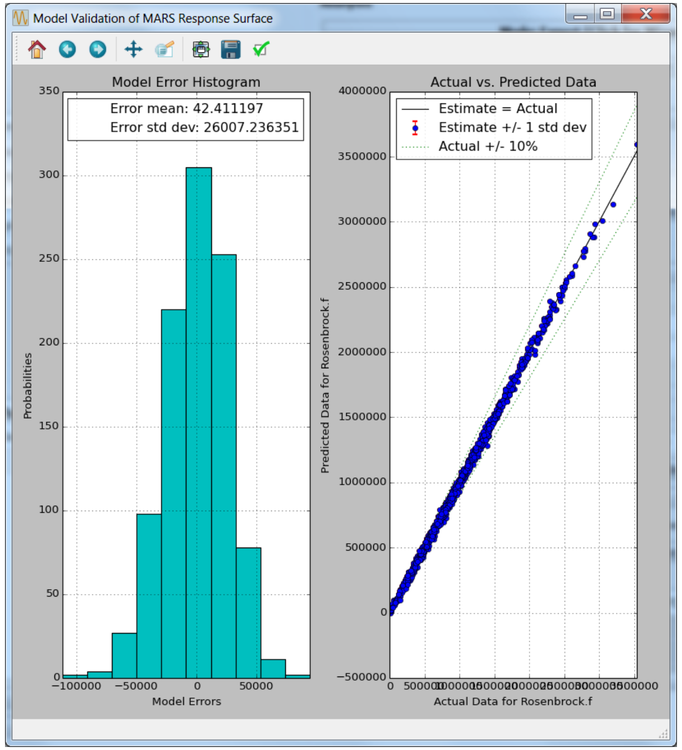
Surrogate-based Parameter Inference

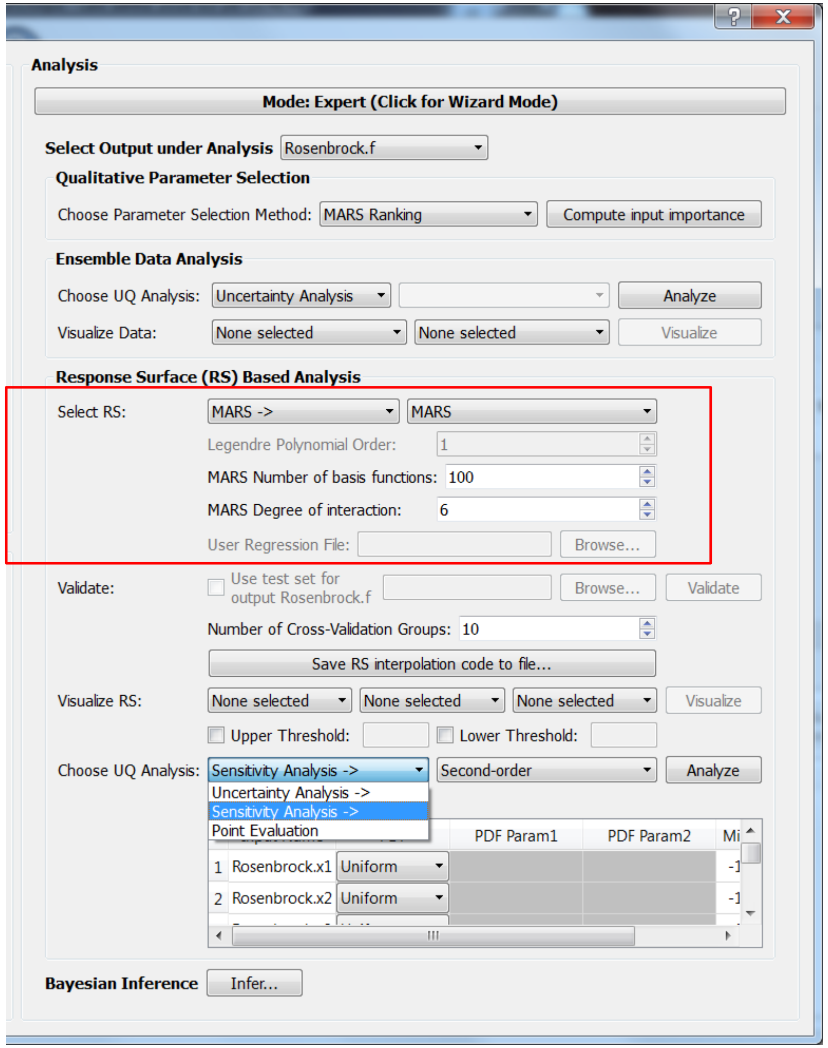


Surrogate Support

UQ

- Train and validate surrogates
- Perform surrogate-based analyses

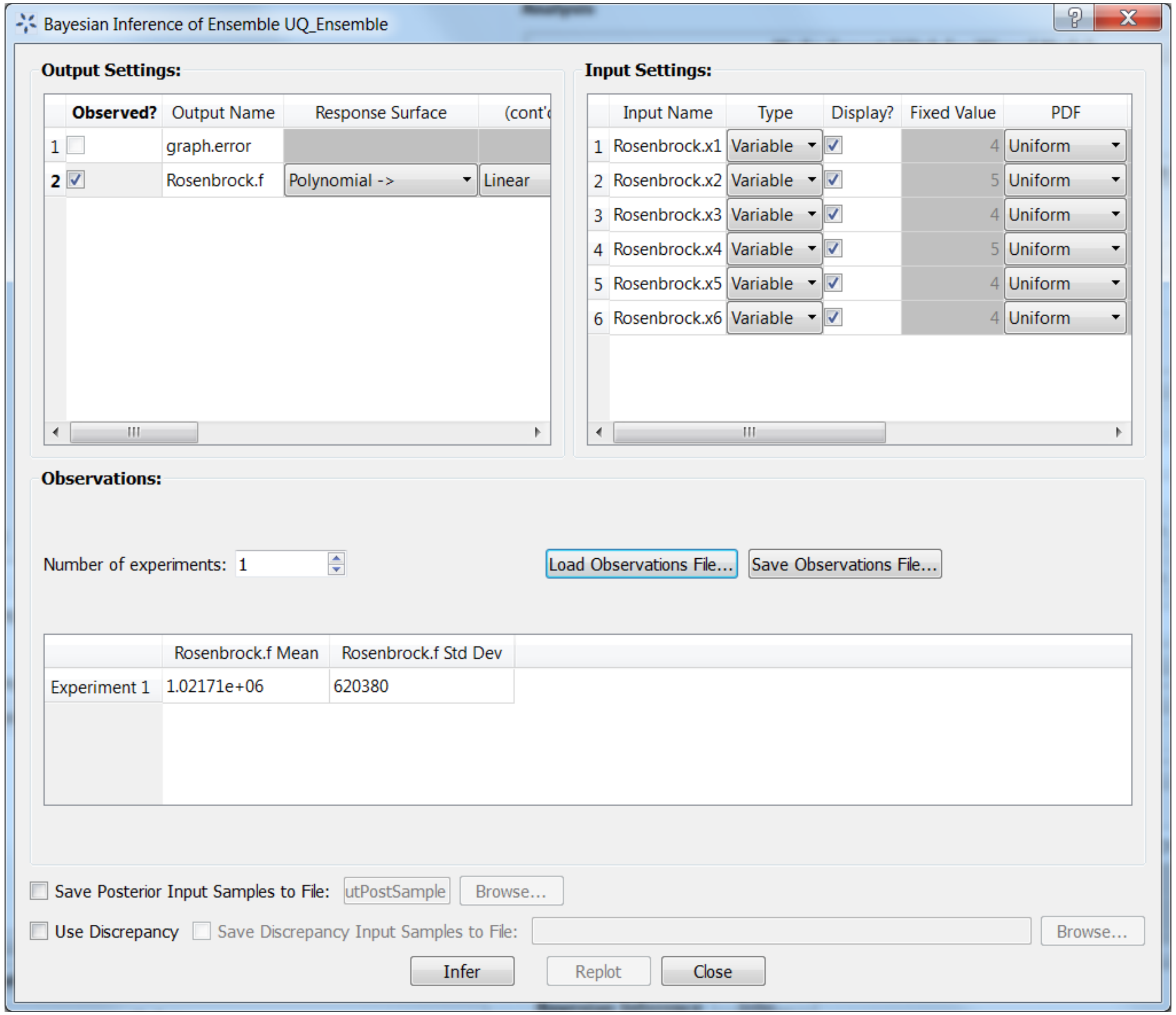




Bayesian Inference

UQ

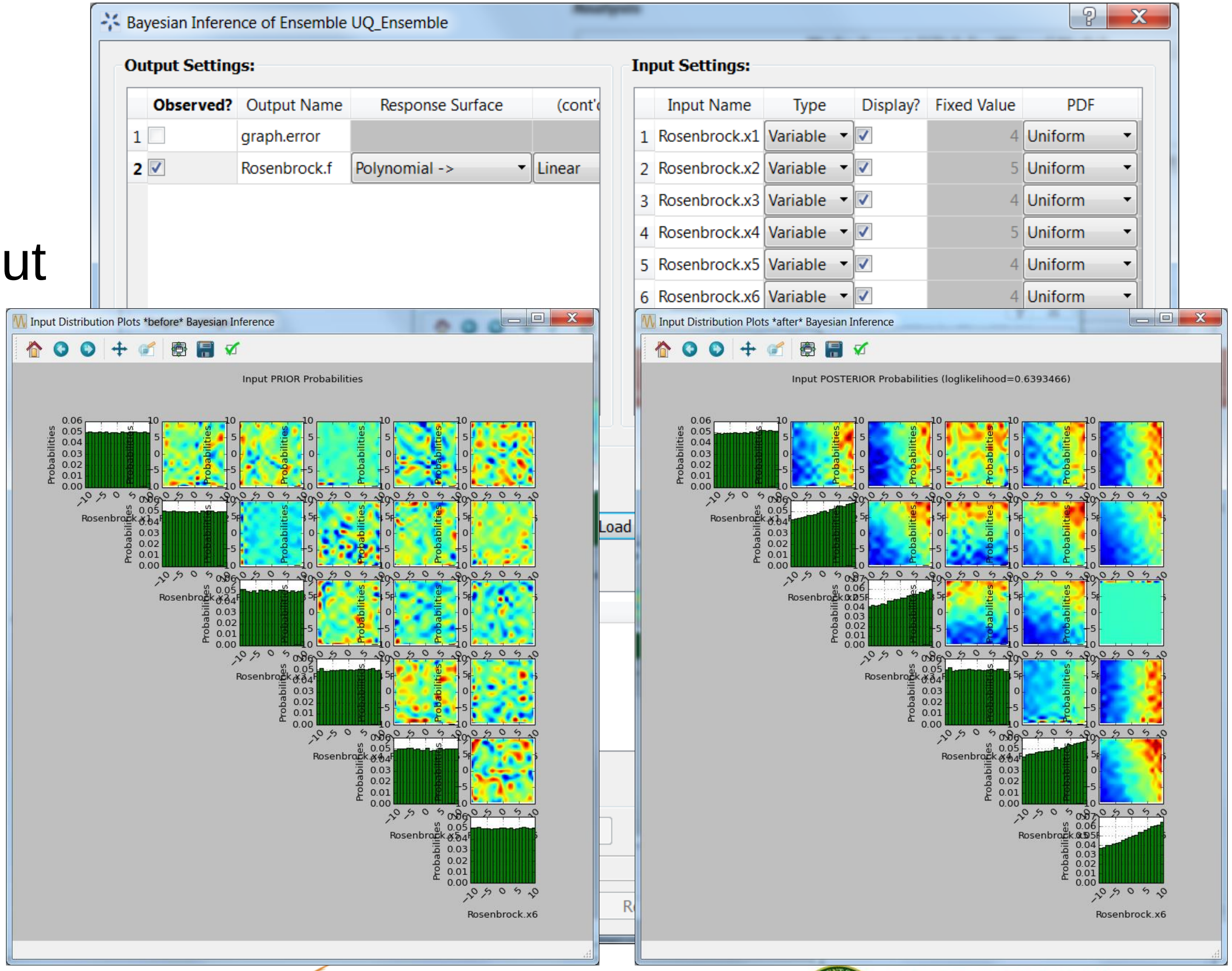
- Import experimental data on observed variables
- Specify prior distribution on input parameters
- Apply surrogate to perform inference
- Save sample of posterior distribution



Bayesian Inference

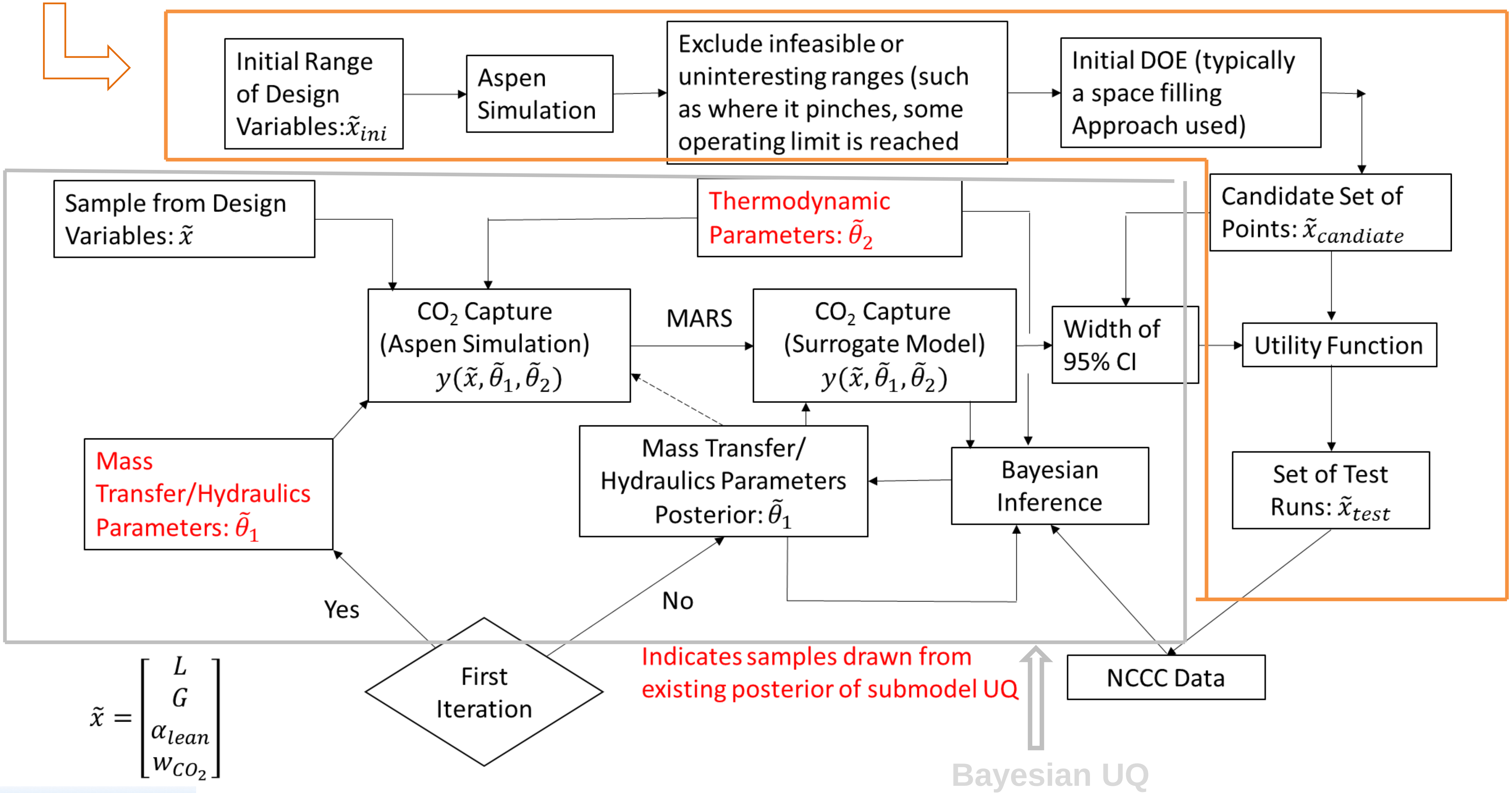
UQ

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



Methodology

Bayesian DOE



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

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

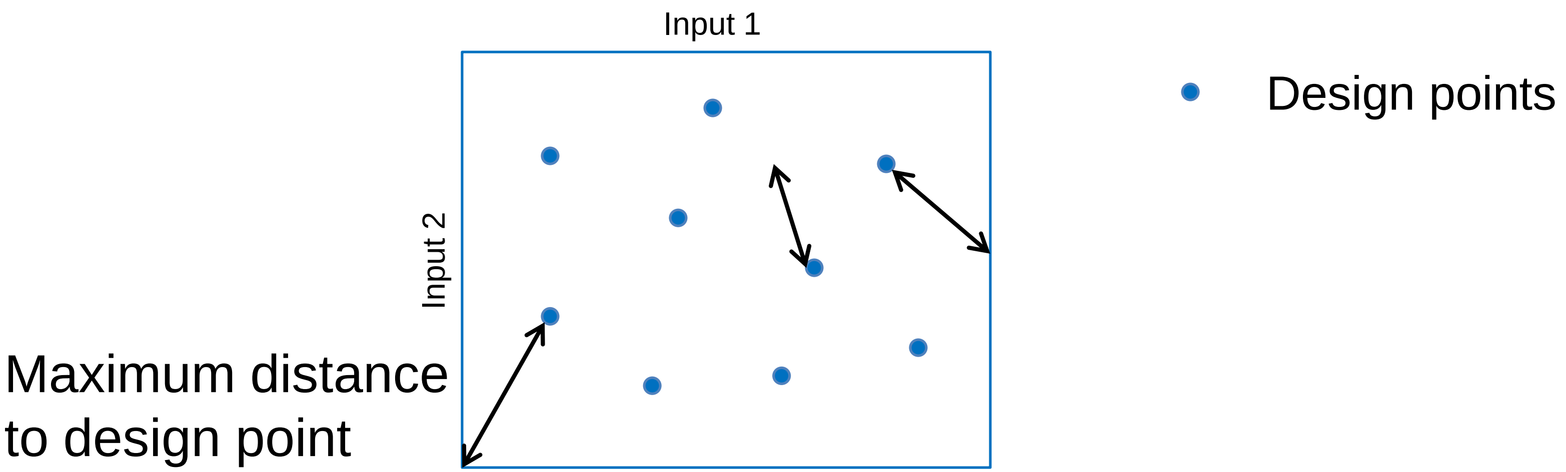
- Flue Gas Flowrate, G in [1000-3000] kg/hr;
- CO_2 weight fraction, w in [0.125-0.175], i.e. (8.4-11.7 mol% CO_2);
- Lean solvent loading, lldg in [0.1-0.3] and;
- Lean solvent flowrate L in [3000-12000] kg/hr

Explore constraints, dependencies, experimental realities.

Designing NCCC Experiments

Initial goal is *exploration* of the input space

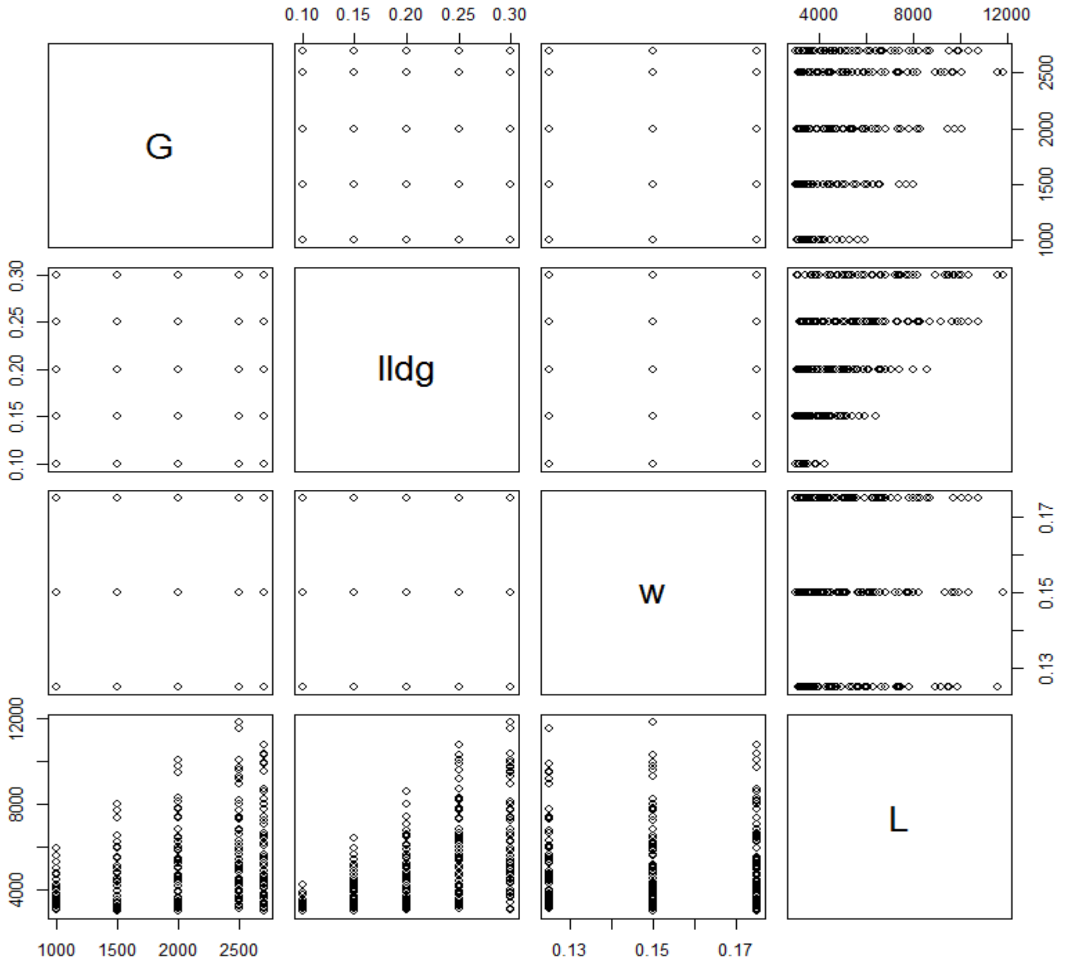
- Criterion used was "minimax" = minimize the largest distance from any point in the input space to a design point



Candidate input combinations

For NCCC experiment:

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

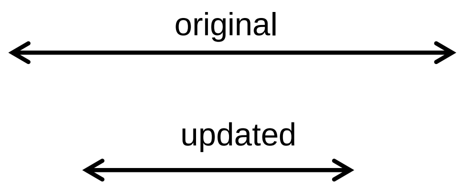


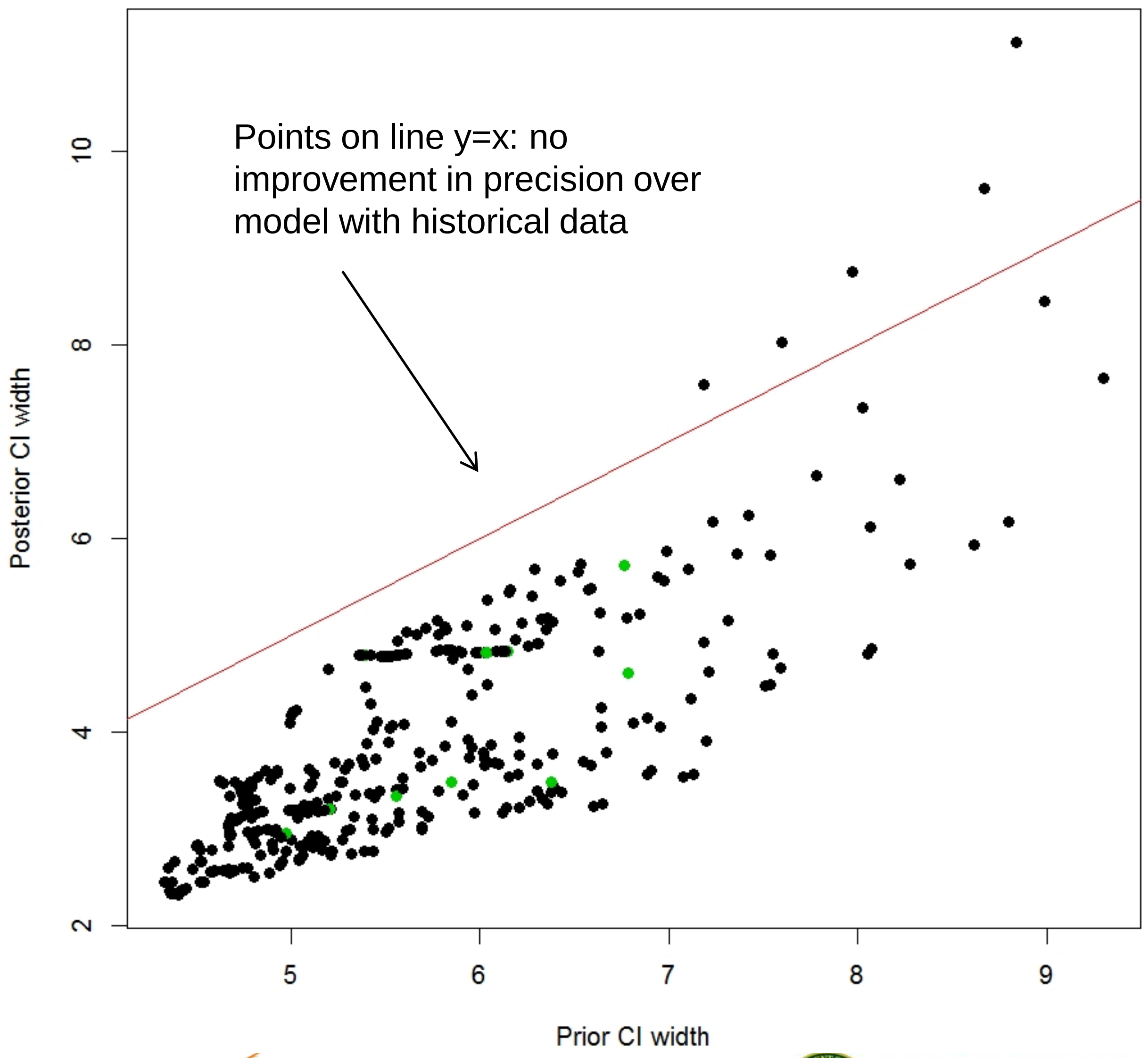
Balance richness of potential experiments against the computation of model evaluation

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

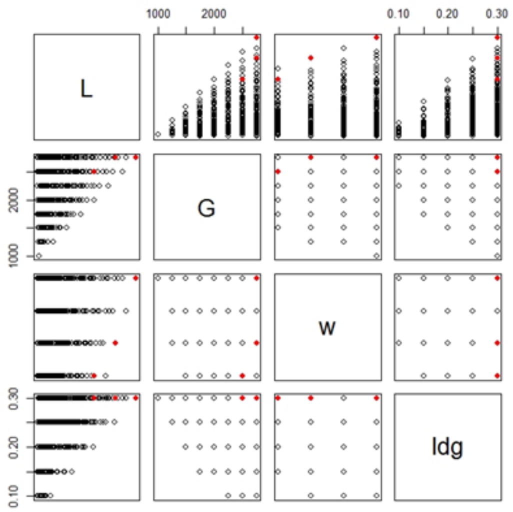
- From: exploration of the design space and clarifying regions of exclusion
- To: improving the precision of prediction for new observations

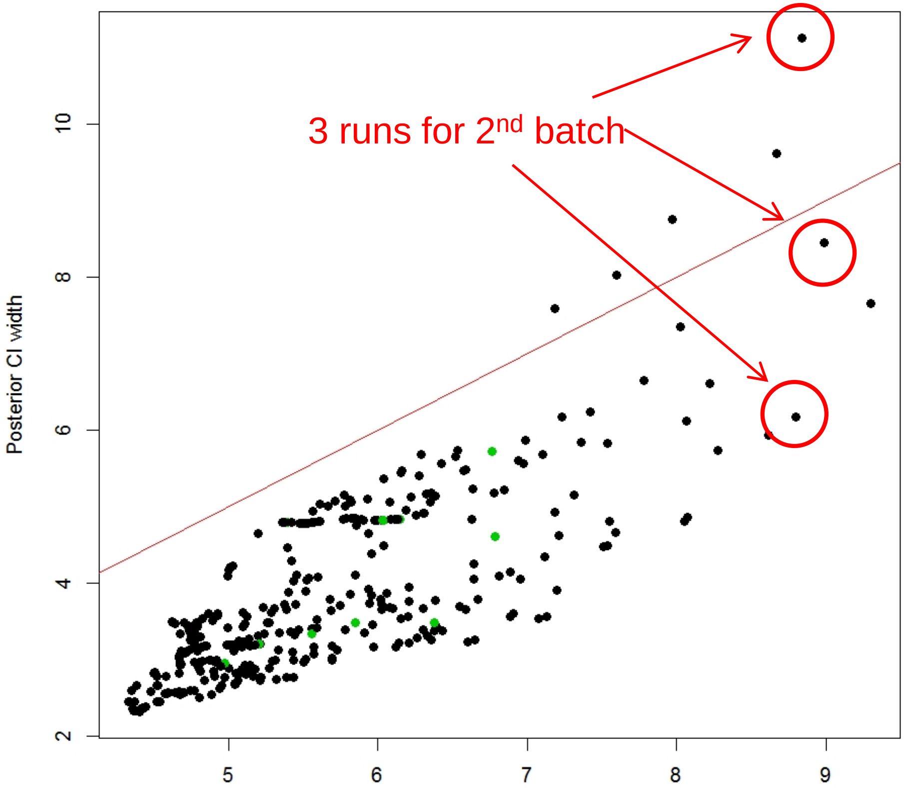




Generate Next Set of Experiments

- 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).

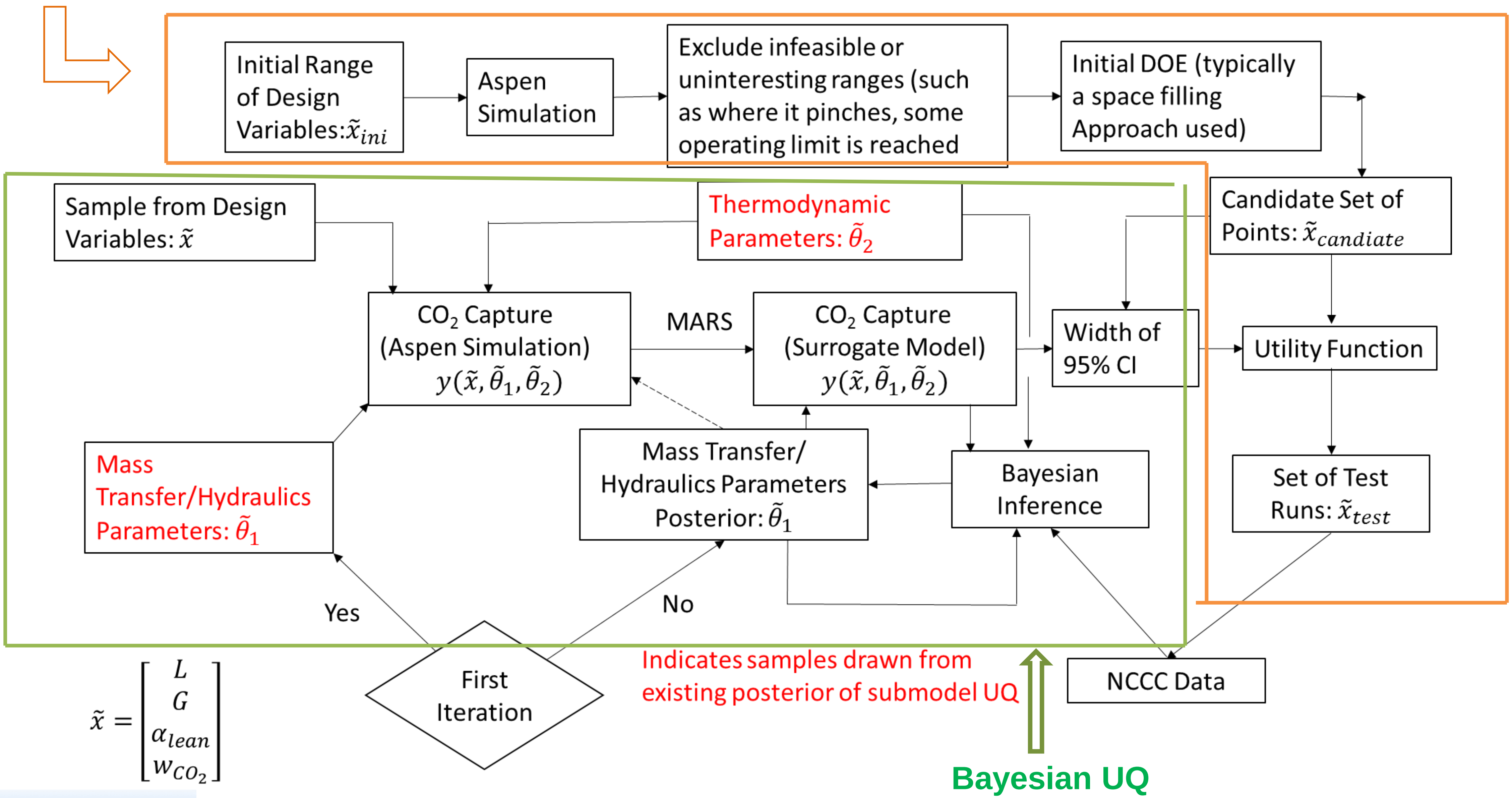




L	G	w	ldg
7971	2500	0.1250	0.3
9881	2750	0.1417	0.3
1675	2750	0.1750	0.3

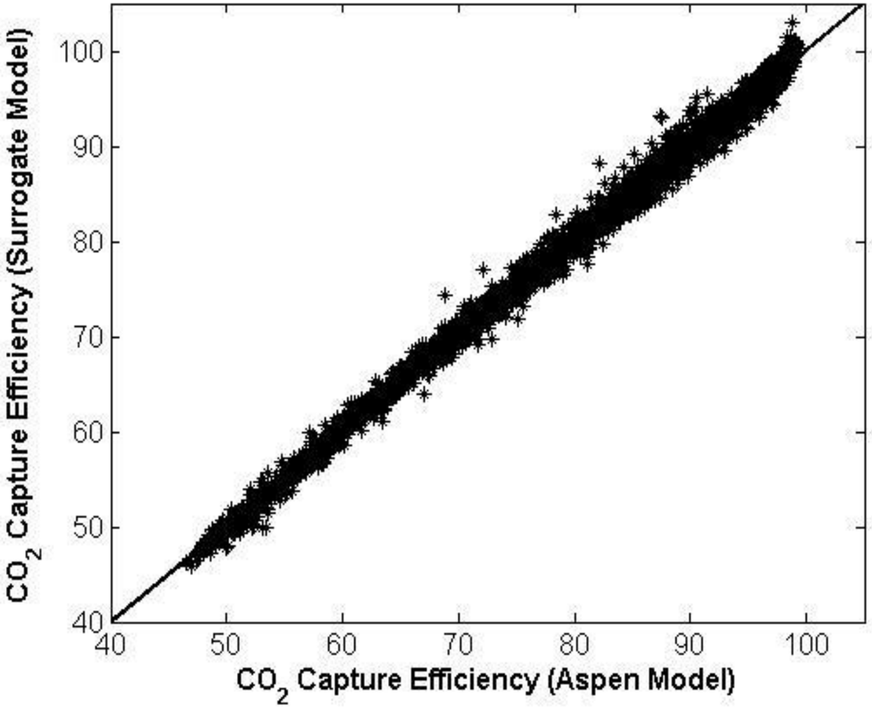
Bayesian DOE

Implementation of Methodology for NCCC DOE



Process Surrogate Model (MARS)

$\hat{\mathbf{y}} = \hat{\mathbf{y}}(\tilde{\mathbf{x}}, \tilde{\boldsymbol{\theta}}_1, \tilde{\boldsymbol{\theta}}_2)$ **y is CO_2 capture percentage**



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

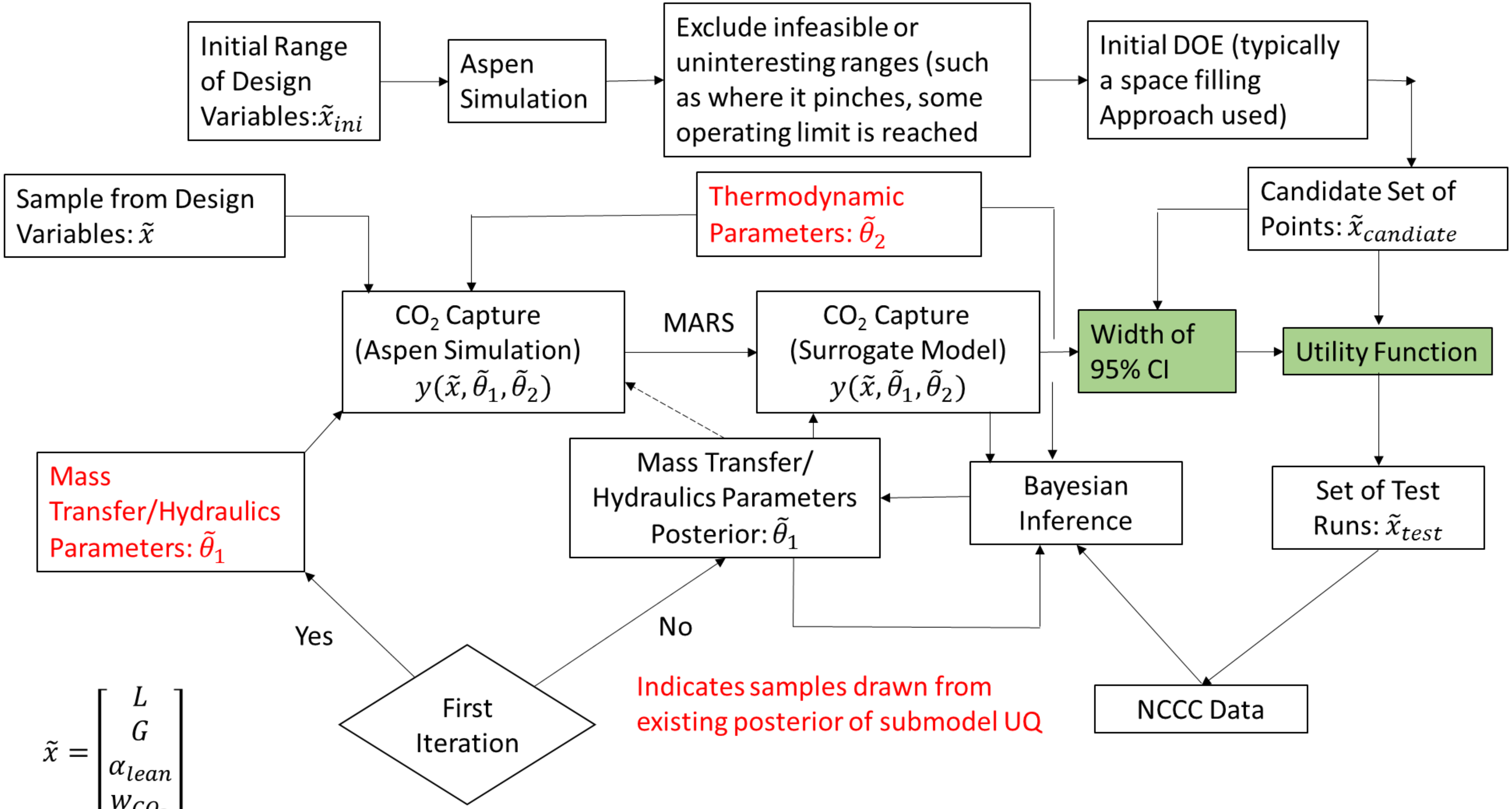
Parameters for which uncertainty is updated (mass transfer + hydraulics): $\tilde{\boldsymbol{\theta}}_2$

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

$$\begin{gathered} 3000 \leq L \leq 13000\ kg/hr \\ 1000 \leq G \leq 3000\ kg/hr \\ 0.1 \leq \alpha_{lean} \leq 0.35\ mol\ CO_2/MEA \\ 0.1 \leq w_{CO_2} \leq 0.175 \end{gathered}$$

Ranges for lean loading and CO_2 weight fraction modified to accommodate all experimental data

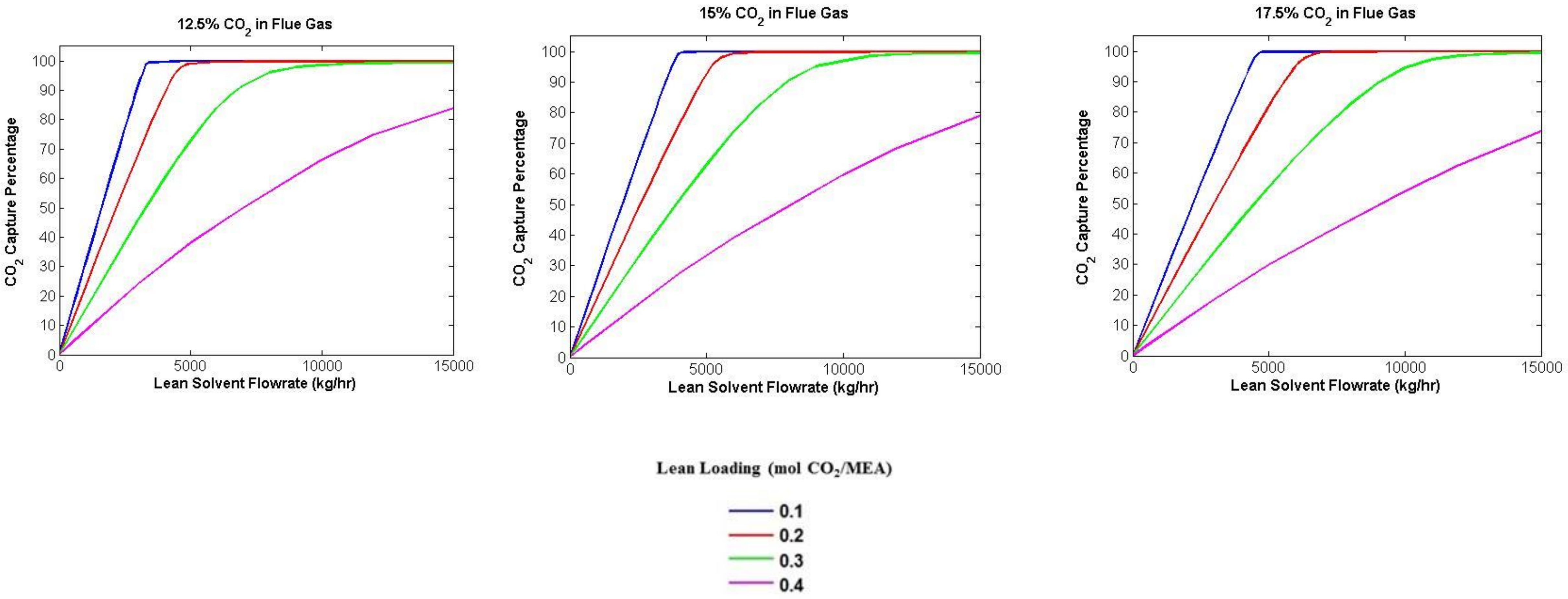
Utility Function



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

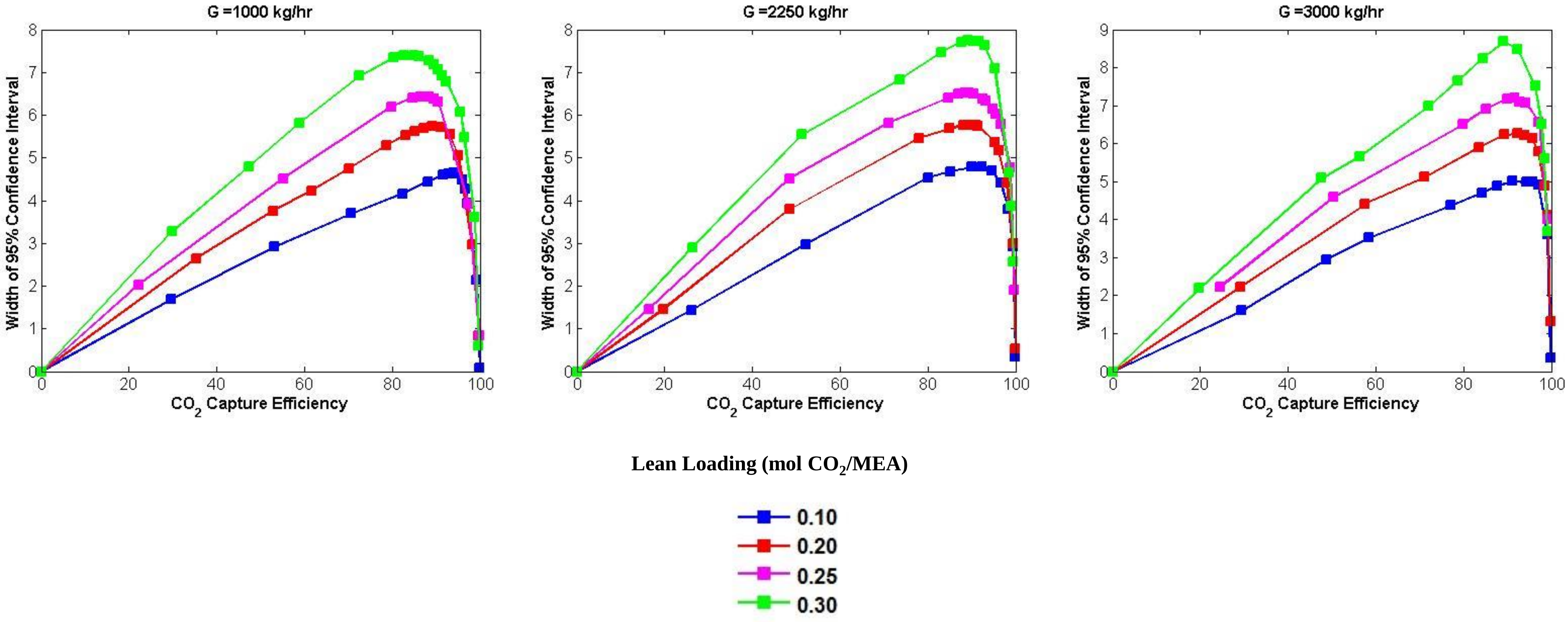
Absorber Model Performance

G = 2250 kg/hr

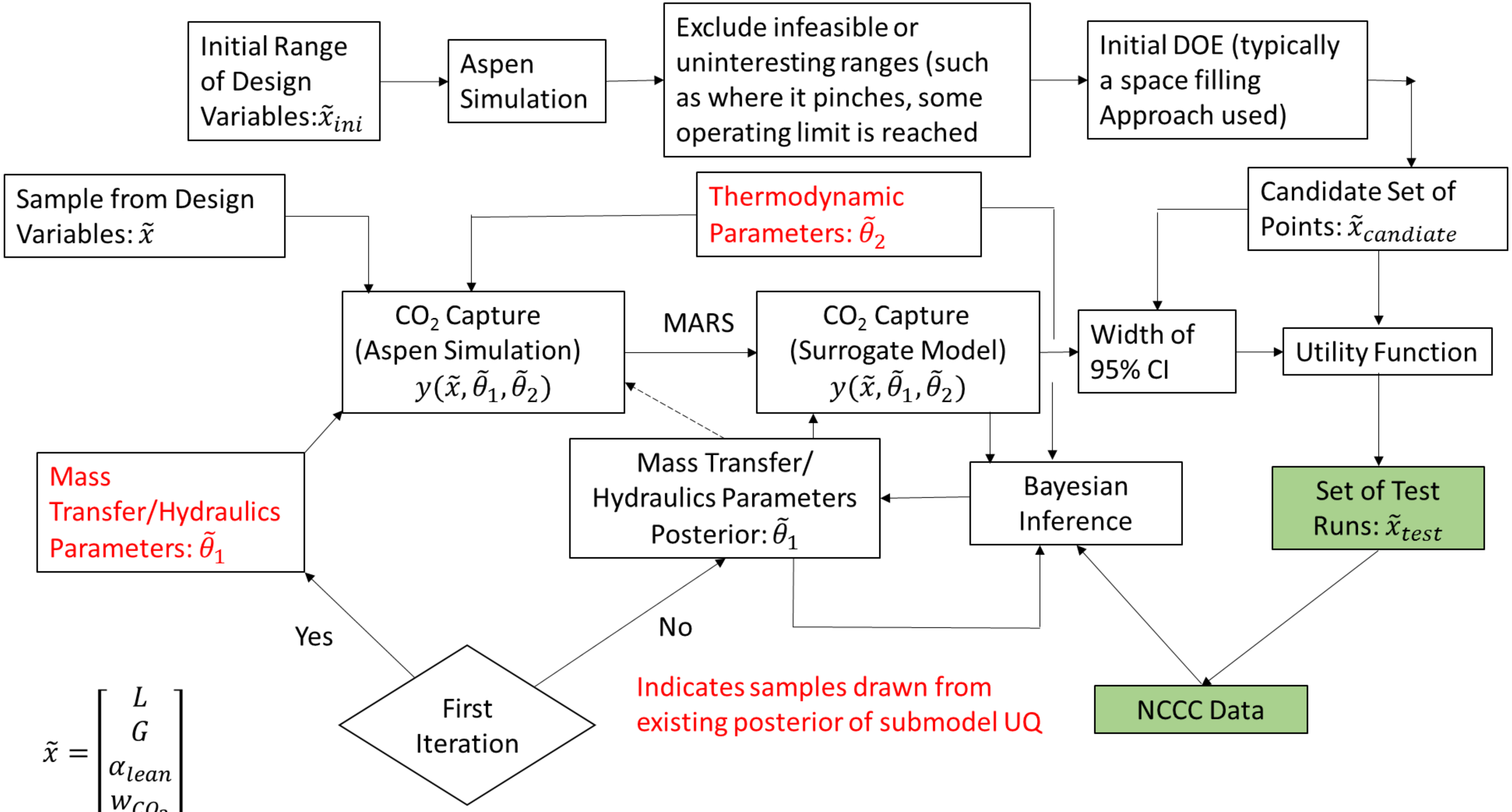


Width of 95% Confidence Intervals

15 wt% MEA



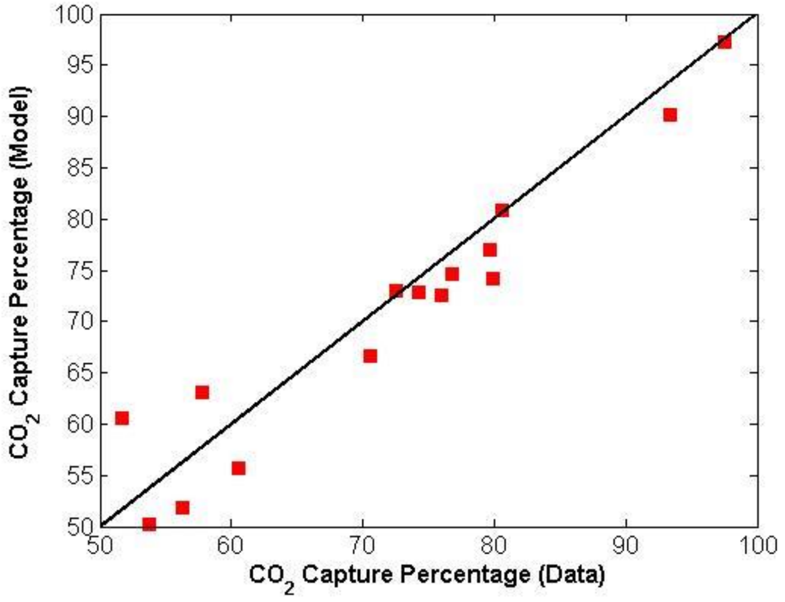
Implementation of Test Runs at NCCC



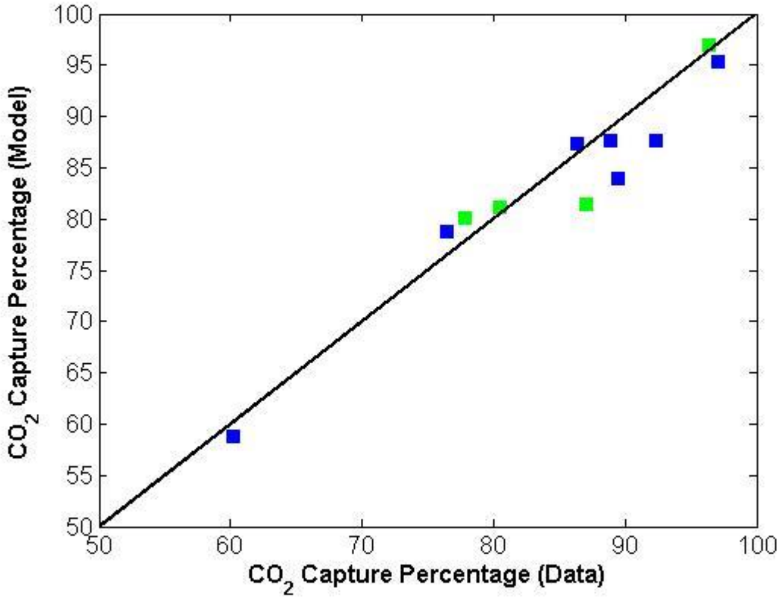
$$\tilde{x} = \begin{bmatrix} L \\ G \\ \alpha_{lean} \\ w_{CO_2} \end{bmatrix}$$

Absorber Performance – Parity Plots

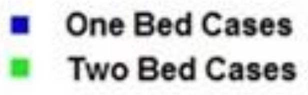
Three Beds (With Intercooling)



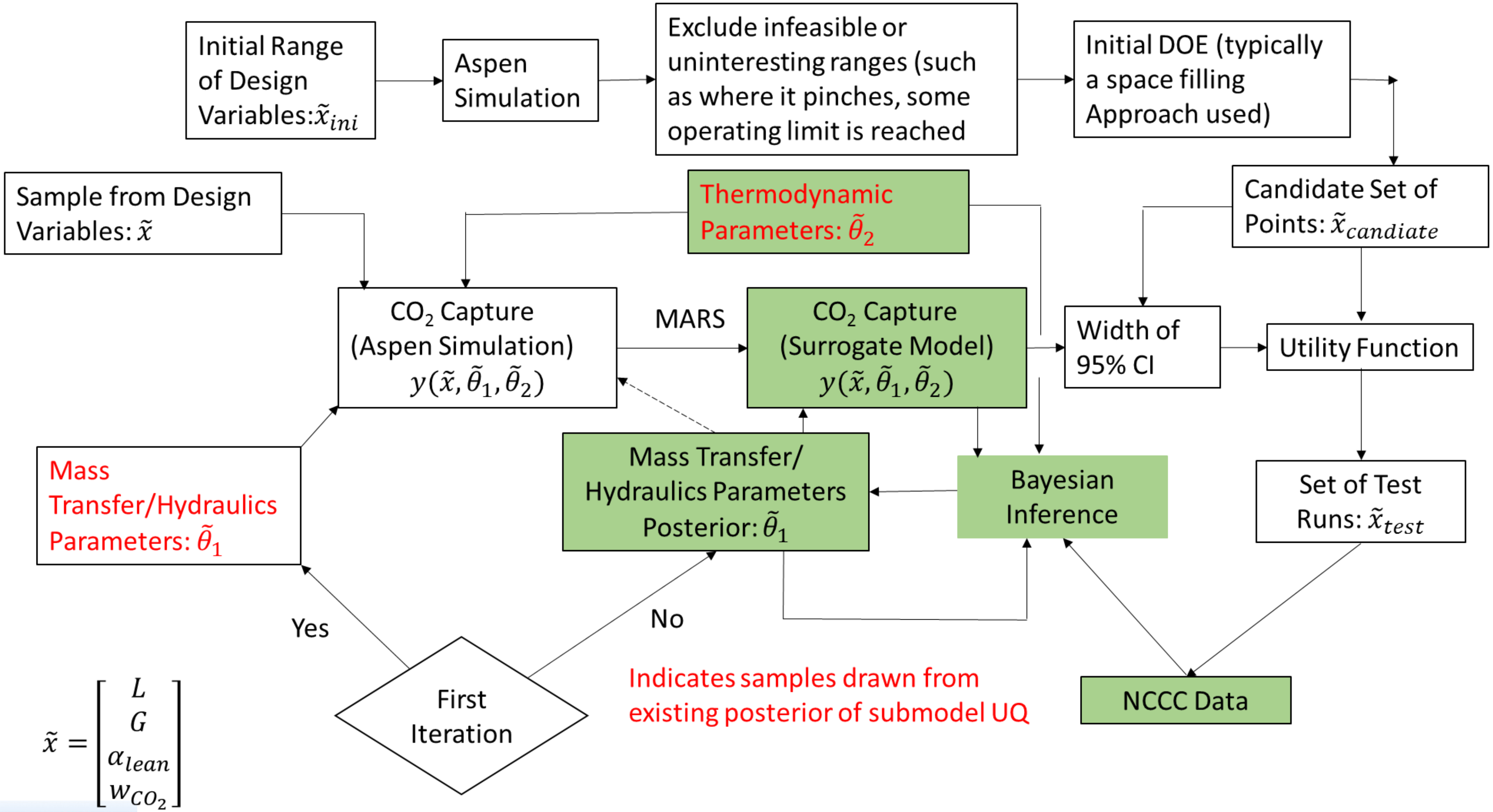
One or Two Beds (Without Intercooling)



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

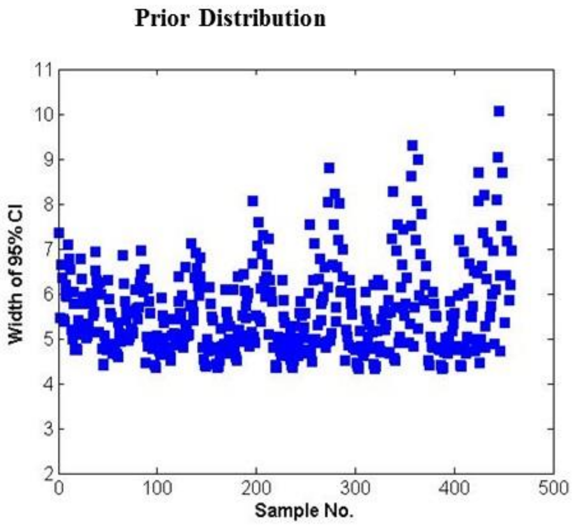


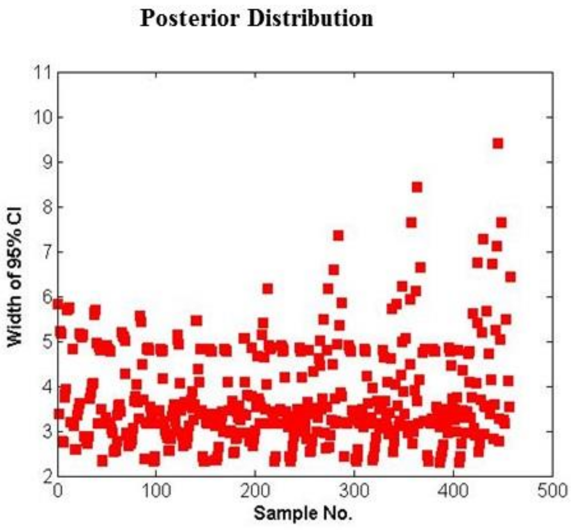
Learning from the Experimental Data: Updating Quantified Uncertainty



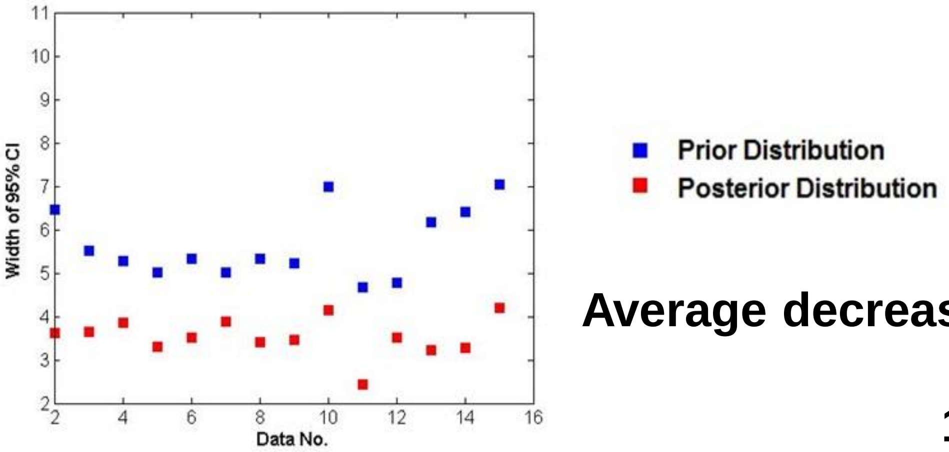
Effect of Bayesian Inference on CI Width (1st Iteration)

Candidate Points





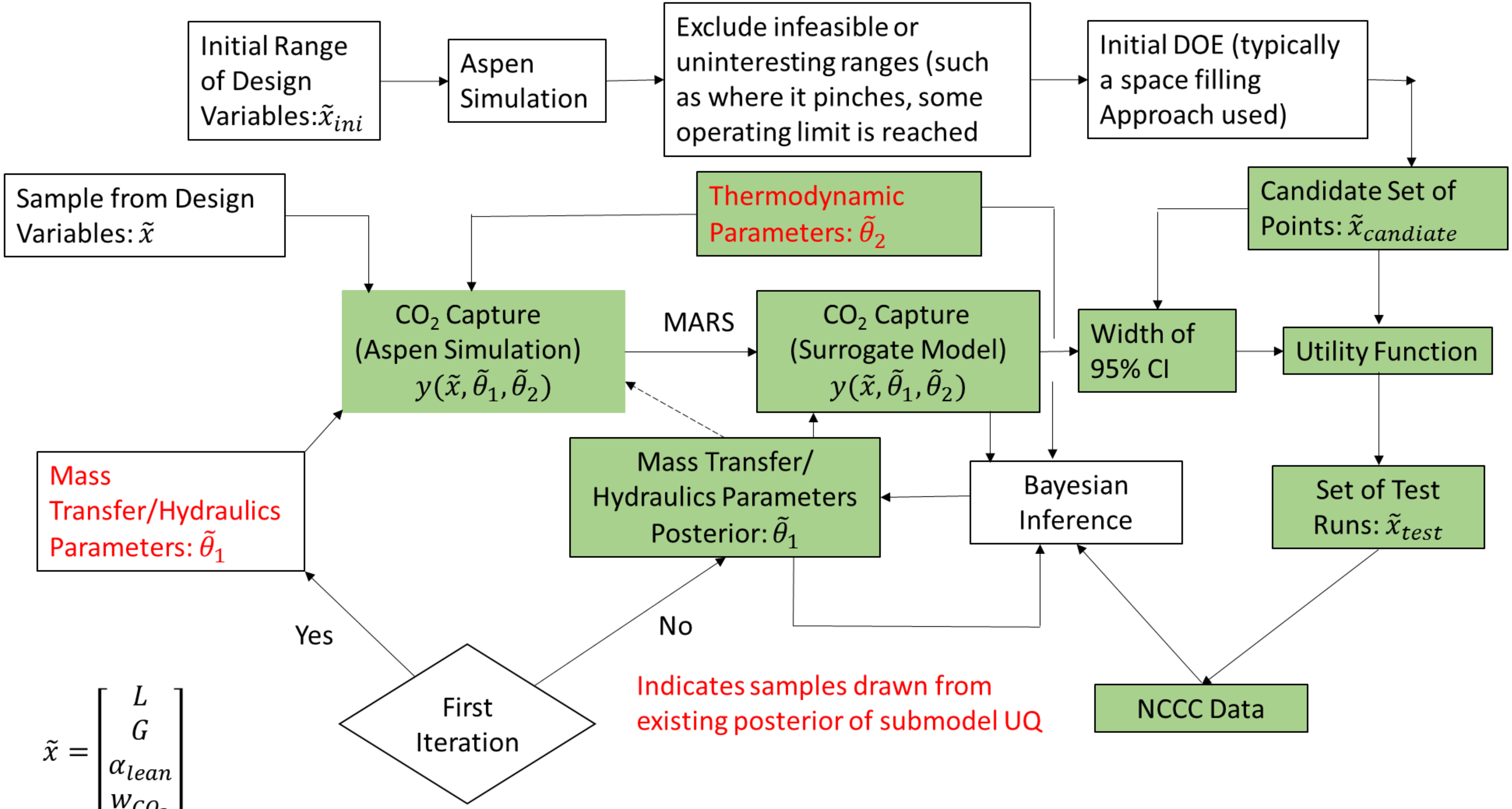
Points with Experimental Data



Average decrease in CI width (% CO_2 Capture):

1.79

Next Iteration

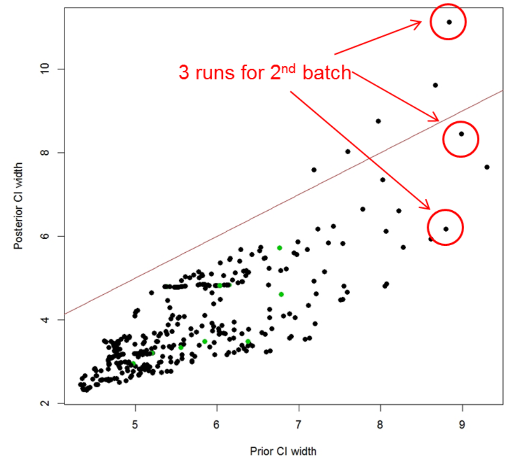


$$\tilde{x} = \begin{bmatrix} L \\ G \\ \alpha_{lean} \\ w_{CO_2} \end{bmatrix}$$

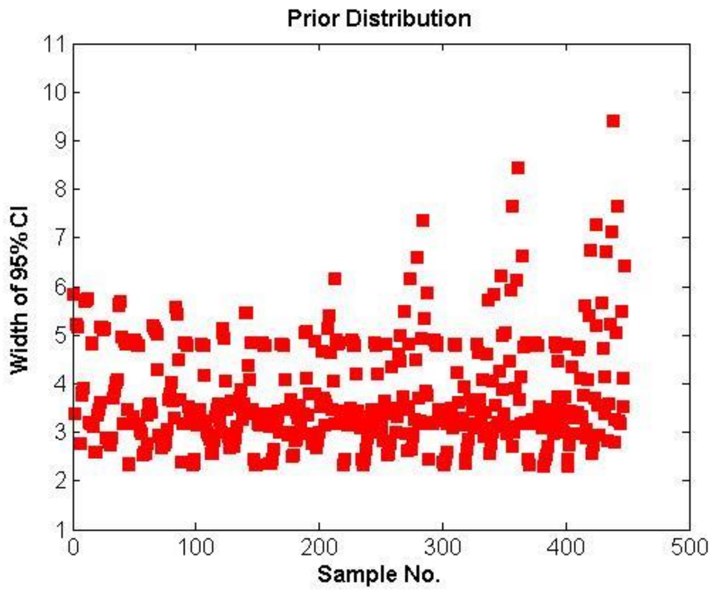
Effect of Bayesian Inference on CI Width (2nd Iteration)

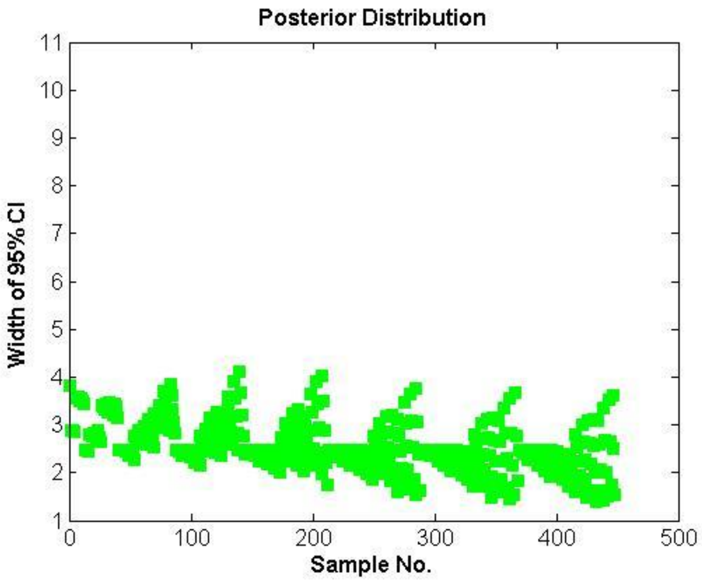
Test Cases

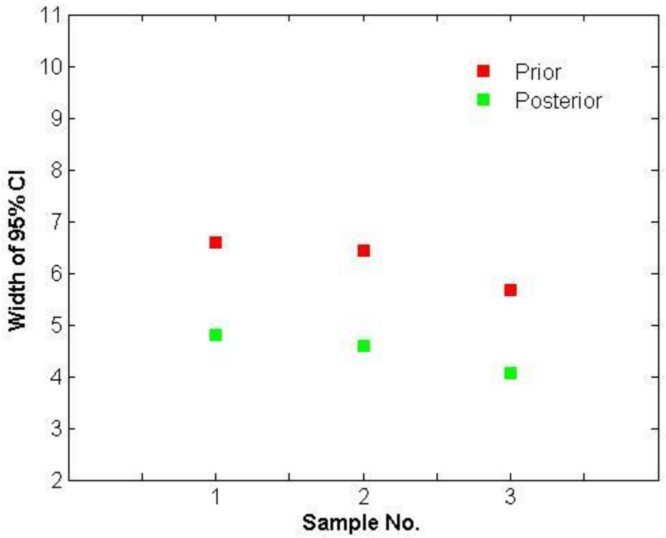
Case No.	L (kg/hr)	G (kg/hr)	α_{lean}	w_{CO_2}	CO_2 Capture
1	7959	2497	0.3	0.118	96.1
2	9871	2746	0.3	0.133	97.7
3	11412	2748	0.3	0.162	94.9



Update in CI Width







Average decrease in CI width (% CO_2 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