CCSI²

Carbon Capture Simulation for Industry Impact

Sequential Design of Experiments

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Outline

- What is Sequential Design of Experiments
  - How can it be helpful?

- Example – The Technology Centre Mongstad (TCM) Experiment
  - Implementation of SDoE for Model Calibration and Optimization

- What tools are under development
  - FOQUS SDoE Module

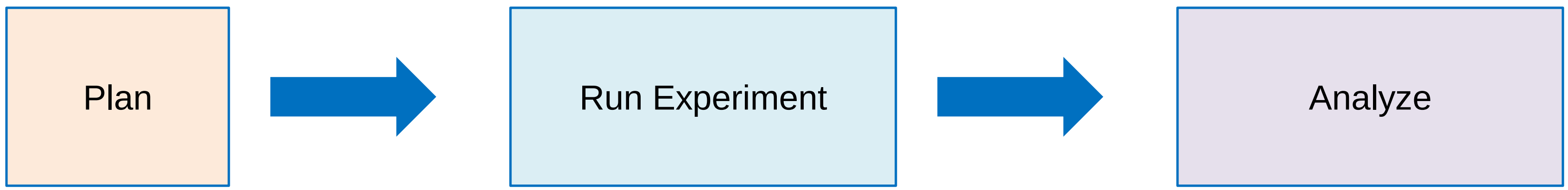
CCSI[2] Carbon Capture Simulation for Industry Impact NETL Berkeley Lab Lawrence Livermore National Laboratory Los Alamos National Laboratory Pacific Northwest National Laboratory U.S. Department of Energy

Statistical Design of Experiments

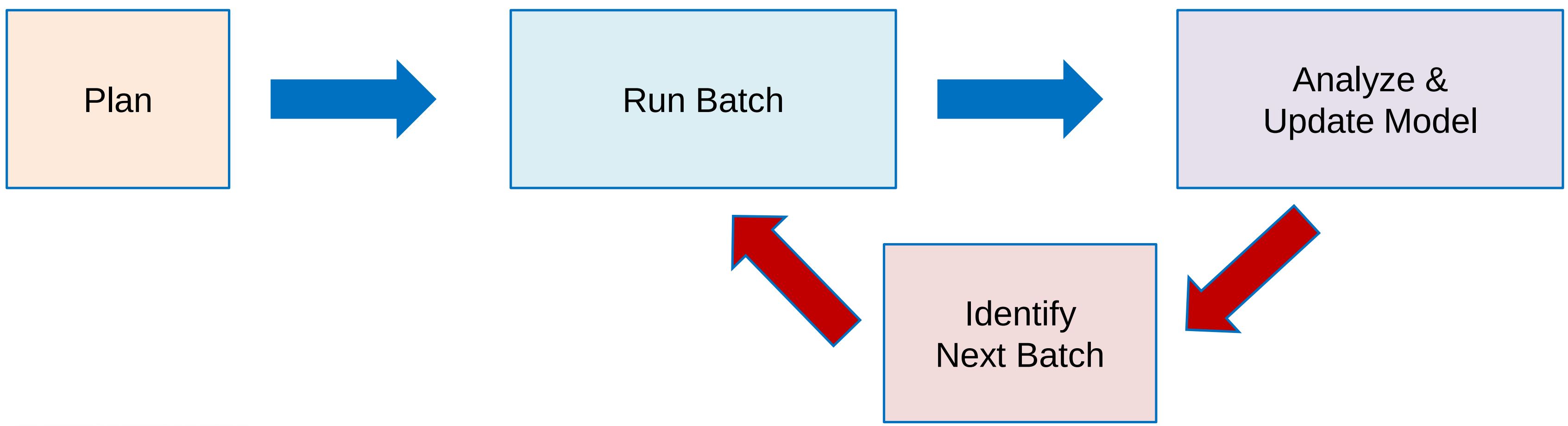
Statistical Design of Experiments is a way to accelerate learning by collecting a ***strategic*** sample of data:

- Help reach required precision or understanding faster
- Help learn more with a fixed set of resources

One-shot experiment



Sequential experiment



Possible Criteria to use from SDoE

1. Exploration
   – Space-filling designs

2. Model Calibration
   – Data to check how well the model and observed data match

3. Improving the quality of prediction for new observations
   – Using a measure of precision of prediction, seek to improve worst case or average prediction uncertainty (eg. Minimize the width of a confidence interval for new observations)

4. Optimization of response value
   – Find the location in the input space that optimizes a performance criteria and verify its performance relative to nearby points

Process for Sequential DoE

Planning Phase

1. Identify one or more criteria over which to design the experiment.
2. Develop a working model of the process to calculate the criteria values based on currently available knowledge and data.
3. Define the inputs (with their ranges) to be explored during the experiment.
4. Identify candidate input combinations.
5. Decide on initial batch of input combinations for experiment setup.
6. Develop a working model of the process able to receive data and update the calculated criteria values.
7. Determine feasible size of the sequential batches, based on runtime requirements.

During Experiment

8. Run the initial batch of runs [using input combinations from (5).
9. Apply data to update the working model in (6) and calculate criteria values.
10. Select the next batch of input combinations for next set of runs.
11. Repeat steps 8-10 for subsequent batches.

Technology Centre Mongstad Experiment

- Sequential Design of Experiments was used throughout the 5 weeks of testing at TCM in June-July 2018
- Priorities of the Experiment were:
  - Exploration over the ranges of inputs of interest (initial)
  - Improving the quality of prediction (reducing the worst case uncertainty of predicting new observations – G-optimality)
  - Optimization of a performance metric (finding the most cost-effective location to operate the facility subject to constraints)
- There were several different sub-questions that were considered in different portions of the experiment
  - For each of them, we applied a customized version of SDoE

TCM Test Plan

- Test runs completed
- 24 m absorber packed height
- Simple stripper configuration

Phase 1

Space-filling design for model validation

Phase 2

Selection of points for testing based on economic objective function

Phase 3

Sequential test point selection for model refinement

- 12-18 m absorber packed height
- Stripper operated with solvent bypass system

Phase 4-5

Optimization of specific reboiler duty

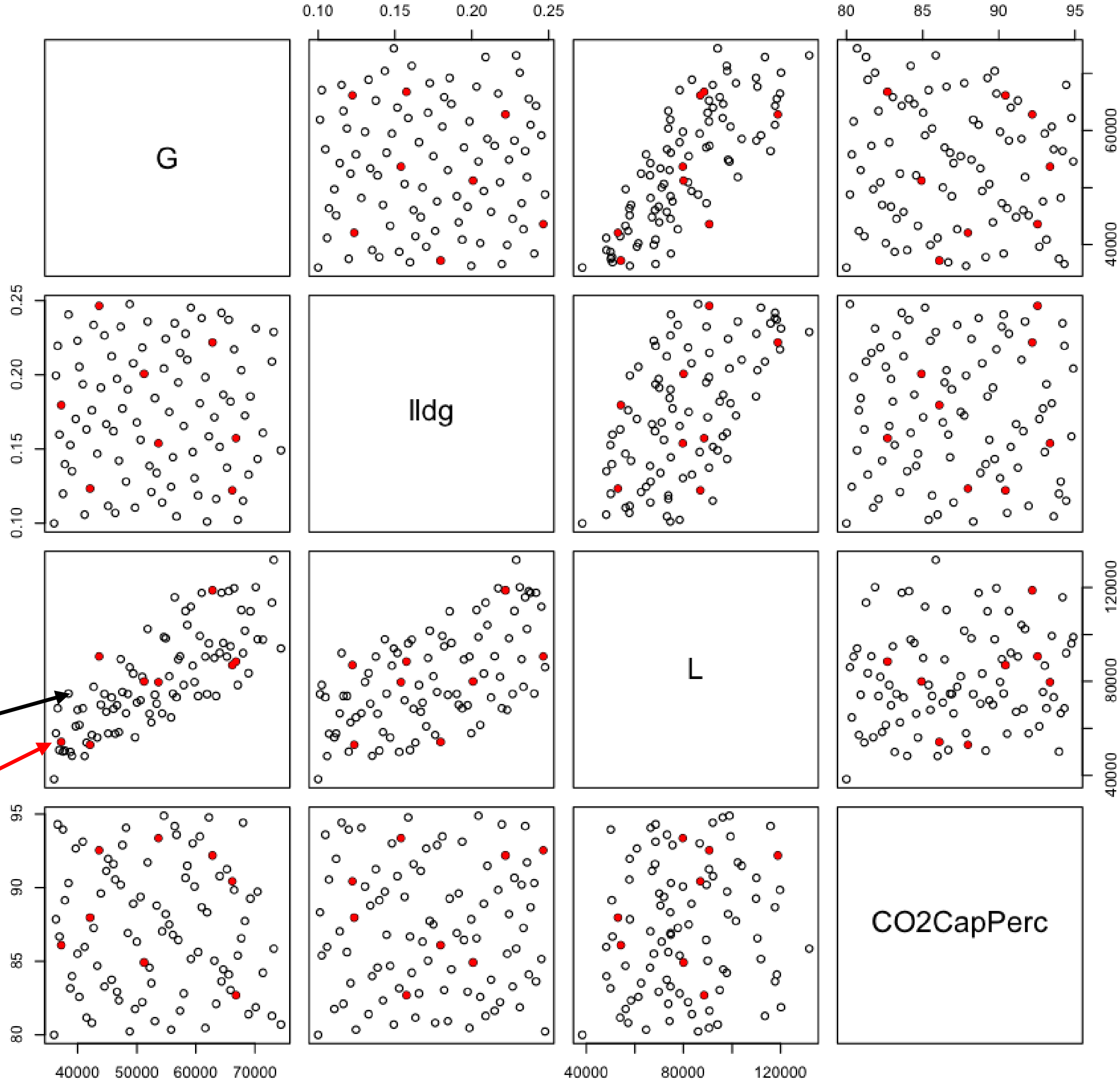
Phase 1 – 24m Absorber Packed Height
Goal: Space-filling of 4-D space (minimax)

Scenario:
8 mol% CO_2 in flue gas

3. Define input region of interest

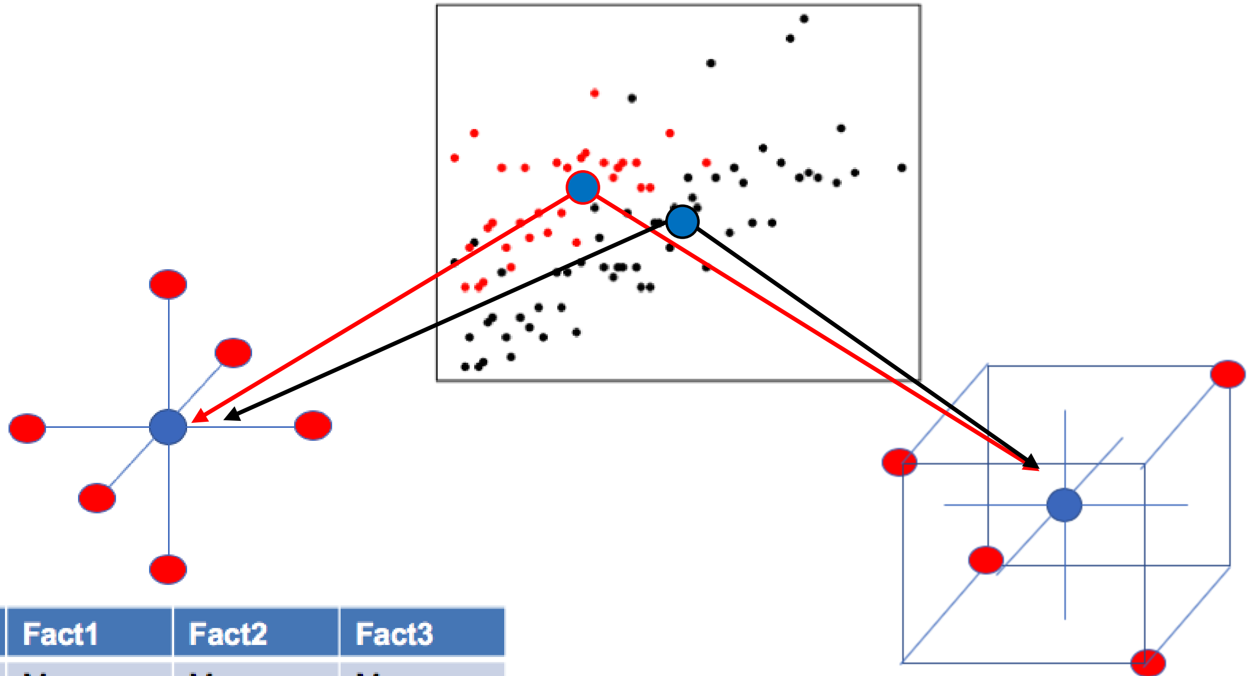
4. Identify candidate points from which to choose

5. Create space-filling design of the required size (here 8 runs)



Phase 2 – Confirmation of Optimal Run Locations

For each of 8 mol% CO_2 + 10 mol% CO_2 in flue gas, an optimal economic location was identified based on the updated models

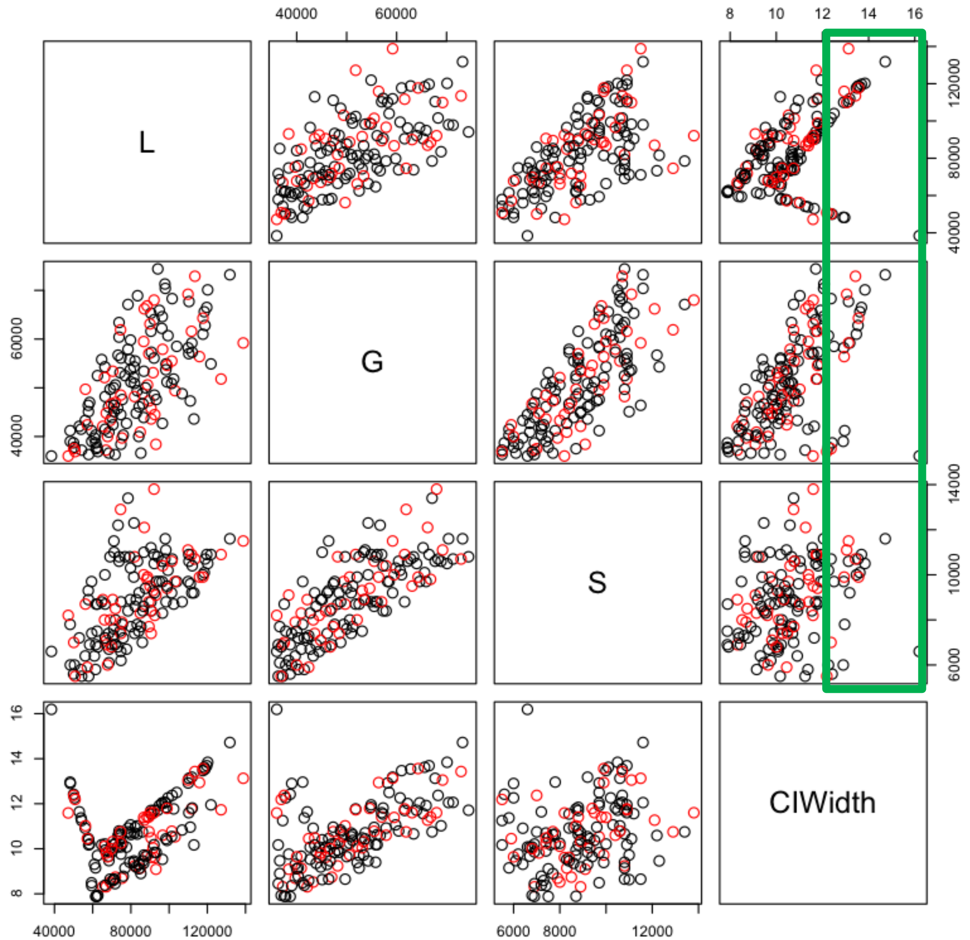


Run	Fact1	Fact2	Fact3
Optimal	M	M	M
Adjust F1	L	M	M
	H	M	M
Adjust F2	M	L	M
	M	H	M
Adjust F3	M	M	L
	M	M	H

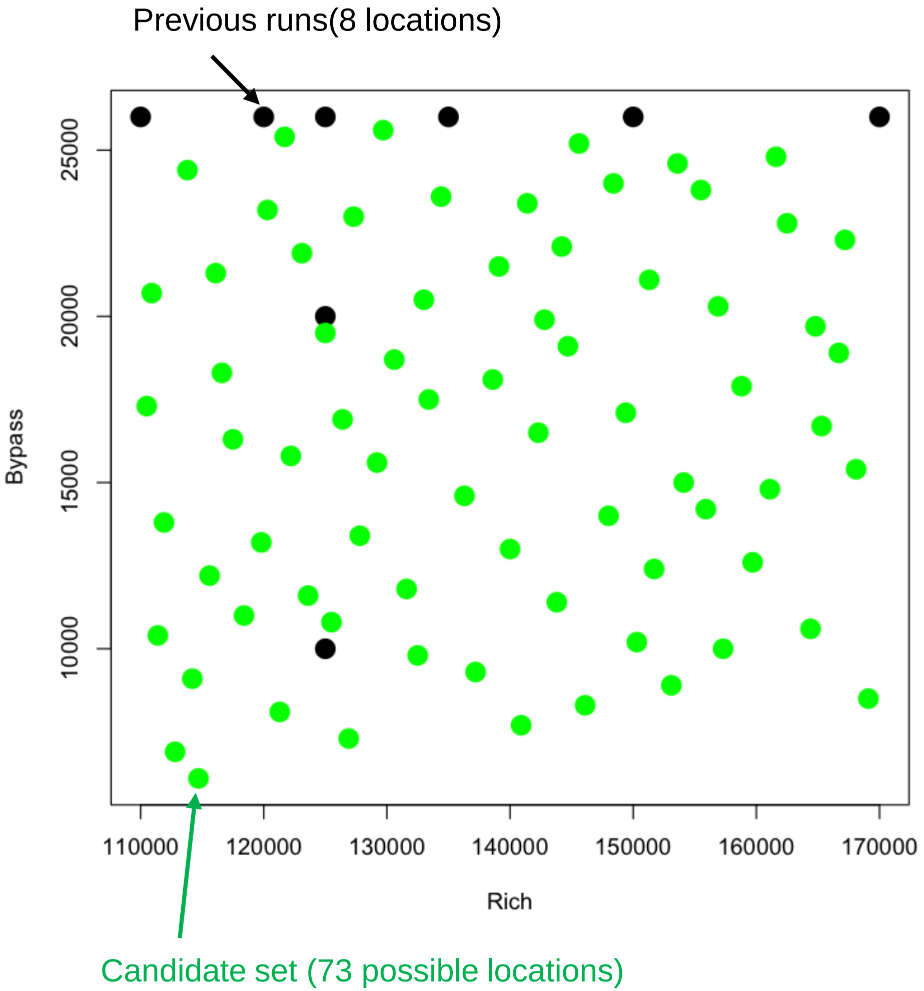
Run	Fact1	Fact2	Fact3
Optimal	M	M	M
Corner1	L	H	L
Corner2	H	L	L
Corner3	L	L	H
Corner4	H	H	H

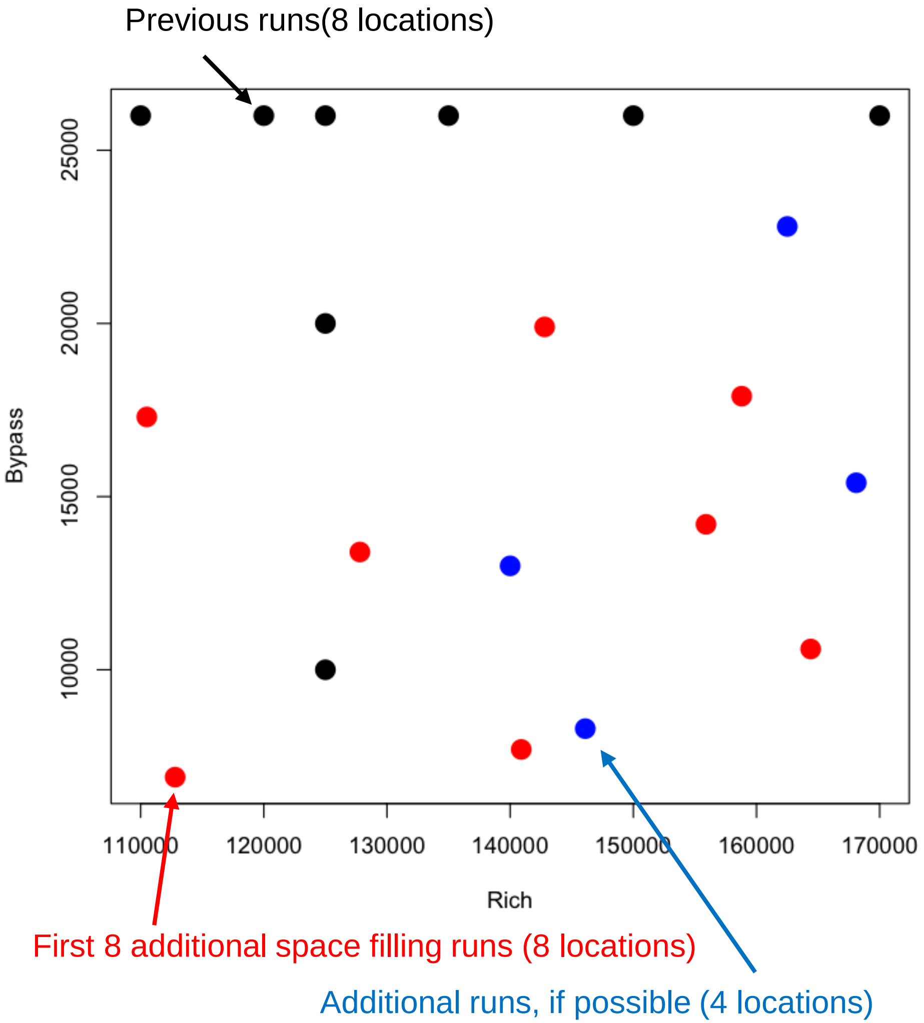
Phase 3 – Improving the Precision of Prediction
Goal: Reduce width of Confidence Intervals for new prediction

Target input combinations with large C.I. Widths
–> Most significant reduction in model uncertainty



Phase 5 – 12m Absorber Packed Height (rich solvent bypass system)
Goal: Space-filling of 2-D space (minimax)



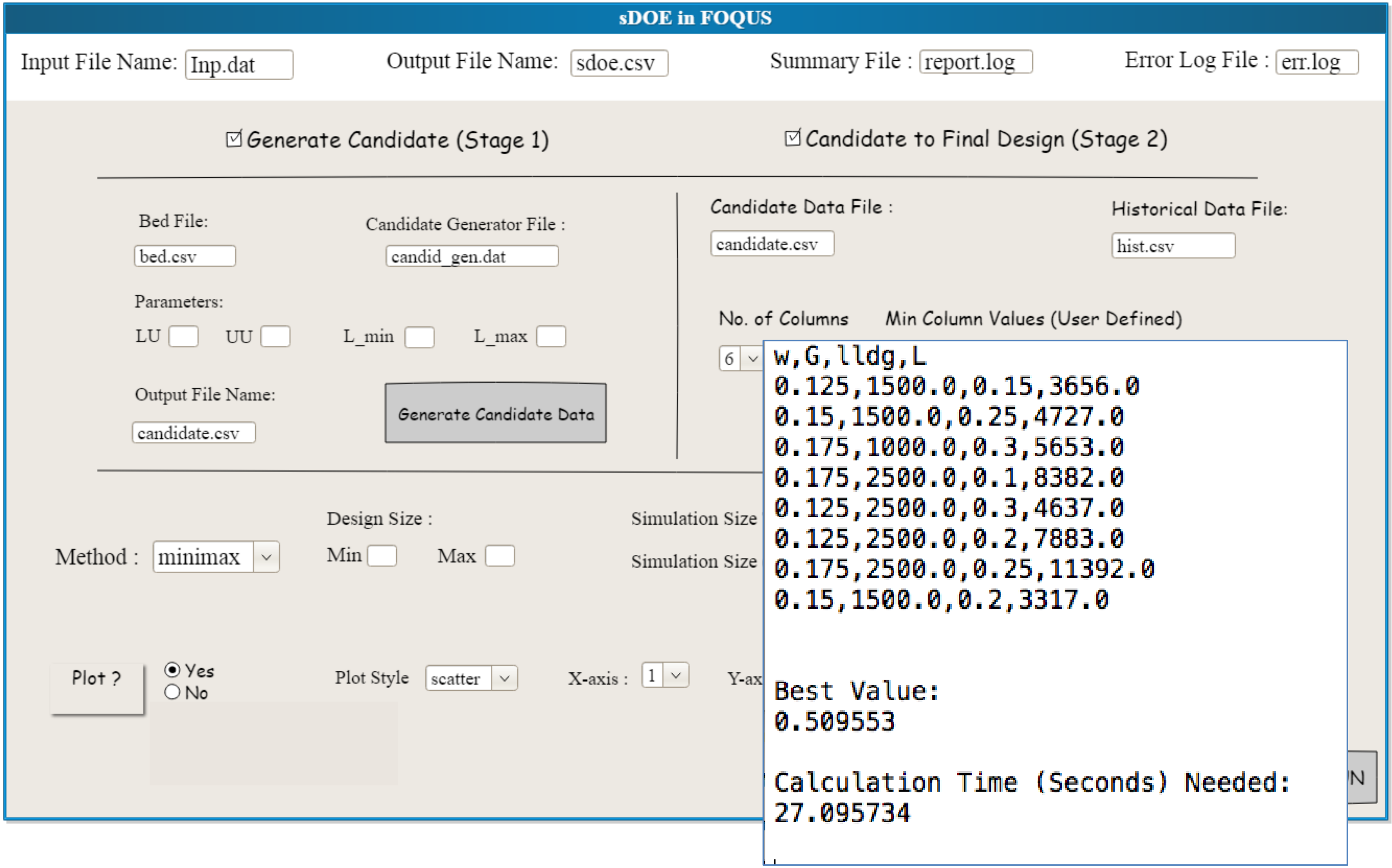


SDoE in FOQUS

- A multi-year plan is being implemented to make SDoE capabilities more easily available
- Phase 1 (target: end of 2018):
  - Exploration
  - Model Calibration
  - Improving Quality of Prediction (simple version)
- Phase 2 (target: end of 2019):
  - Improving Quality of Prediction (more advanced version)
  - Optimization of Response Value

See poster **"Sequential Design of Experiments in FOQUS to Maximize Learning from Experiments"** by T. Ahmed & C. Anderson-Cook **today at 5:30** for more details

GUI Mockup for Phase 1



Conclusions

- Design of experiments is a powerful tool for accelerating learning, by targeting maximally helpful input combinations for experiment goals.
- Sequential DoE incorporates (in near real-time) empirical information from an experiment as it is being run.
- The criteria over which to optimize should be chosen to match the goals of the experiment.
  a) Exploration
  b) Model calibration
  c) Improving the precision of prediction for new observations
  d) Optimizing the value of responses of interest.
- CCSI2 is developing a set of tools within FOQUS to make running SDoE more straightforward.

- Remember, all experiments are designed – just some are poorly designed!