CCSI^2 Project Overview

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Executive Summary

- **Overview**
  - •50+ personnel accelerating CCS technology understanding and development
  - •Engagement with International Test Center Network (ITCN) and ~50 Industrial/Academic Stakeholders
- **Industrial Collaborations**
  - •CCSI^2 Supports 10 CO_2 Capture Program projects $60MM+ in total project value (TRL 3-7)
    - Three DOCCSS projects, four Developers Testing at TCM, LLNL MECS Technology, UT Austin AFS, UKy Process Control
  - •Additional external industrial agreements (executed or in progress)
    - GE, ADA-ES, Test Centre Mongstad (TCM), SINTEF, Canada's Oil Sands Innovation Alliance (COSIA)
- **Strategic Design of Experiments**
  - •Improves model while optimizing experimental data collection
  - •Demonstrated success in MEA campaigns at NCCC and TCM
- **DOCCSS Collaboration**
  - •Materials Characterization → Equipment Design → Process Optimization

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
WestVirginiaUniversity
THE UNIVERSITY OF TEXAS AT AUSTIN
U.S. DEPARTMENT OF ENERGY

CCSI²: Accelerating Rate of RD&D

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
National Energy Technology Laboratory
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
CAER

Industry

Google
ADA Environmental Solutions
Alstom
B&W the babcock&wilcox company
GE
CO2 Technology Centre Mongstad
AEP American Electric Power
Fluor
Phillips 66
EPRI Electric Power Research Institute
Southern California Edison An EDISON INTERNATIONAL Company San Onofre Nuclear Generating Station
Southern Company
ExxonMobil
Chevron
URS
Air Products
Eastman
NC National Carbon Capture Center
aspentech
ANSYS
Schneider Electric
PSE

CCSI² Carbon Capture Simulation for Industry Impact
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West Virginia University
The University of Texas at Austin
U.S. Department of Energy

CCSI Toolset: New Capabilities for Modeling

Maximize the learning at each stage of technology development

- **Early stage R&D**
  - Screening concepts
  - Identify conditions to focus development
  - Prioritize data collection & test conditions
- **Pilot scale**
  - Ensure the right data is collected
  - Support scale-up design
- **Demo scale**
  - Design the right process
  - Support deployment with reduced risk

2016 R&D 100 Awards

Complete Toolset Available at github.com/CCSI-Toolset

FOQUS - Framework for Optimization and Quantification of Uncertainty and Surrogates

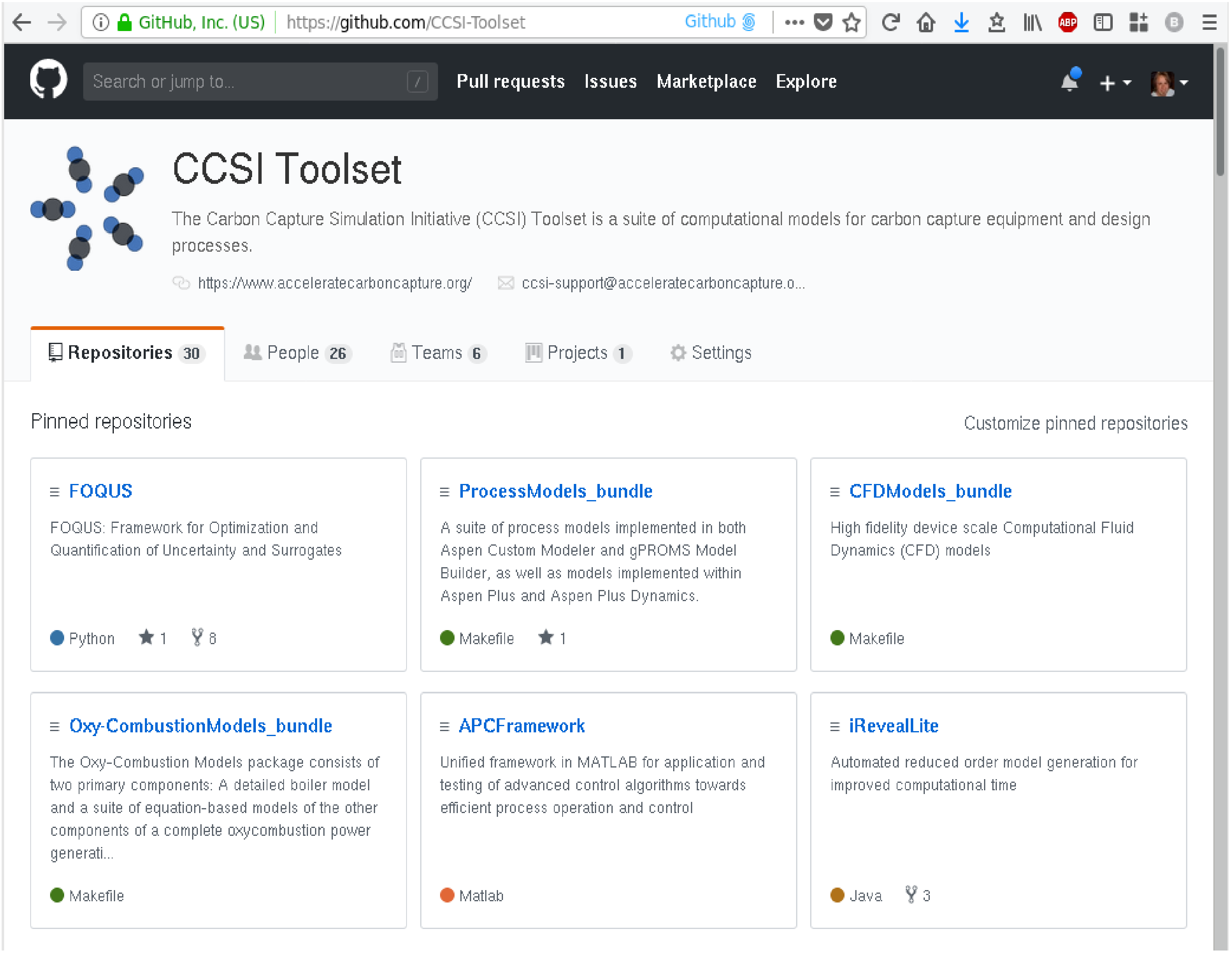
3 Toolset Bundles:

CFD Models: High fidelity device scale Computational Fluid Dynamics (CFD) models

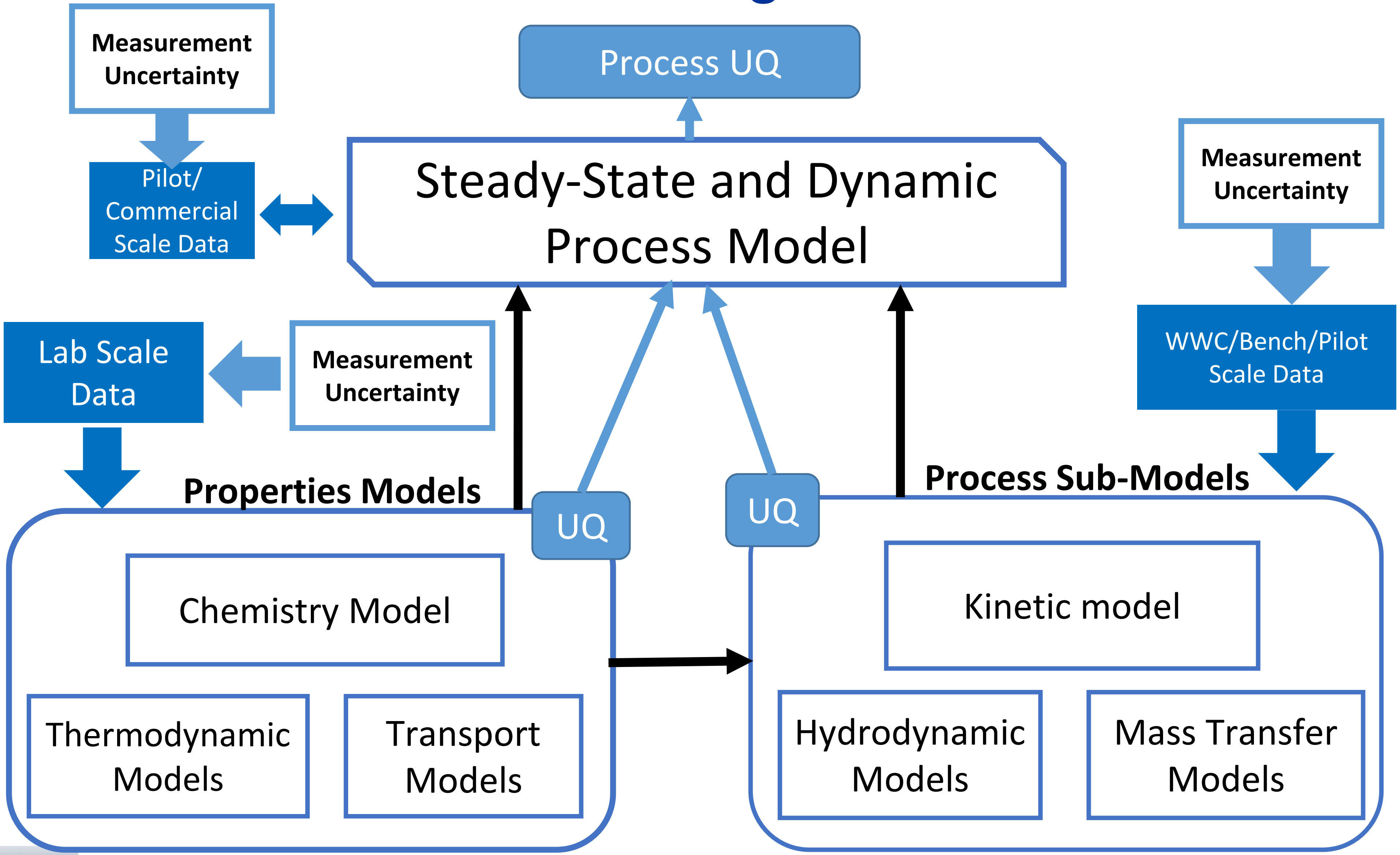
Oxy-Combustion Models: Boiler model and a suite of equation-based models

Process Models: A suite of process models implemented in gPROMS, Aspen Custom Modeler, Aspen Plus and Aspen Plus Dynamics

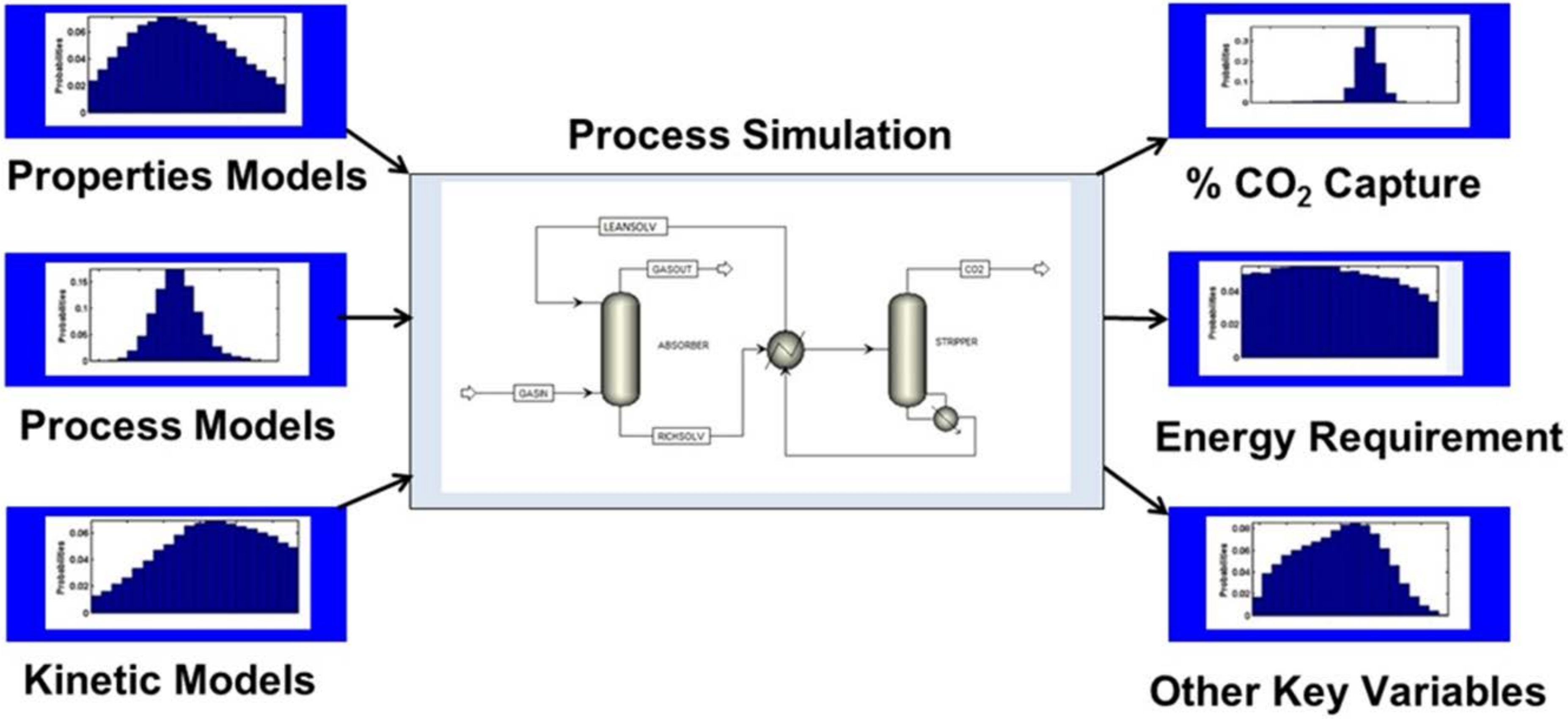
Many more...



Baseline Modeling Framework



Integrated Multi-Scale Model Approach



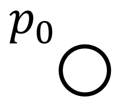
Test Campaigns to Reduce Uncertainty

- **Pilot Test Campaigns Are Costly!**
- **Uncertainty evaluated in the following models:**
  - Transport models (surface tension, viscosity, diffusivity)
  - Thermodynamic models (density, VLE, heat capacity)
  - Hydraulic models (pressure drop, holdup)
  - Mass transfer models (mass transfer coefficients, interfacial area)
  - Kinetic model
- **Model Validation with Data and propagation of all parametric uncertainties through the model**
  - UQ methodology is leveraged to improve models and test plans
- **Optimize Campaign to Maximize Value…**

Required Experiments

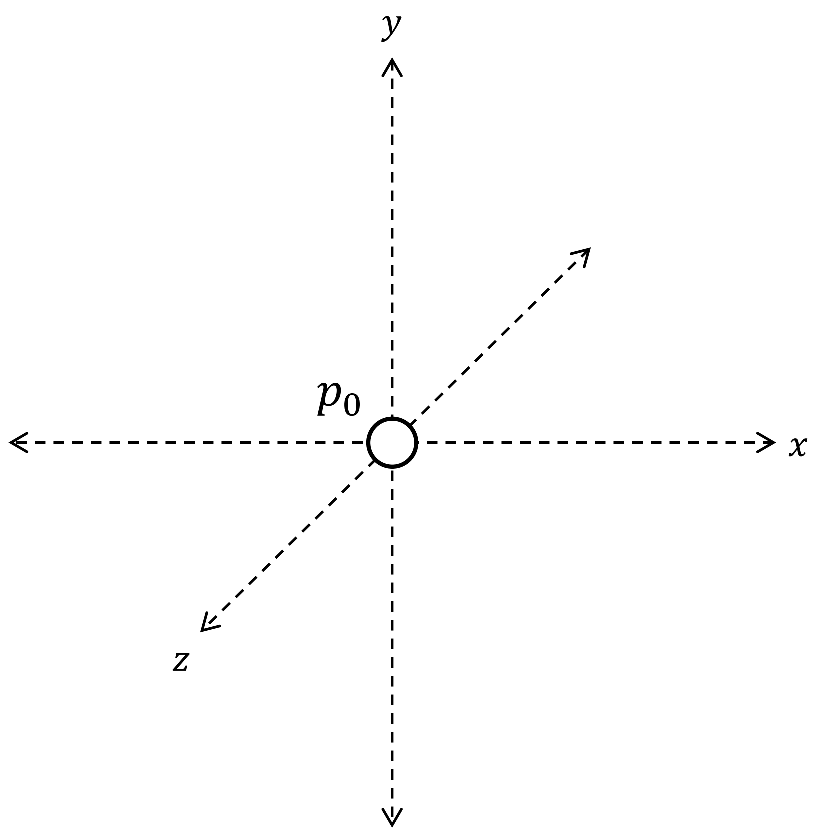
Required Experiments

$p_0 = (startingpoint)$



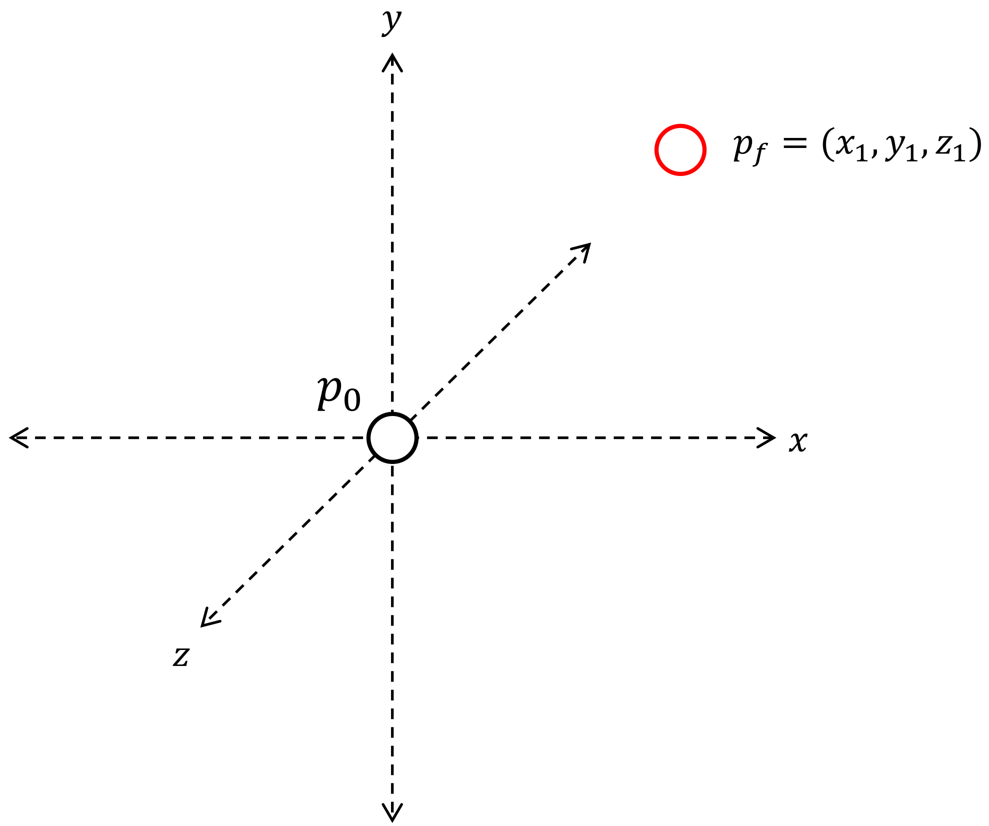
Required Experiments

$p_0 = (x_0, y_0, z_0)$



Required Experiments

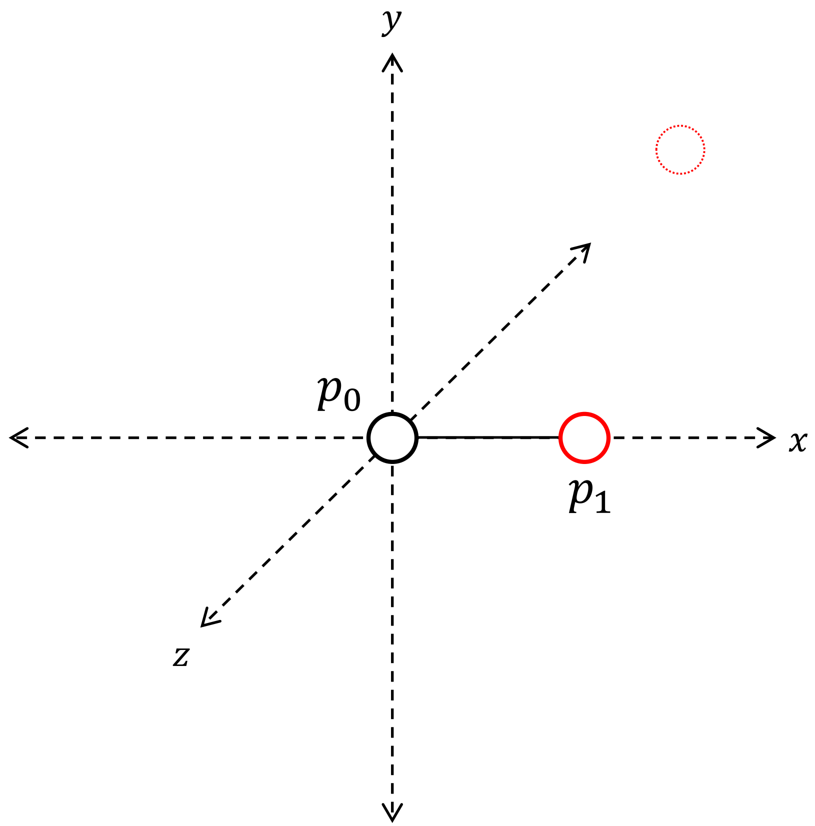
$p_0 = (x_0, y_0, z_0)$



Required Experiments

$p_0 = (x_0, y_0, z_0)$

$p_1 = (x_1, y_0, z_0)$

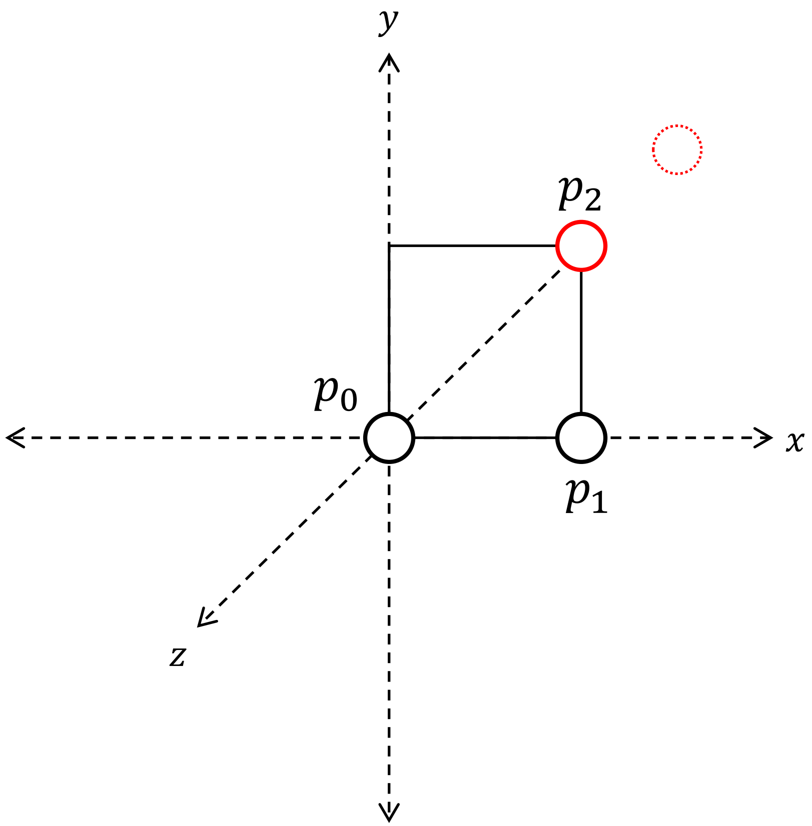


Required Experiments

$p_0 = (x_0, y_0, z_0)$

$p_1 = (x_1, y_0, z_0)$

$p_2 = (x_1, y_1, z_0)$



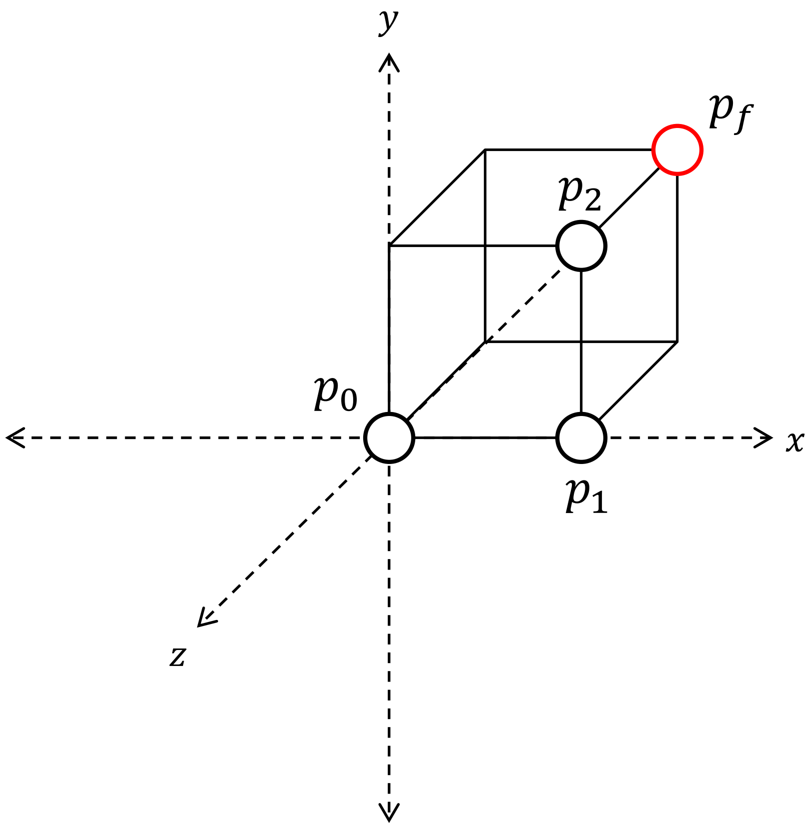
Required Experiments

$p_0 = (x_0, y_0, z_0)$

$p_1 = (x_1, y_0, z_0)$

$p_2 = (x_1, y_1, z_0)$

$p_f = (x_1, y_1, z_1)$

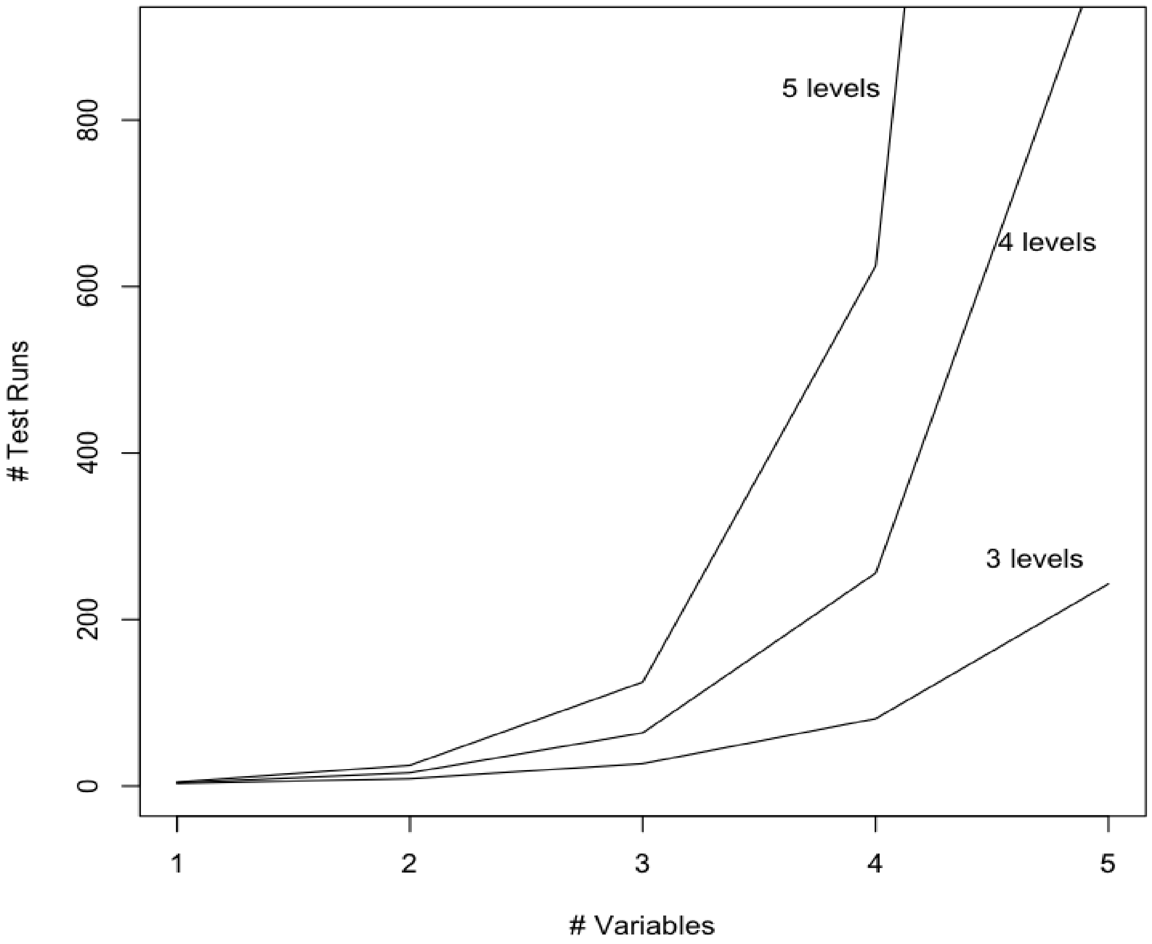


To get to next desired point, p_f:

$$\#\,Tests \approx \#\,Variables$$

p_1 & p_2 may not be desired…

Traditional Design of Experiments*



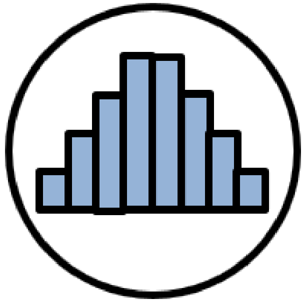
- Brute force approach
- 3-5 increments for each variable
- Exponential increase in test runs as variables increase

How can we maximize value of a practical test campaign?

We must minimize suboptimal experiments!

***Zero Engineering Insight**

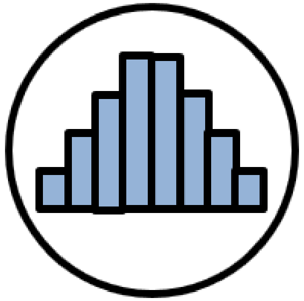
Sequential Experimentation: Optimal Test Conditions



Initially-assumed parameter distributions

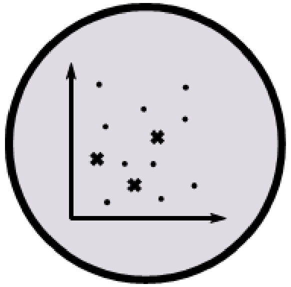
→ G-optimality criterion

Sequential Experimentation: Optimal Test Conditions



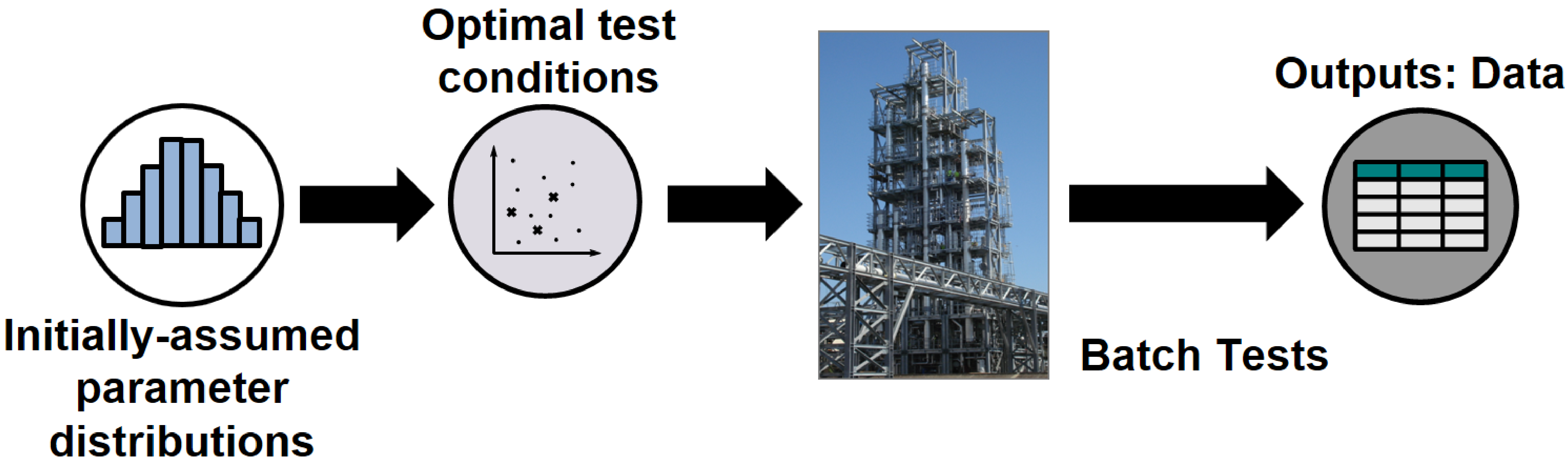
Initially-assumed parameter distributions

Optimal test conditions

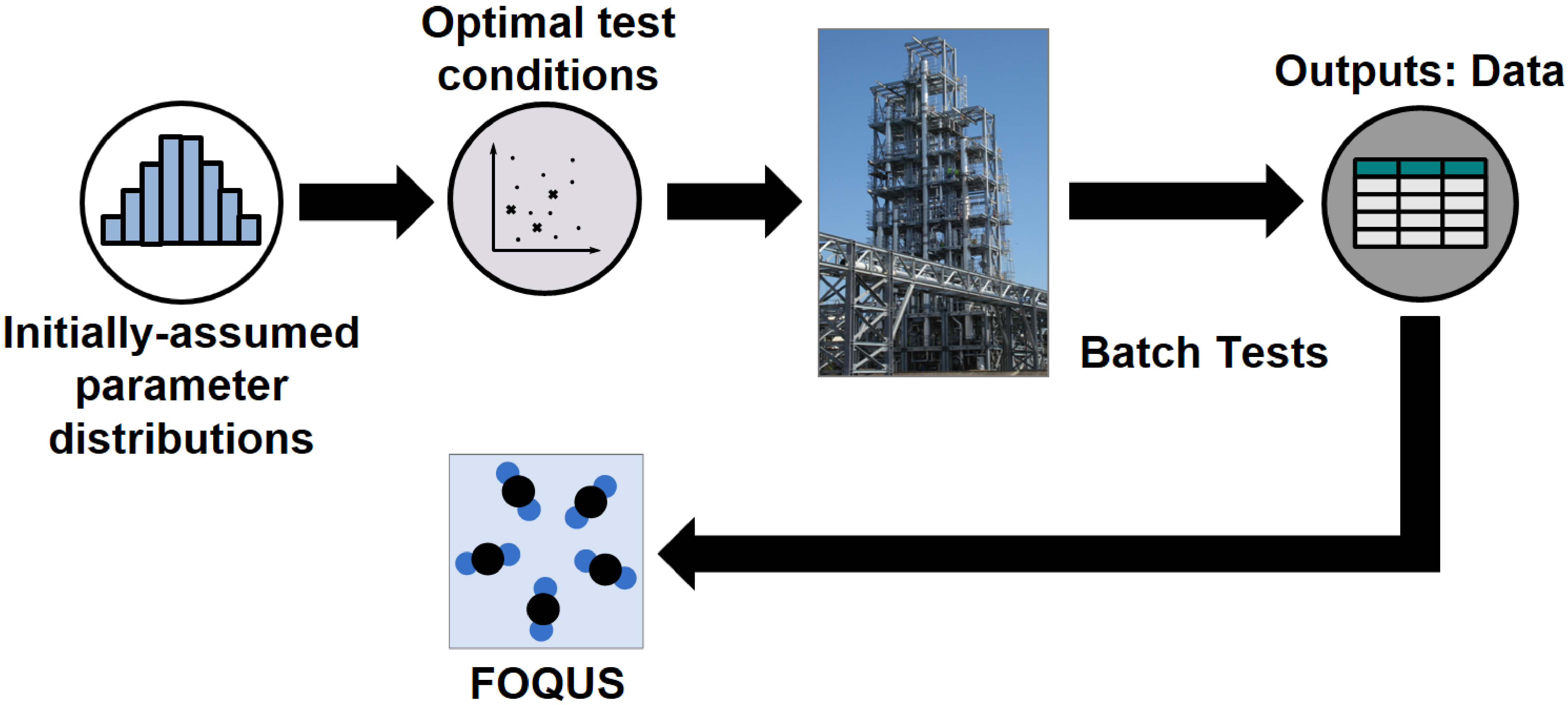


Batch Tests

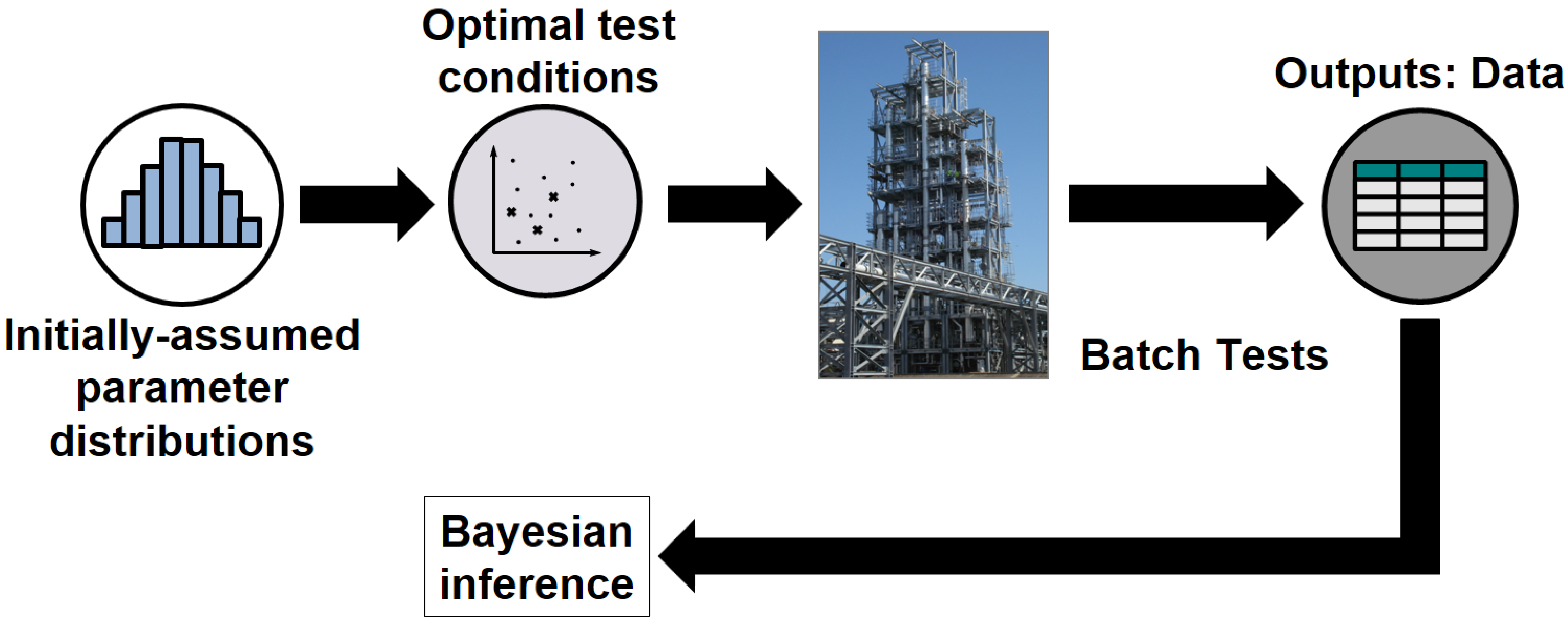
Sequential Experimentation: Optimal Test Conditions



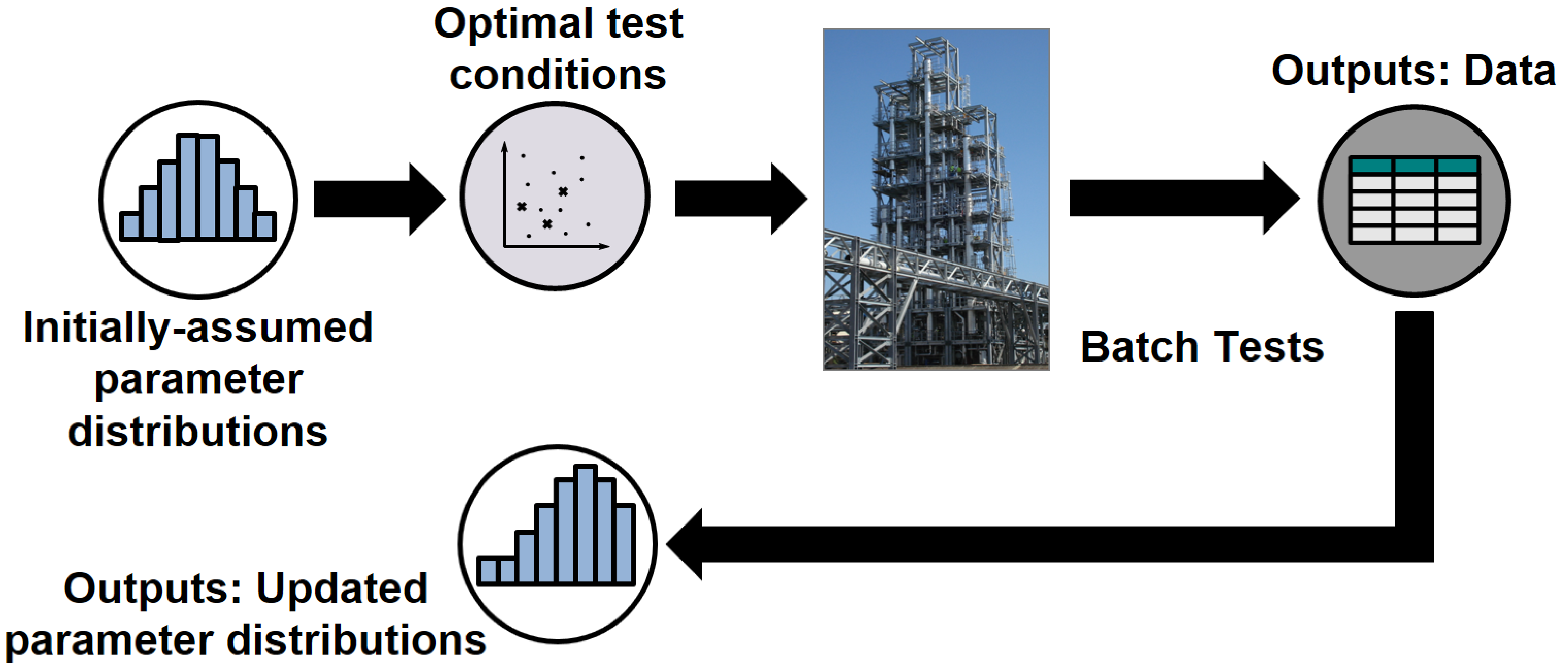
Sequential Experimentation: Optimal Test Conditions



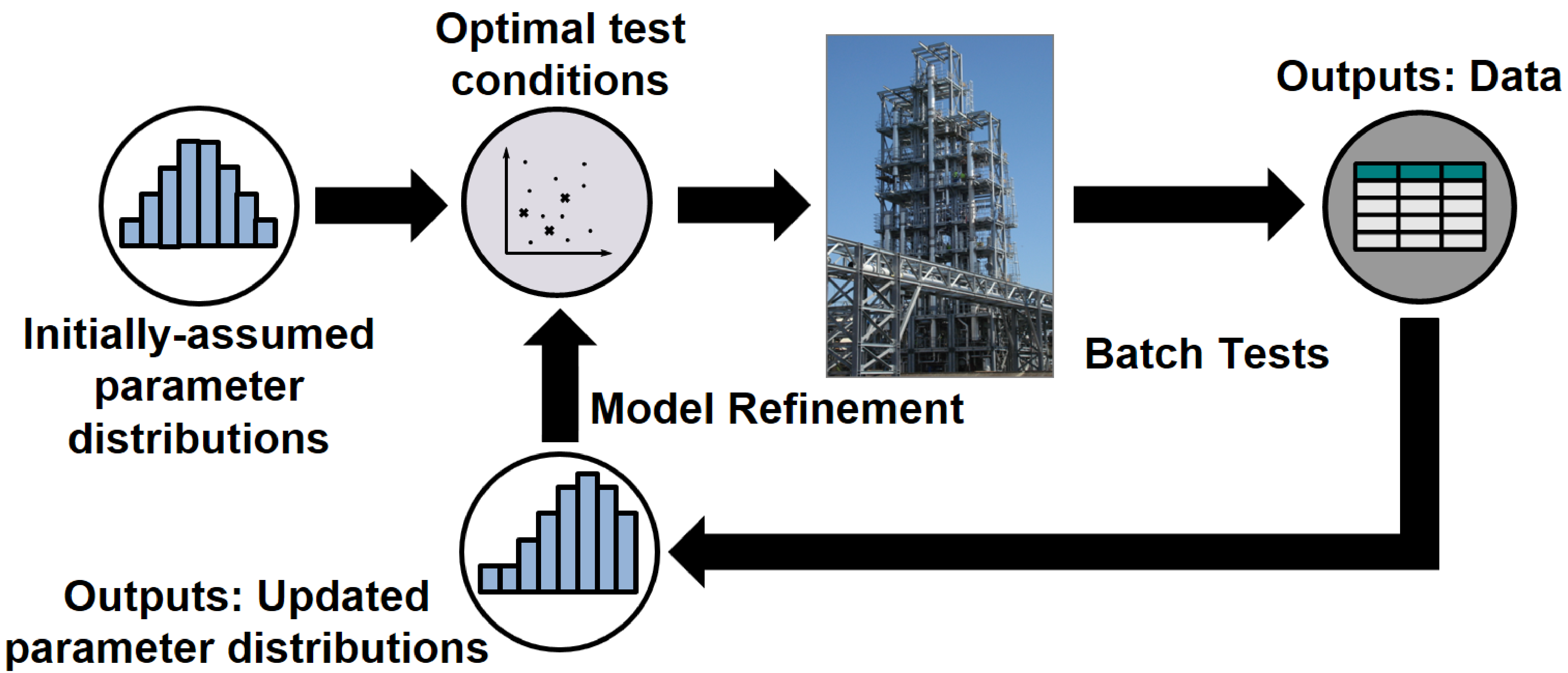
Sequential Experimentation: Optimal Test Conditions



Sequential Experimentation: Optimal Test Conditions

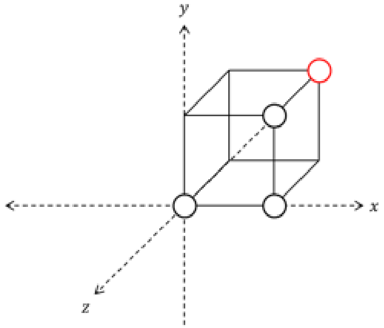


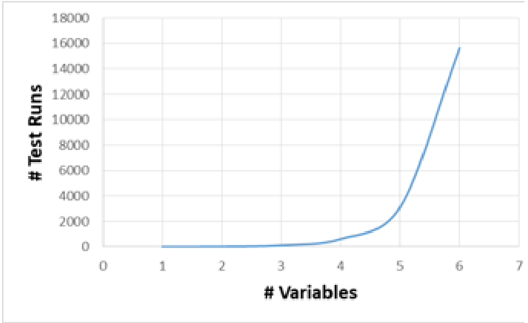
Sequential Experimentation: Optimal Test Conditions



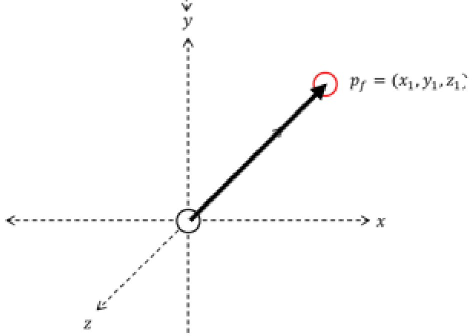
Effective Test Campaigns

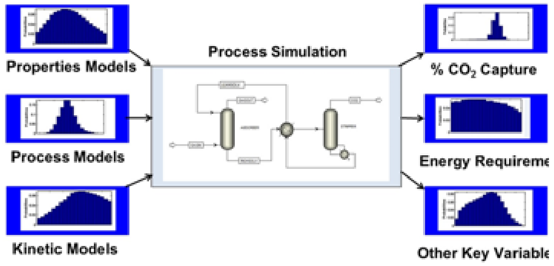
- **Campaign Progression Varying One Dimension at a Time:**
  - INSUFFICIENT



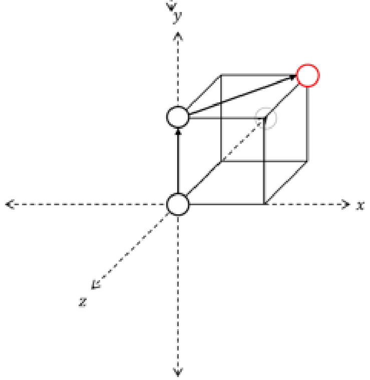


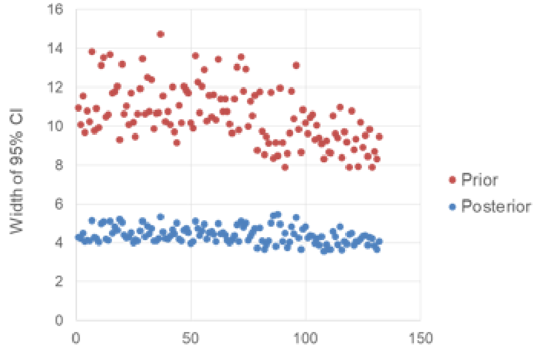
- **Campaign Progression Varying All Dimensions at Once:**
  - Possible with very accurate models/understanding…
  - But Higher Risk with higher dimensions





- **Campaign Progression Varying Multiple Dimensions at a Time:**
  - Practical solution – facility-dependent
  - Less risky with more accurate models – more dimensions possible





Effective Test Campaigns

- **Campaign Progression Varying One Dimension at a Time:**
  – INSUFFICIENT

 # runs = # dim

- **Campaign Progression Varying All Dimensions at Once:**
  – Possible with very accurate models/understanding…
  – But Higher Risk with higher dimensions

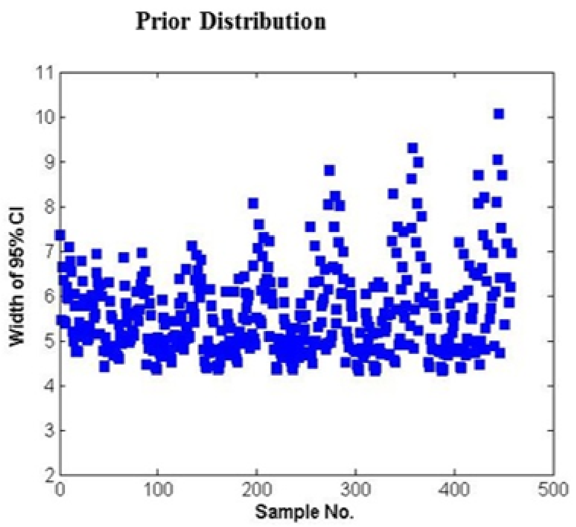
 # runs = 1

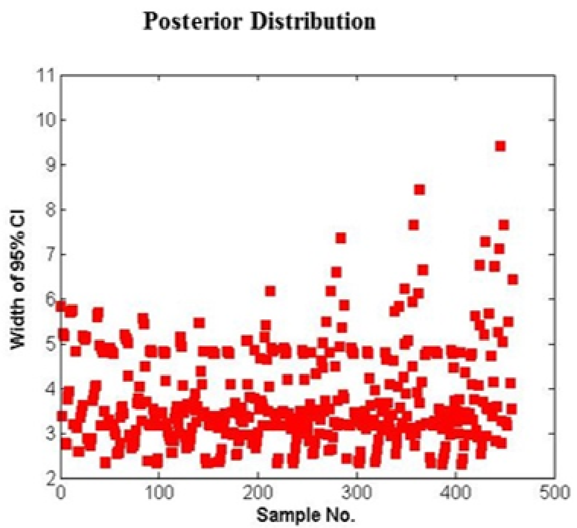
- **Campaign Progression Varying Multiple Dimensions at a Time:**
  – Practical solution – facility-dependent
  – Less risky with more accurate models – more dimensions possible

1 ≤ # runs < # dim

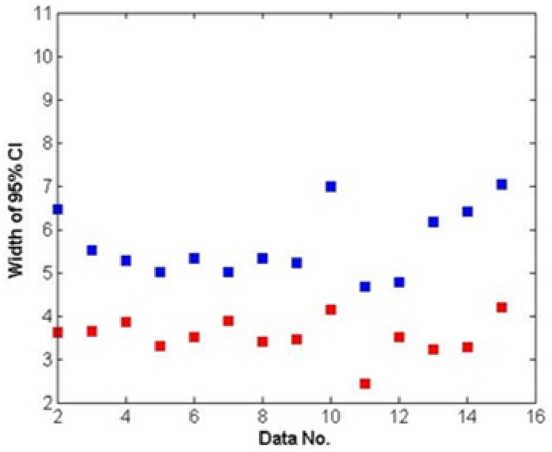
Optimal Design of Experiments: NCCC Trial

Candidate Points



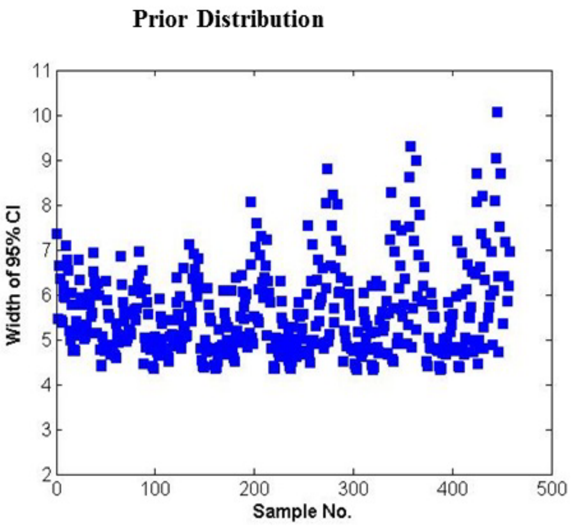


Points with Experimental Data

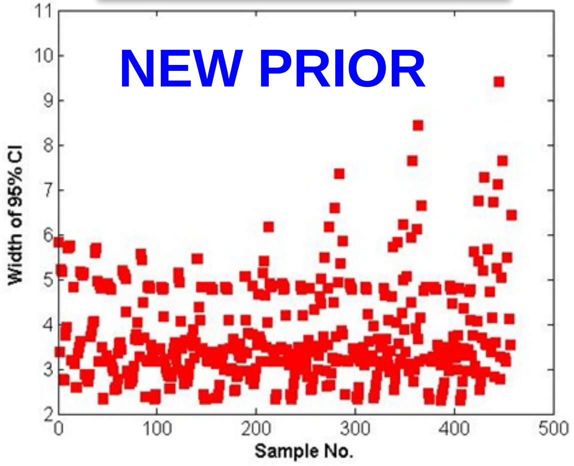


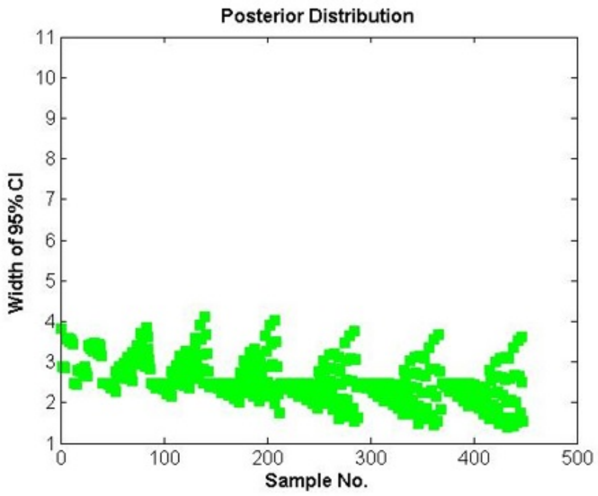
Optimal Design of Experiments: NCCC Trial

Candidate Points

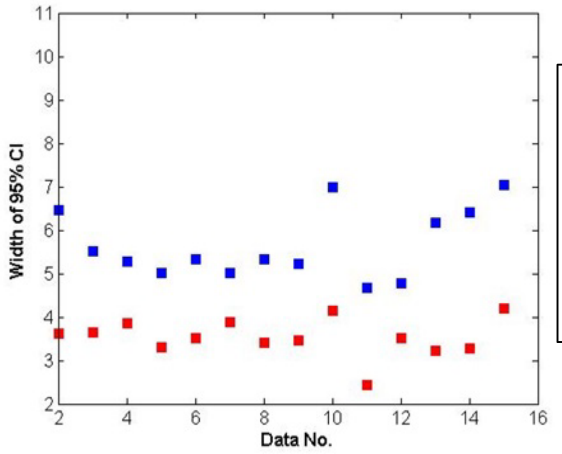


Next iteration

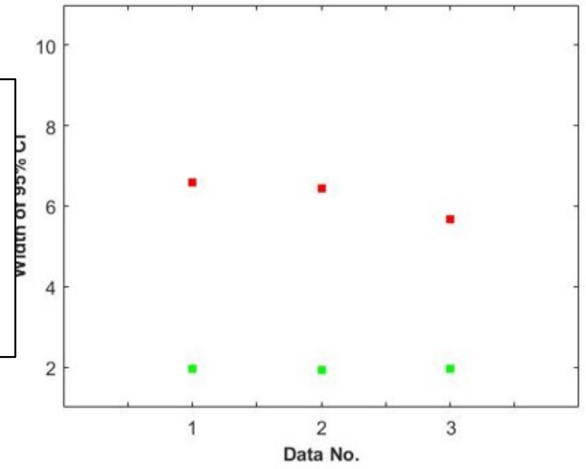




Points with Experimental Data



50-70% Reduction in CO_2 Capture Prediction Uncertainty
(18 total runs)



TCM: Bayesian Inference Continues to Improve Model

Sample No. represents variation in input variables:

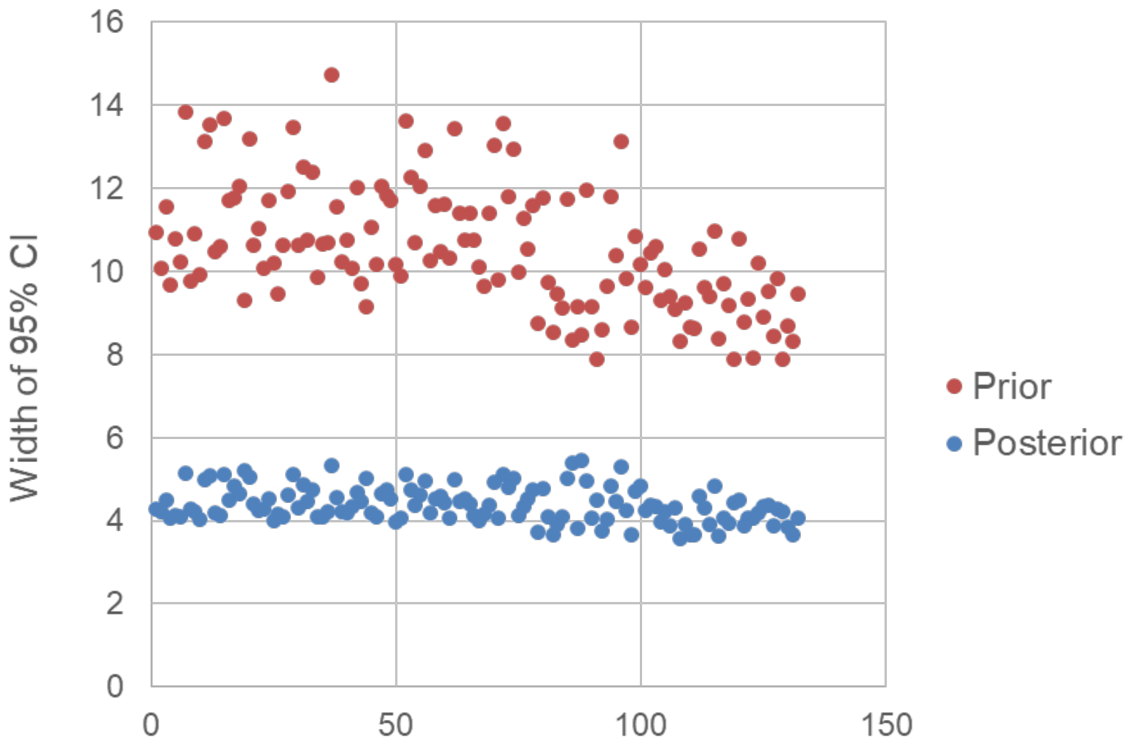
- Liquid Flowrate
- Flue Gas Flowrate
- Lean Loading
- CO_2 Percentage in Flue Gas

Capture Range

- 80-95% CO_2

DoE Results

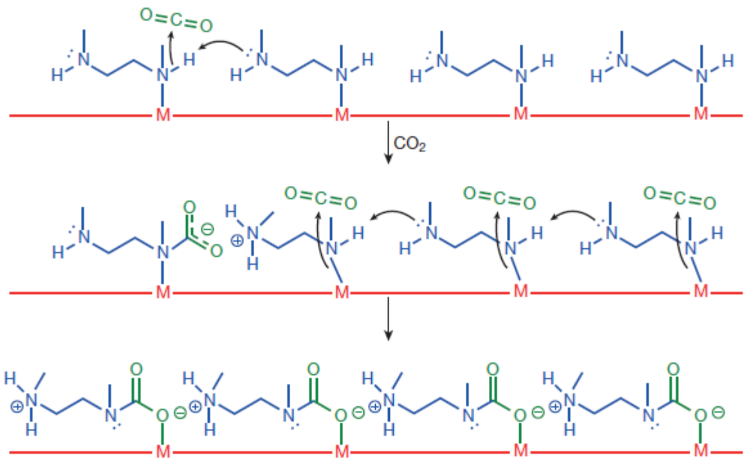
- Precision shown at 2nd iteration – ~2 weeks
- Remaining uncertainty attributed to thermodynamic model

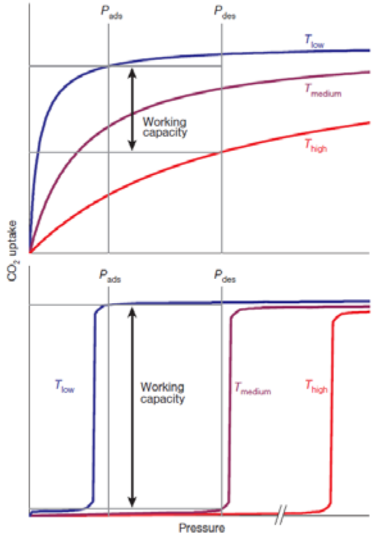


50-70% Reduction in CO_2 Capture Prediction Uncertainty

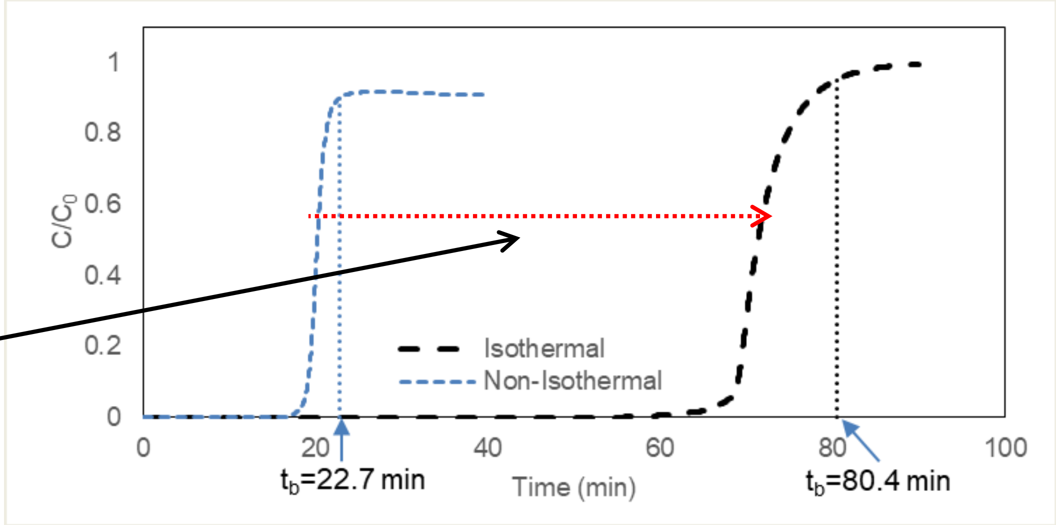
DOCCSS: LBNL Metal Organic Framework

- **Material: Step Isotherm**
  - Amine Functionalization results in cooperative CO_2 adsorption
  - Extremely rapid adsorption – step change in loading
  - Extremely rapid heat liberation



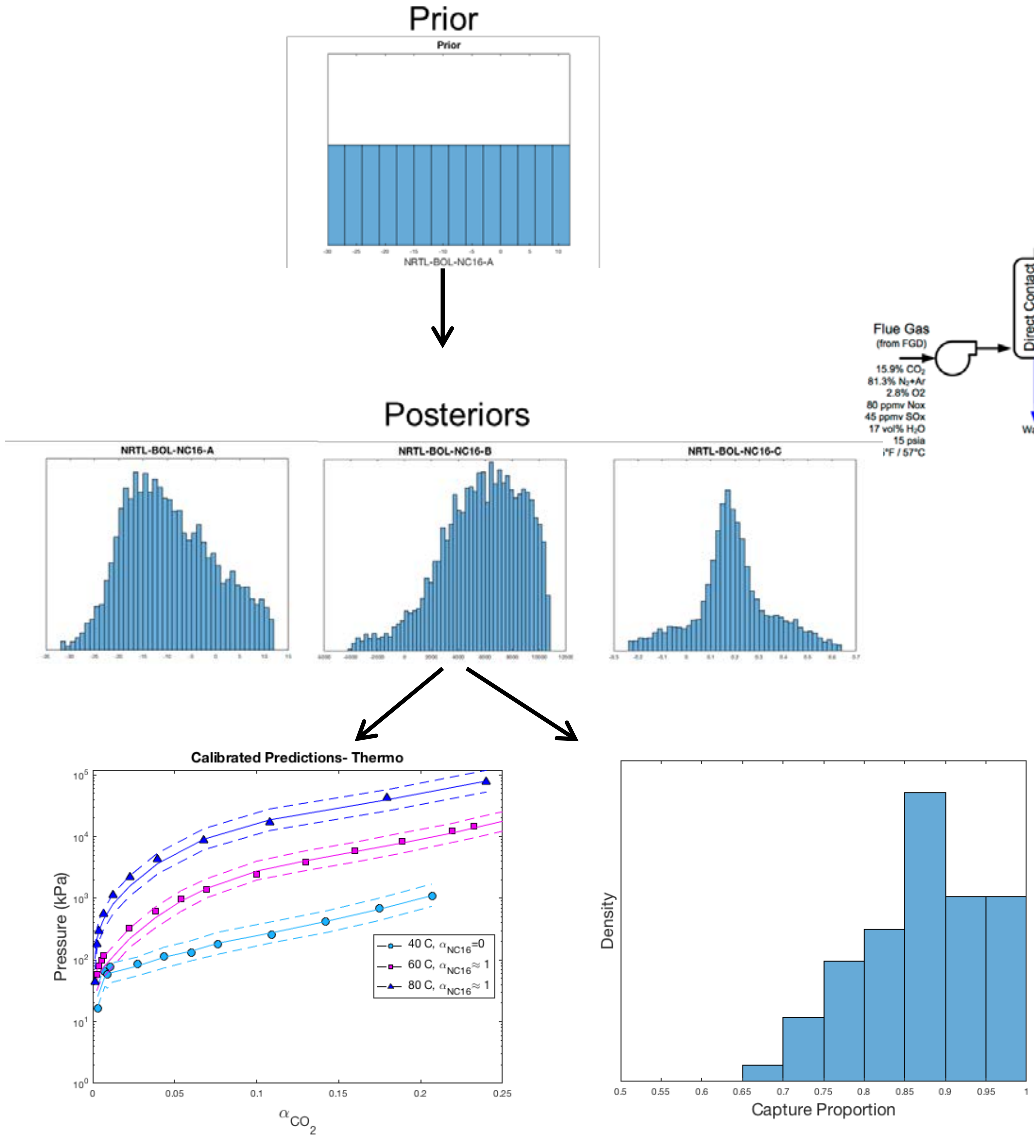


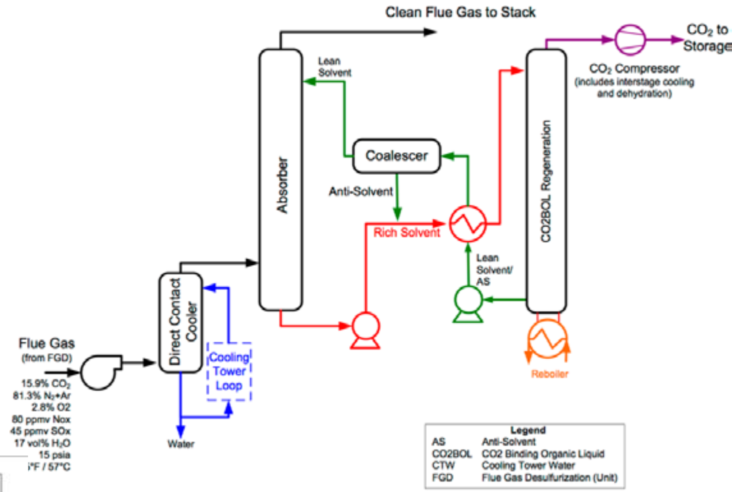
- **Equipment**
  - Heat accumulation undermines performance
  - Bed breakthrough times can be increased by ~4X with ideal design



DOCCSS: PNNL CO_2BOL System Optimization

- **Multi-scale modeling**
  - CO_2BOL Solvent
  - Equipment
  - System
- **Parameter Reduction**
  - 100’s of variables → 41
- **System Analysis**
  - Lost work thermodynamic inefficiency
  - Improvements to novel CO_2BOL system
  - Fully propagated UQ



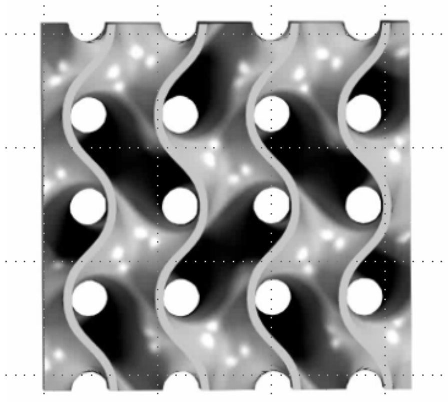


DOCCSS: LLNL Reactor Geometry Optimization

- **Triply Period Minimal Surface Structure (TPMS)**
  - Adjacent, independent, interwoven flow paths
  - Can increase heat transfer per unit surface area per by over 10x

- **CCSI² classifying solvent hydrodynamics**
  - Higher viscosity = more uniform flow path – advantageous for non-aqueous
  - Understanding supports geometry optimization

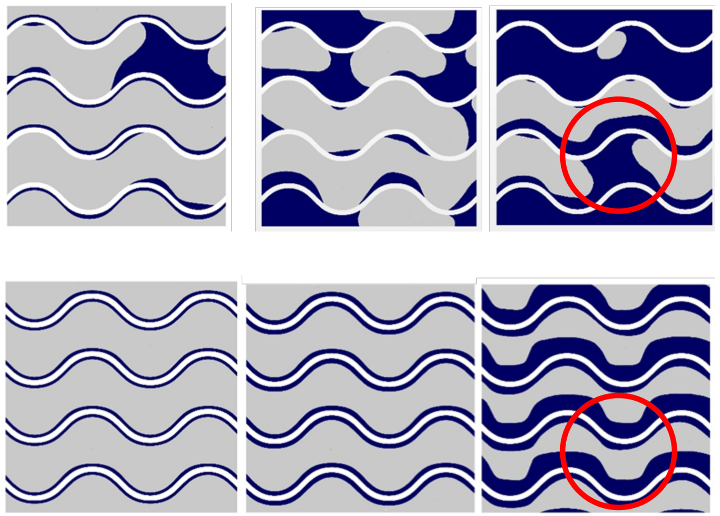
TPMS



$$\sin x \cos y + \sin y \cos z + \sin z \cos x = 0$$

2.5 cP

25 cP



Technology Development Acceleration

- **Many tech development programs incompletely integrated**
    - **Involve sequential steps of experimentation modeling and design relying more on expert judgment than a thorough utilization of available information**
  - **Experimental programs** exploring potential variations in conditions without full analysis of existing information, key data needs
    - inadequate focus on most effective use of time, resources to address key development questions
  - **Modeling programs** based on single best fits to limited data sets. Suboptimal consideration of…
    - All scales of available data for models from fundamental scale to fully integrated plant design
    - Best collection of data for creation of most accurate model,
    - Ranges of possible values of fitting model parameters,
    - Uncertainty analysis of predictions,
    - Identification of most critical gaps to reduce uncertainty
  - **Design** typically limited by…
    - Using a few isolated process conditions gleaned from limited experimental datasets
    - Focused on high-performance steady state conditions
      - Poor ability to understand process startup, shutdowns, dynamics and control issues essential for optimize full design for all anticipated operating conditions
  - **Optimizations** typically done by varying conditions around a presumed satisfactory base design condition.

Fully Integrated Modeling Experimentation Design and Optimization

- **Models created from full utilization of available data**
  - at all scales; validated against all available data
- **Uncertainty quantification integral to model creation**
  - utilized to inform best choices of experimental program to reduce uncertainty, expand predictive ability, focus on key design and optimization features
- **Experimental plans based on best use of prior data**,
  - Enables best choice of experimental program to reduce key model uncertainties, enable design and optimization
- **Designs based on complete evaluation of potential variables, prediction of ranges of potential design choices;**
  - **key uncertainties quantified**
- **Optimizations based on more complete understanding of design options** and varying conditions of operation, enables advanced process control.

CCSI2 applies this approach to carbon capture technology development.

-Toolset contains the essential components to apply to other tech developments.

This Meeting – Examples of CCSI2 "FIMEDO" Approach

- CCSI Toolset developed in collaboration with large group of tech development partners.
- Now being applied to broad range of Carbon Capture Tech Development projects
  - From low-TRL programs to answer key questions sooner
  - To Large Scale Demonstrations (UT, UKy, NCCC, TCM) to focus high-cost test programs on most valuable information to enable next scale design optimization and experimentation.

Approach applicable to many capture technology developments

- Includes "Gold Standard" models for multiple capture technologies

Toolset provides key components to enable application far beyond capture

- You'll need to build your own models
- Toolset provides UQ, Integration, Optimization, Iteration capabilities

CCSI²

Carbon Capture Simulation for Industry Impact

For more information:
https://www.acceleratecarboncapture.org/

For Toolset:
github.com/CCSI-Toolset

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