Carbon Capture Simulation for Industry Impact

Sequential Design of Experiments: Capabilities, Progress, and Applications

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Today's Plan

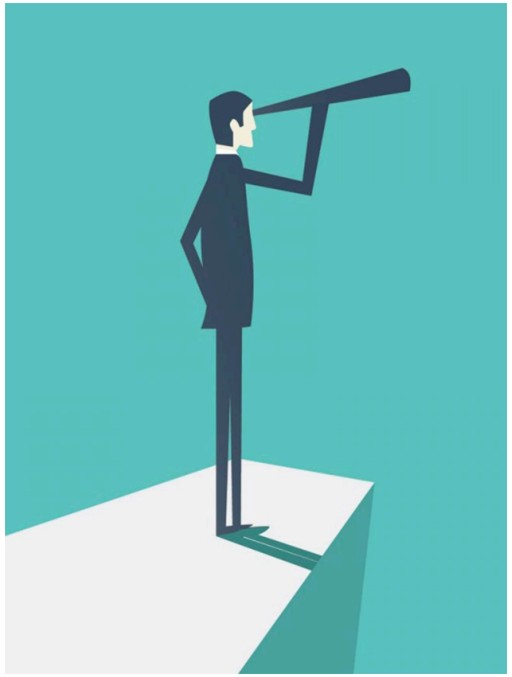
- **SDoE overview: range of SDoE methodologies to support multiple objectives – available in CCSI^2 Toolset**

- **New and in progress additions to CCSI^2 SDoE Toolset**
  - Added capabilities for increased flexibility
  - Targeted problem-solving

- **Applications: SDoE support for scale-up testing of carbon capture technology**

DoE Overview

- **Strategy for selecting input combinations**
  - Compute output (computer experiment)
  - Operate system (physical experiment)
- **Range of inputs form region of interest**
- **Selected inputs form design**

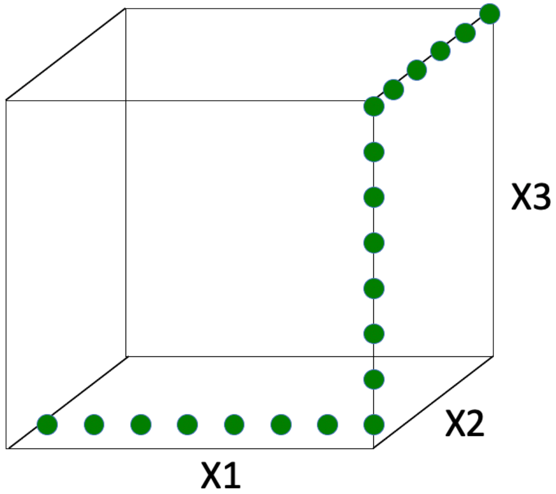


- **DoE produces exceptionally high-quality data**
  - Leads to improved understanding, decision-making, confidence

Design of Experiments not the same as One-Factor-at-a-Time

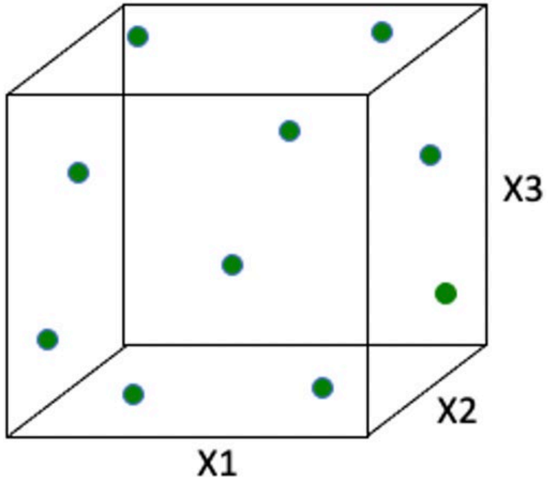
- **In the OFAAT strategy, the experimenter changes only one input (factor) at a time, while all other inputs are held constant**

- **OFAAT approach has drawbacks**



  - Inefficient use of budget
  - Cannot identify interactions
  - Not randomized

DoE avoids these drawbacks



Why a statistically designed experiment (DoE)?

- **Extract maximum information with a fixed budget**
  - Produces exceptionally high-quality data
- **Can save years off of pilot test schedule**
- **Proven track record from past applications**
  - Over 25% reduction in model uncertainty
  - CO_2 Capture percentage within 3-6% with 95% confidence

Why Sequential DoE?

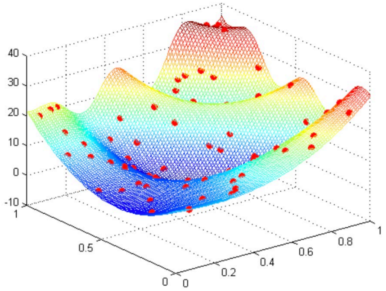
SDoE: directly incorporate knowledge learned in previous stages
Result: strategic data collection across multiple stages

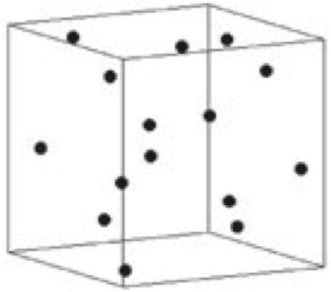
Feasibility study → Exploration of input space → Model building / refinement → Optimization → Confirmation

Feasibility study	Exploration of input space	Model building / refinement	Optimization	Confirmation
Is it possible to collect quality data? Proof of concept	Understand basic relationship between inputs and responses	Verify that the model captures patterns Add data for better model parameter estimation or prediction	Focus on region of maximum interest Close to most desirable operation conditions	Verify results for production or operational use Ability to duplicate results

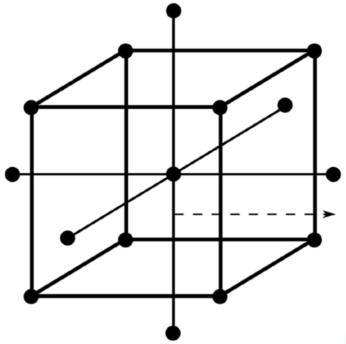
Range of strategies provides flexibility

- **Space-filling designs:**
  - Useful when relationship between inputs and response(s) of interest not well understood
  - Good precision for predicting new results at any new location





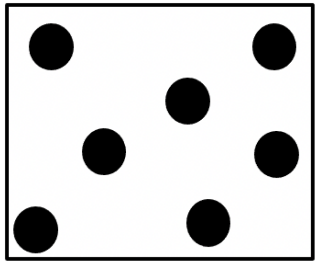
- **Model-based designs:**
  - Can specify correct form for model of interest to characterize relationship between inputs and response(s)
  - Relationship can be well approximated by a low-order polynomial

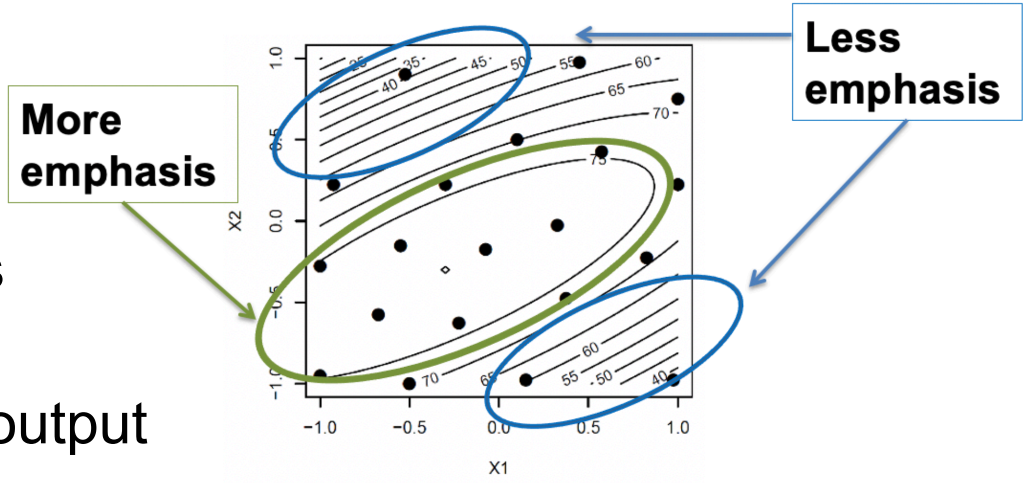


- **CCSI² Toolset supports both approaches**

CCSI² Space-Filling Design Capabilities

1. **Uniform Space-Filling (USF)**
   - Design points are evenly spread throughout space of interest
   - Collect information throughout region
2. **Non-Uniform Space-Filling (NUSF)**
   - Design points still spread out
   - Emphasize some regions more than others
   - For more in-depth exploration of certain areas
3. **Input Response Space-Filling (IRSF)**
   - Used when information is known about likely output values
   - Select design points likely to results in good distribution of output values
   - Balance with good space-filling properties in input space





***Recent additions: New/enhanced functionality for all 3 methods**

CCSI² Model-Based Design Capabilities

Robust Optimally-Based Design of Experiments (ODoE)

- Construct designs based on empirically fit models
- Choose desired mathematical optimality criterion for design construction (based on assumptions about the problem)

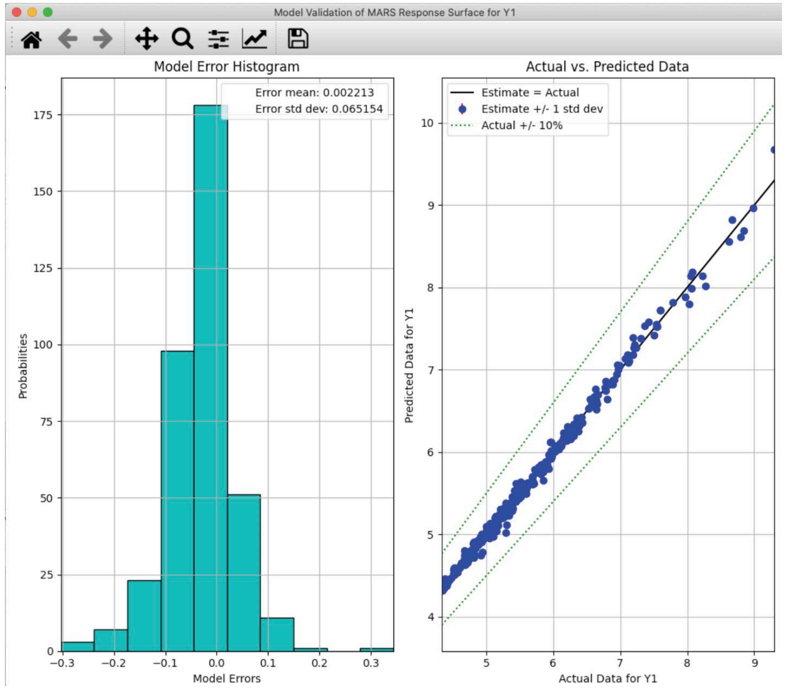
– D-optimal
– A-optimal
– E-optimal

Focus: Parameter estimation

*Recent addition

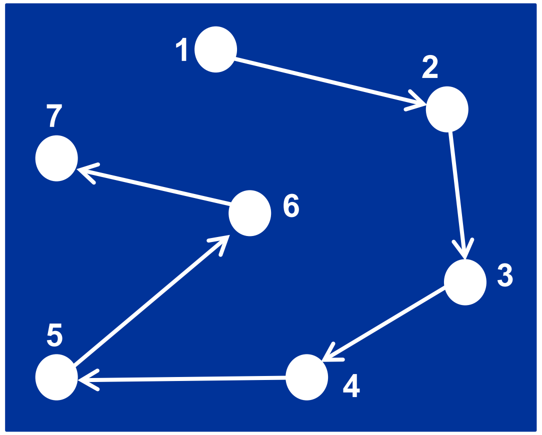
– G-optimal
– I-optimal

Focus: Response prediction

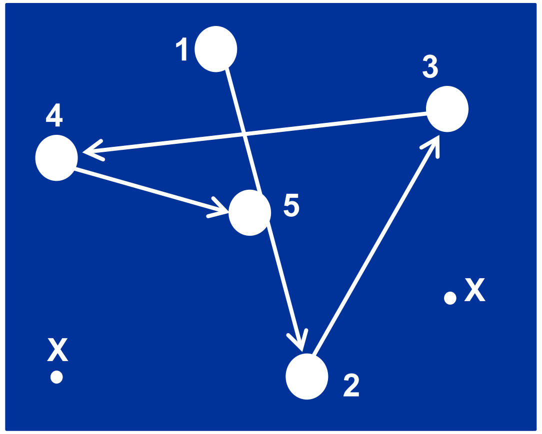


Other Capabilities

- **Design ordering algorithm:**
  - Orders the experimental runs
  - Improves efficiency of operations
- **Missing value imputation**
  - Estimates values for missing weights (NUSF) or missing response values (IRSF) in the candidate set
  - Fully utilize all candidate set points
- **Graphical tools for design evaluation and comparison**
  - Facilitates comparison among design options
  - Allows users to quickly assess design coverage and properties



Ordered



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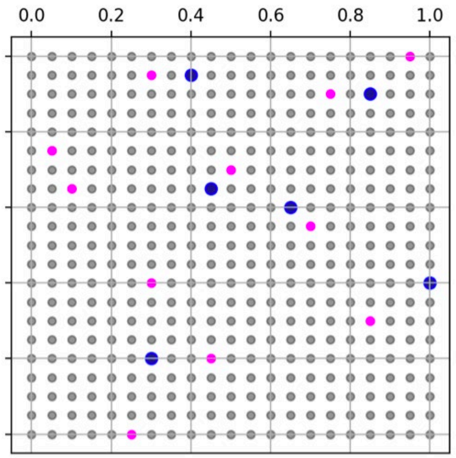
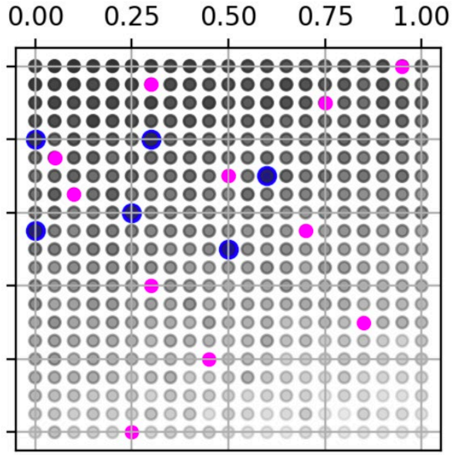


MRW = 1



MRW = 10

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SDoE Support Tools

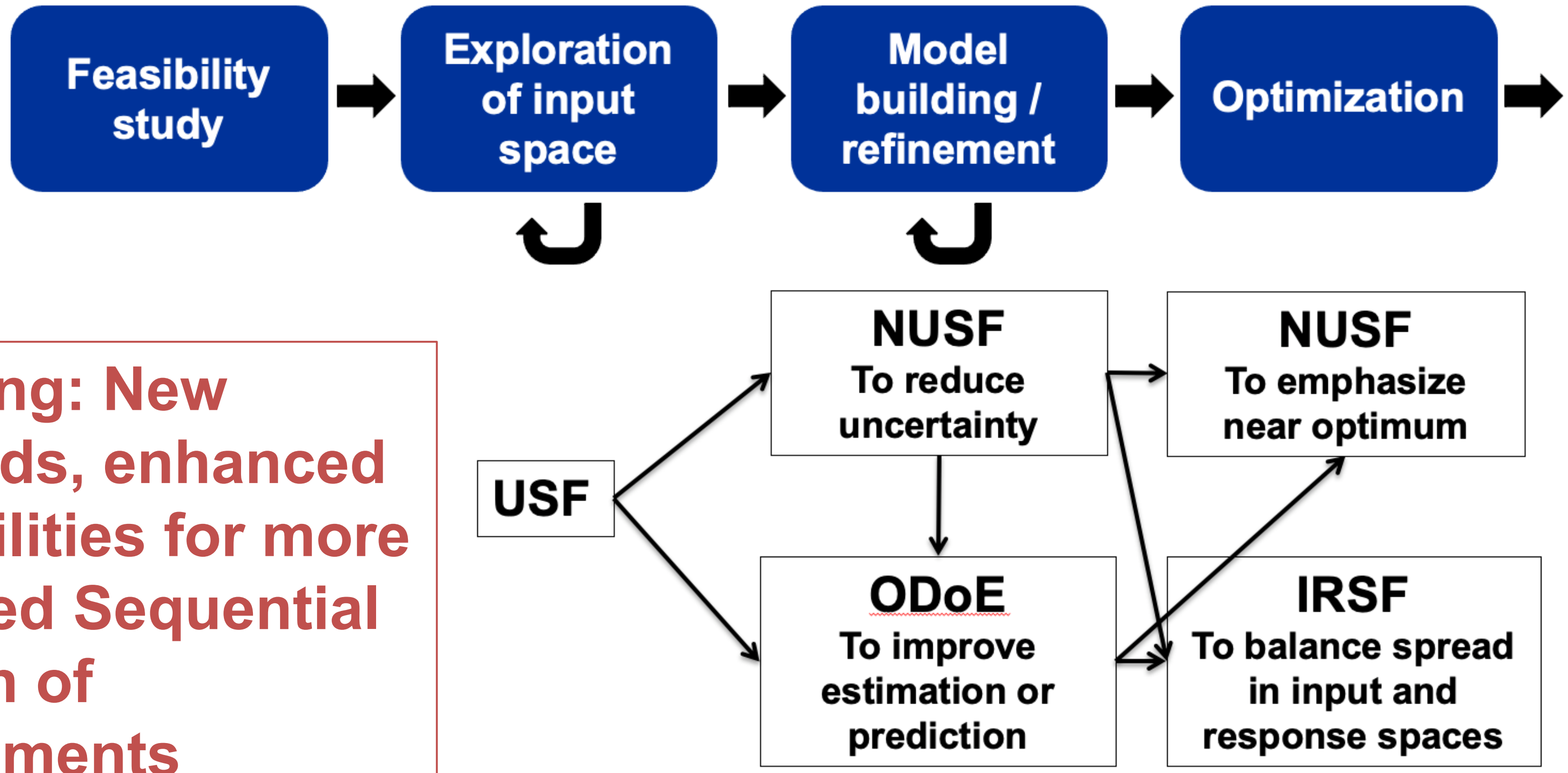
Recently added support tools for improved user experience

- **Series of tutorial videos to guide users through SDoE process and demonstrate module capabilities**
- **In total, over 75 minutes of detailed SDoE guidance**

	First Phase	Sequential
Uniform Space-Filling (USF)	✓	✓
Non-Uniform Space-Filling (NUSF)	✓	✓
Input-Response Space-Filling (IRSF)	✓	✓

One continuous example – can be watched individually

Build a sequence that works for each experiment



Ongoing: New methods, enhanced capabilities for more targeted Sequential Design of Experiments problem solving

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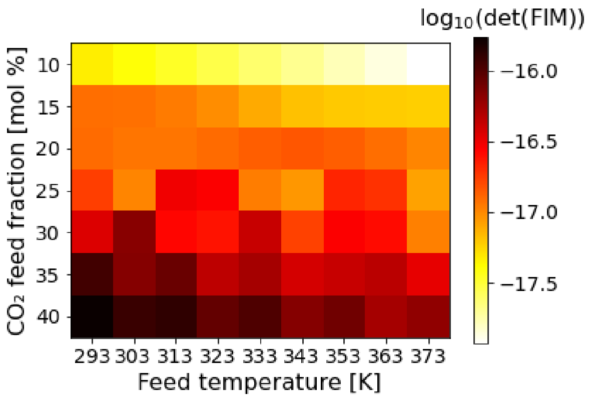
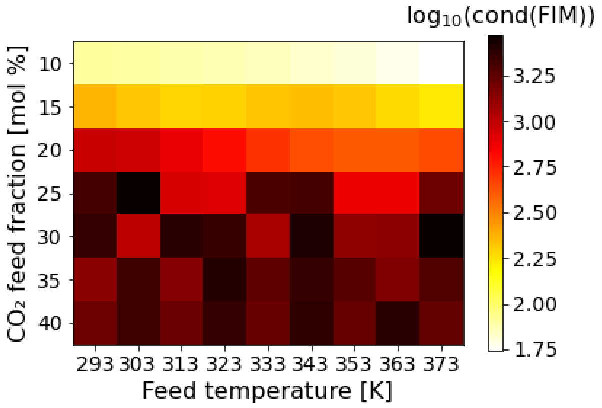
New Capability: Science Model-Based Design of Experiments

- **Main Idea:** use full model equations <u>directly</u> to optimizing experimental campaigns to improve parameter estimates
  - Avoids need to build/validate surrogates
  - Discriminate between alternative mechanistic models
  - Requires access to equations (e.g., Pyomo)

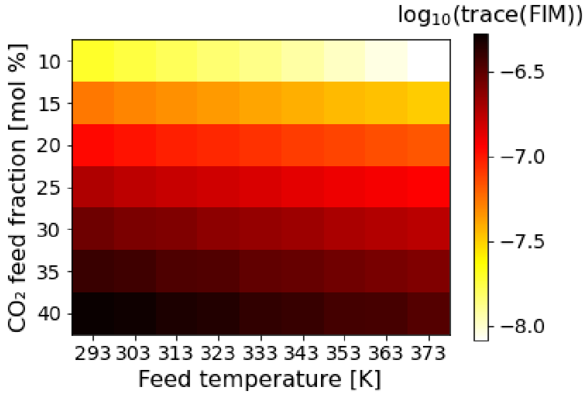
- **Example:** What is the optimal CO_2 feed composition and feed temperature for next Metal Organic Framework MOF fixed bed experiment?



D-optimality



A-optimality



E-optimality

Darker regions indicate choices that lead to greater improvement in parameter estimation criterion

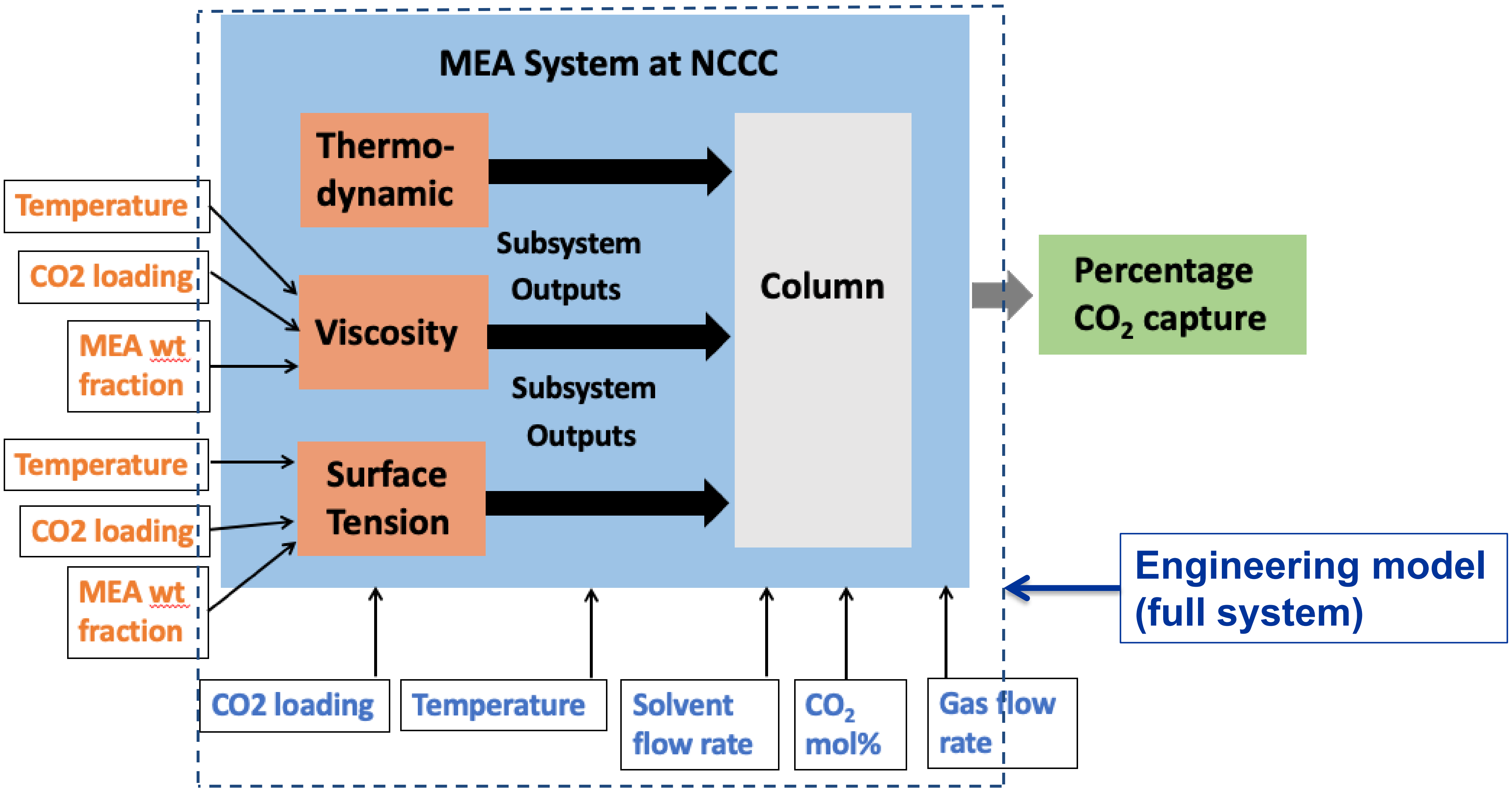
New Capability: Science Model-Based Design of Experiments

- **Developed an MBDoE package in Python called Pyomo.DOE**
  - Combines Pyomo.DAE to solve dynamic problems (e.g. DAE and PDE)

- **Pyomo.DOE automatically formulate and solve MBDoE problems**
  - Does not require user to have extensive DoE expertise

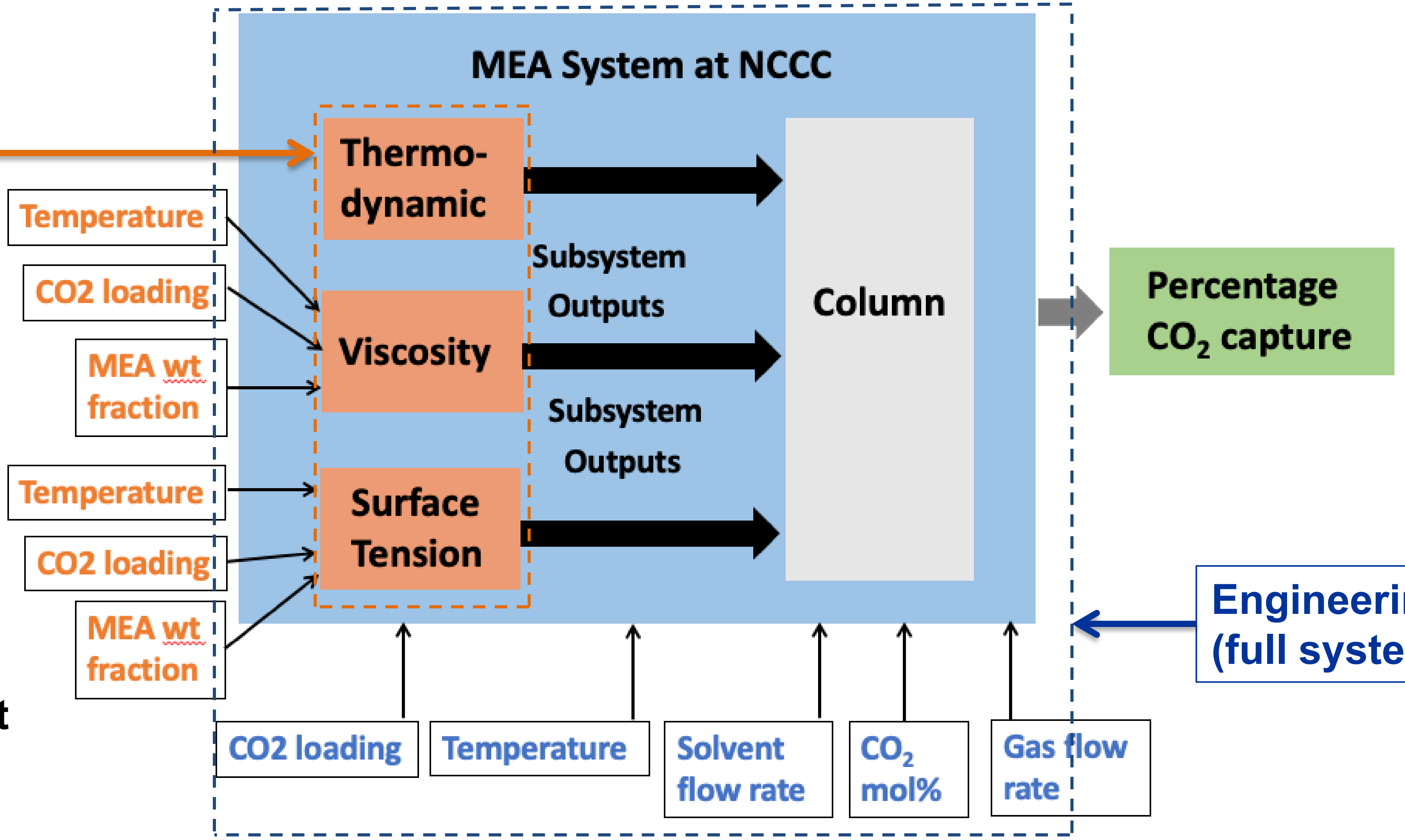
- **Demonstrated Pyomo.DOE package and method to optimize fixed-bed breakthrough experiments for Metal Organic Framework (MOF) sorbent characterization**

Under Development: Design for multi-level conglomerate models



Under Development: Design for multi-level conglomerate models

Fundamental science models (sub system)



Subsystems can be operated, studied separately

Goal: **Best prediction throughout input space of NCCC system model**

Engineering model (full system)

How to plan an experiment using available budget?
Different approaches; different associated costs and utility

Other possibilities?

Approach 1: Full system tests

Approach 2: Subsystem tests

Higher cost
(Fewer tests)
Collect data to inform system response directly

Lower cost
(More tests)
Collect subsystem info to inform system response

How to plan an experiment using available budget? Different approaches; different associated costs and utility

Partition total available budget
- Some full system tests
- Some subsystem tests
- Likely unequal split

Approach 1: Full system tests

Approach 2: Subsystem tests

Higher cost (Fewer tests)

Lower cost (More tests)

Example:
- 30% available budget for full system
- Divide remainder among sub systems

Most efficient partitioning?
✓ Use DoE to answer

Under Development: Design of Experiments for Conglomerate Models

Using MEA system model case study

- ✓ Develop methodology for resource allocation decisions for engineering models within a first stage experiment
- ✓ Demonstrate with case study
- ✓ Enhancements to methodology for wider application

Approach 1: Full system tests

Approach 2: Subsystem tests

Higher cost
(Fewer tests)

Lower cost
(More tests)

Under Development: Space Filling Designs for Hard-to-Change Factors

Motivation: Operating constraints encountered by industry partners

- **Some factors are hard-to-change – take a long time to change**

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No factors are hard to change

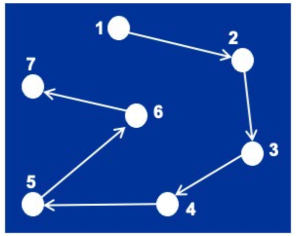
All factors are hard to change

Use a completely randomized design

- **DoE gold standard**

Use design ordering algorithm in CCSI² toolset

- **Trade-off**
- **Lose DoE advantages associated with randomization**



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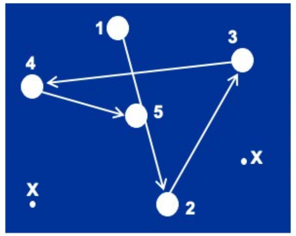

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Under Development: Space Filling Designs for Hard-to-Change Factors

No factors are hard to change

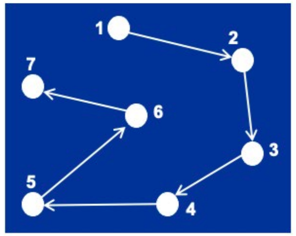
Only certain factors are hard to change

All factors are hard to change

Use a completely randomized design
- **DoE gold standard**

Need a third approach: Designs for Hard-to-Change Factors
- **Directly account for operating constraints**
- **Middle ground: retain as much randomization as possible**

Use design ordering algorithm in CCSI² toolset
- **Trade-off**
- **Lose DoE advantages associated with randomization**



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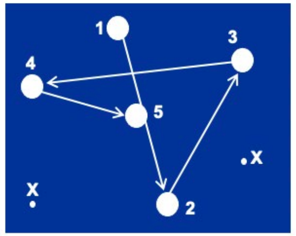


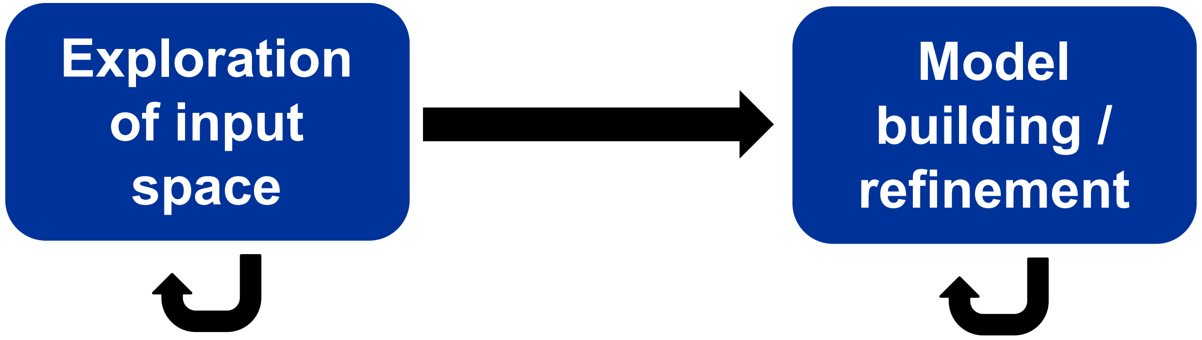
Unordered

CCSI²
Carbon Capture Simulation for Industry Impact

Applications: MTR Field Test at TCM

- CCSI^2 supported MTR's engineering-scale advanced membrane field test at the Technology Centre Mongstad (TCM) (DE-FE0031591)
- Test objective: Identify optimum operating conditions for CO_2 capture rates from 50 – 90%
- 4 inputs
  - Flue gas flowrate
  - Sweep air flowrate
  - Temperature
  - Recycle stream flowrate
- Budget: 25 – 35 experimental runs
  - Depends on time per run

CCSI² Team leveraged SDoE tools to make the most of the experimental budget – Learn as we go, increase efficacy



	Phase 1	Phase 2	Phase 3
Primary Objective: **Optimization**	Method: **USF** Budget allocation: **10 runs**	Method: **Sequential USF to refine exploration of input space** Budget allocation: **5 runs**	Method: **Sequential NUSF to reduce uncertainty** Budget allocation: **Remaining available**

Field test completed March 2022

Applications: RTI Test Campaign at TCM

- **Ongoing test campaign at TCM for RTI NAS solvent system**
  - Start date: February 2022
- **CCSI^2 team contributed separate designed experiments for two sets of conditions**
  - Gas-fired combined heat and power (CHP)
  - Residual fluidized catalytic cracker (RFCC) flue gas sources
- **Each designed experiment includes a series of designs ranging in size from 12-22 to account for flexibility in budget**
  - Designs increase sequentially, so only 1 new run is added at a time to allow for flexibility

Applications: RTI Test Campaign at TCM

- **Design factors of interest and their ranges**
  - CO_2 Capture: 85 - 95%
  - Absorber L/G Ratio: 3.5 – 6.0 kg/sm^3
  - Stripper Pressure: 0.9 – 3.2 barg
- **Objective: model refinement and validation**
  - Development and improvement of thermodynamics and other sub-models of NAS solvent system, followed by validation of process models for TCM (12 MWe) and Tiller (60 MWe) pilot plant facilities
- **SDoE provides tools for strategic data collection to support objectives**
  - USF for initial exploration
  - Sequential NUSF for targeted model refinement and validation

Additional Ongoing and Future Applications

- **CCSI[2] teams leverage advantages of SDoE methods across applications ranging from lab scale to bench scale to pilot scale**

- **Ongoing and future SDoE work to support applications in**

  - **Membrane modeling**
  - **Metal Organic Framework (MOF) Sorbent Materials**
  - **CO_2 Absorber Intensification Prototyping and Experimentation**

- **Enables strategic data collection at every stage of the process to scale up technologies**
  - Reduce risk; increase confidence in results

Recap

- **Capabilities: Range of SDoE tools to support multiple objectives; available to everyone**
  - Uniform Space-Filling Designs
  - Non-Uniform Space-Filling Designs
  - Input Response Space-Filling Designs
  - Model-based Optimal Design of Experiments
- **Progress: New and developing capabilities for more targeted problem solving**
  - Science-based Design of Experiments
  - DoE for Conglomerate Models
  - Space-Filling Designs for Hard-to-Change Factors
- **Applications: CCSI^2 collaborations supporting Design of Experiments**
  - MTR, RTI, MOF

Questions?

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CCSI^2

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For more information

https://www.acceleratecarboncapture.org/

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