OPTIMIZATION OF CO_2 CAPTURE SIMULATIONS

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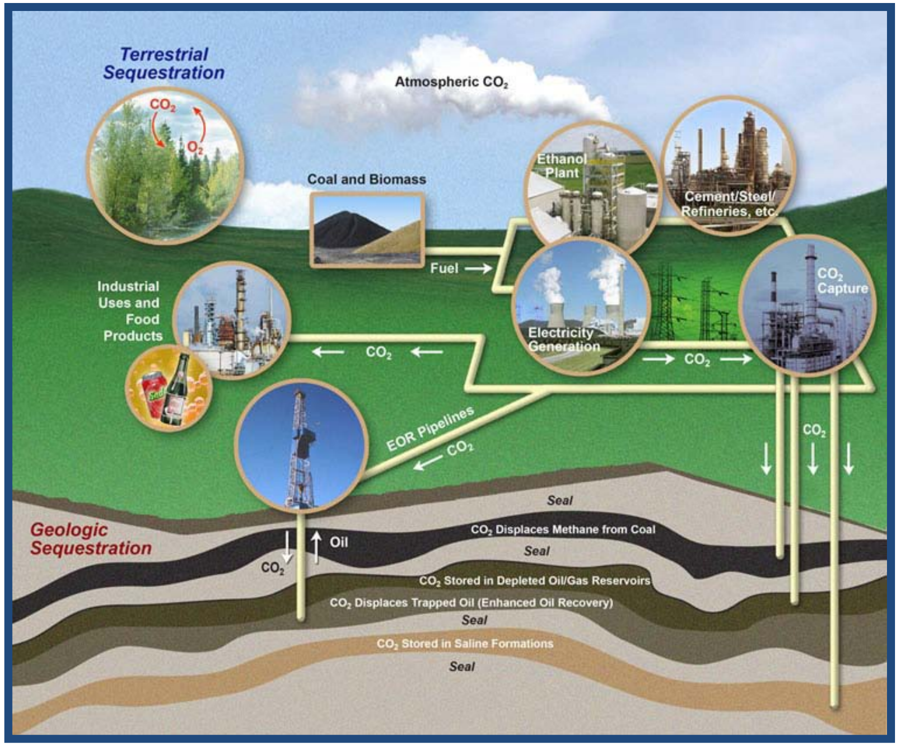
MOTIVATION

- **One-third of U.S. CO_2 emissions come from power plants and other point sources**

- **Available carbon capture technologies would increase electricity costs**
  - **Pulverized coal plants**
    - ***Currently: 75% increase***
    - ***Goal: <30% increase***



http://www.netl.doe.gov/technologies/carbon_seq/index.html

OVERVIEW

1. **Carbon capture process**
2. **Method overview**
3. **Surrogate model generation**
4. **Preliminary results**
5. **Conclusions**

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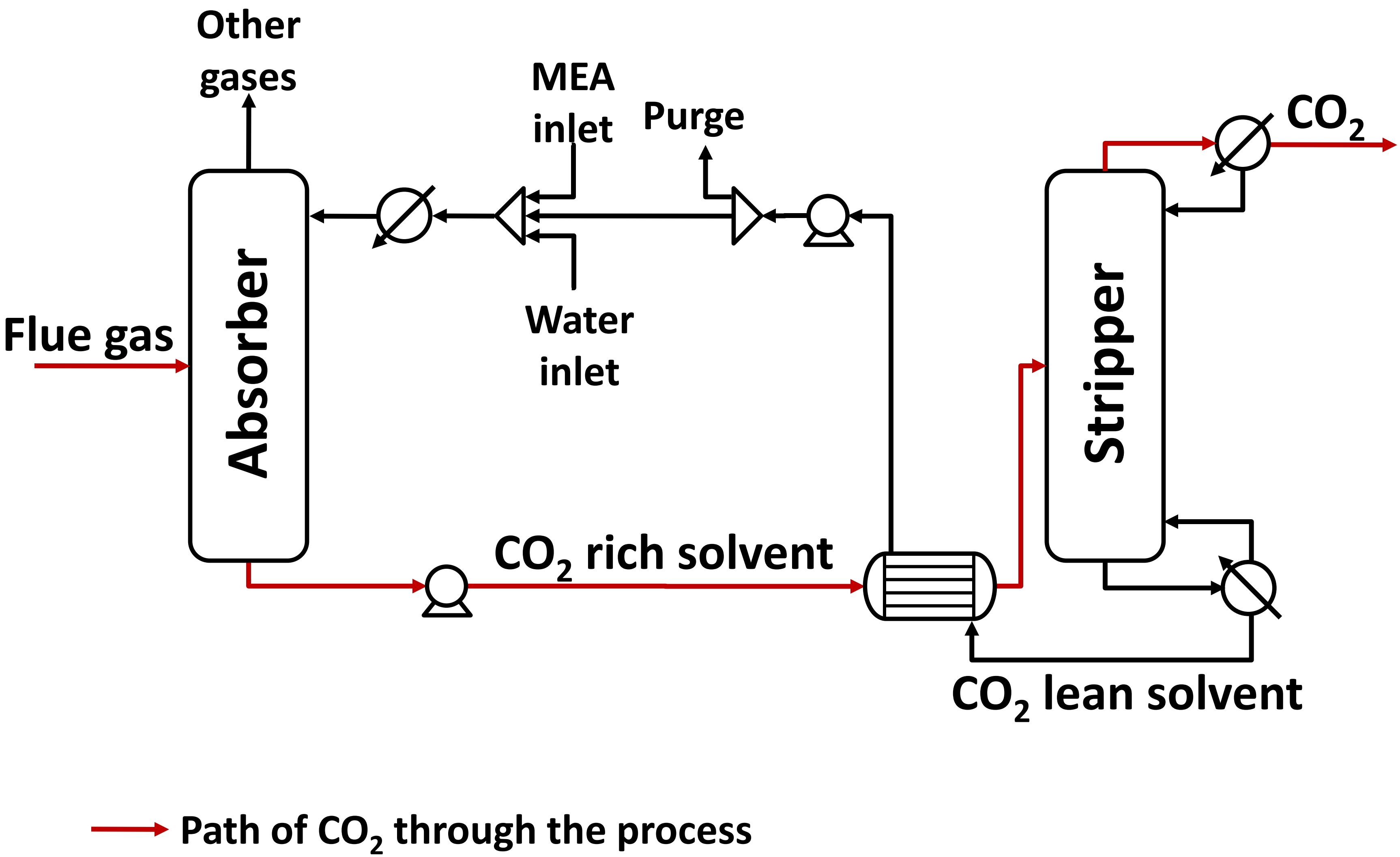
MEA CARBON CAPTURE PROCESS



CURRENT METHODS

- **Simulation methods**
  - **Aspen Plus**
    - *(Amann and Bouallou, 2009)*
    - *(Fashami et al., 2007)*
    - *(Abu-Zahra et al., 2007)*
    - *(Alie et al., 2005)*
    - *(Chang and Shih, 2005)*
    - *(Corradetti and Desideri, 2005)*
    - *(Fisher et al., 2005)*
    - *(Alie, 2004)*
    - *(Freguia and Rochelle, 2003)*
    - *(Report DOE/NETL, 2002)*
    - *(Desideri and Paolucci, 1999)*
    - *(Desideri and Corbelli, 1998)*
  - **HYSYS**
    - *(Amann and Bouallou, 2009)*
    - *(Oi, 2007)*
    - *(Singh et al., 2003)*
  - **MATLAB**
    - *(Mofarahi et al., 2008)*
  - **Fortran code**
    - *(Tobiesen et al., 2007)*
    - *(Tobiesen and Svendsen, 2006)*

CURRENT METHODS

- **Simulation optimization methods**
  - **Direct**
    - ***(Emun, Gadalla, Majozi, and Boer, 2010)***
    - ***(Chen, Shao, and Qian, 2009)***
    - ***(Leboreiro and Acevedo, 2004)***
    - ***(De Simon, Parodi, Fermeglia, and R. Taccani, 2003)***
    - ***(Ernst, Garro, Winkler, Venkataraman, Langer, Cooney, and Sasisekharan, 1997)***
  - **Surrogate model based**
    - ***(Henao and Maravelias, 2010)***
    - ***(Zhou, Xinping, Kefa, and Fan, 2004)***

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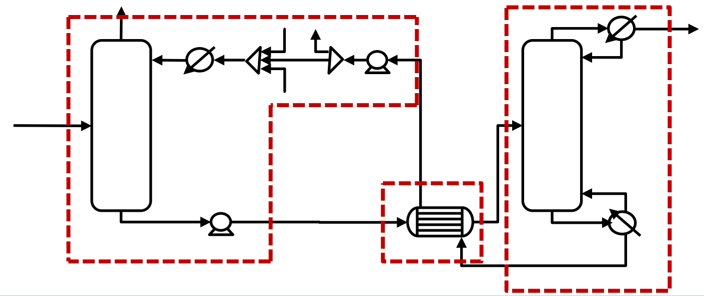
OVERVIEW OF THE METHOD

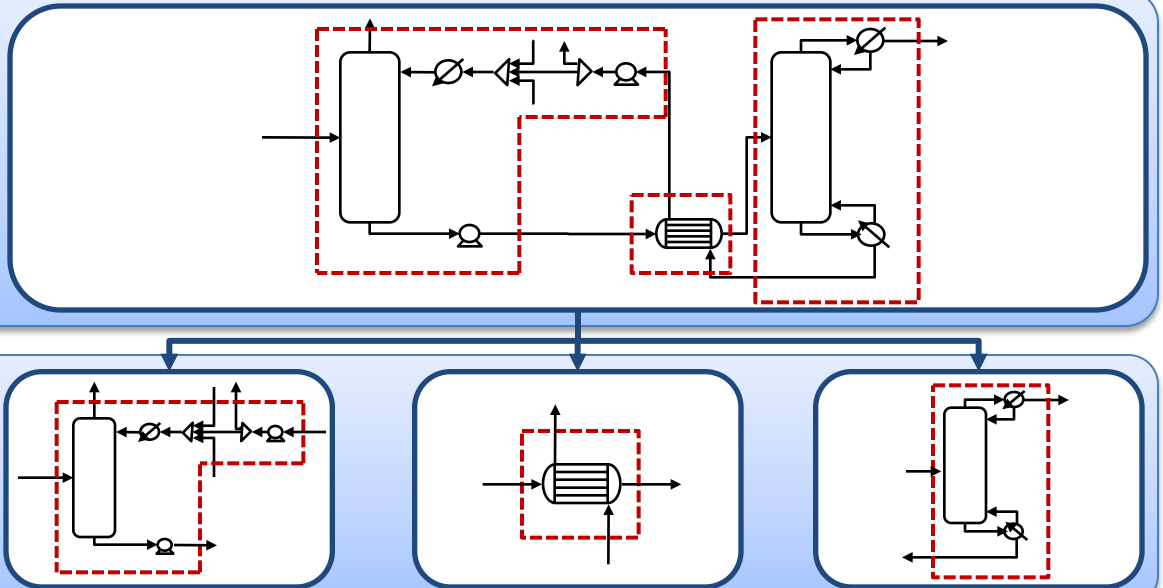
Simulation



OVERVIEW OF THE METHOD

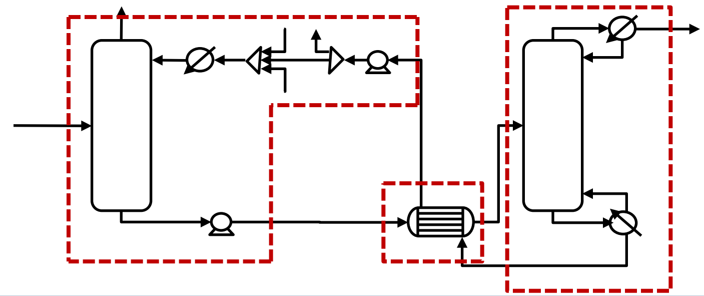
Simulation

Disaggregated blocks of process unit(s)

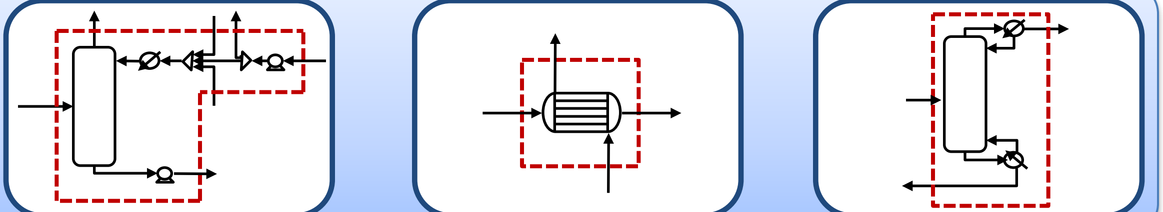


OVERVIEW OF THE METHOD

Simulation



Disaggregated blocks of process unit(s)



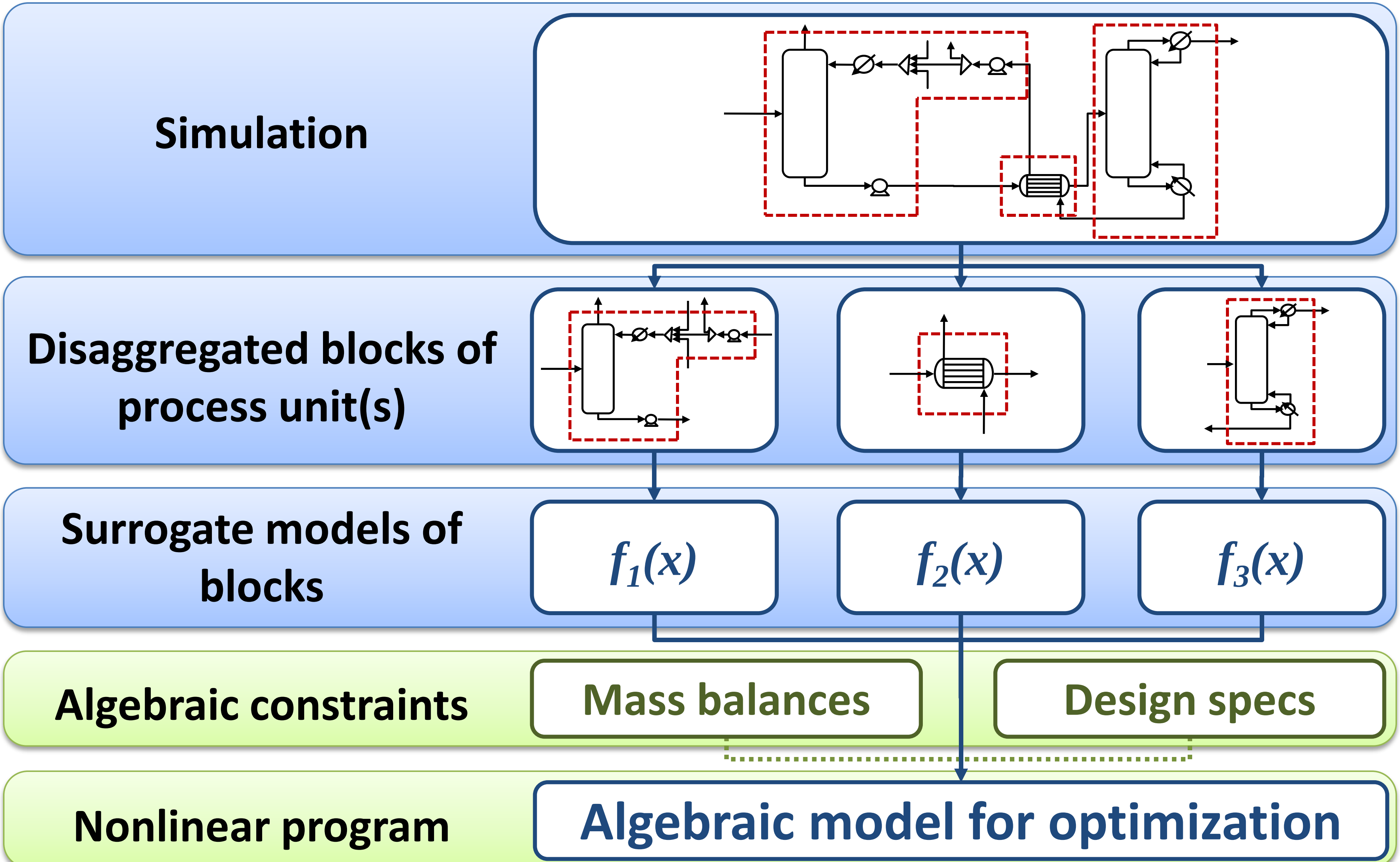
Surrogate models of blocks

$f_1(x)$

$f_2(x)$

$f_3(x)$

OVERVIEW OF THE METHOD



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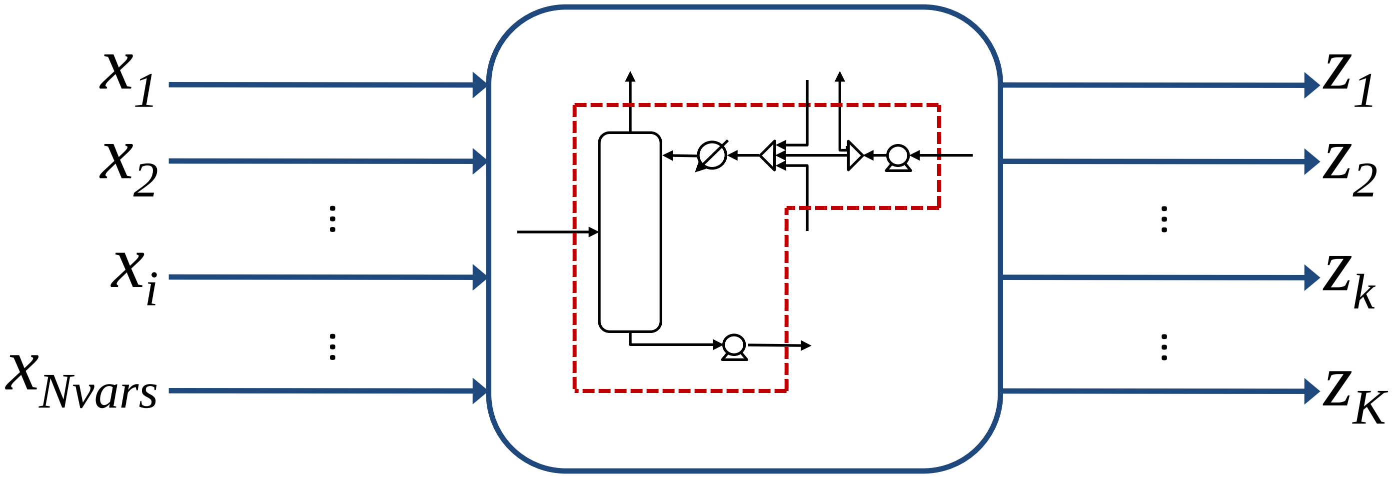
Disaggregated blocks



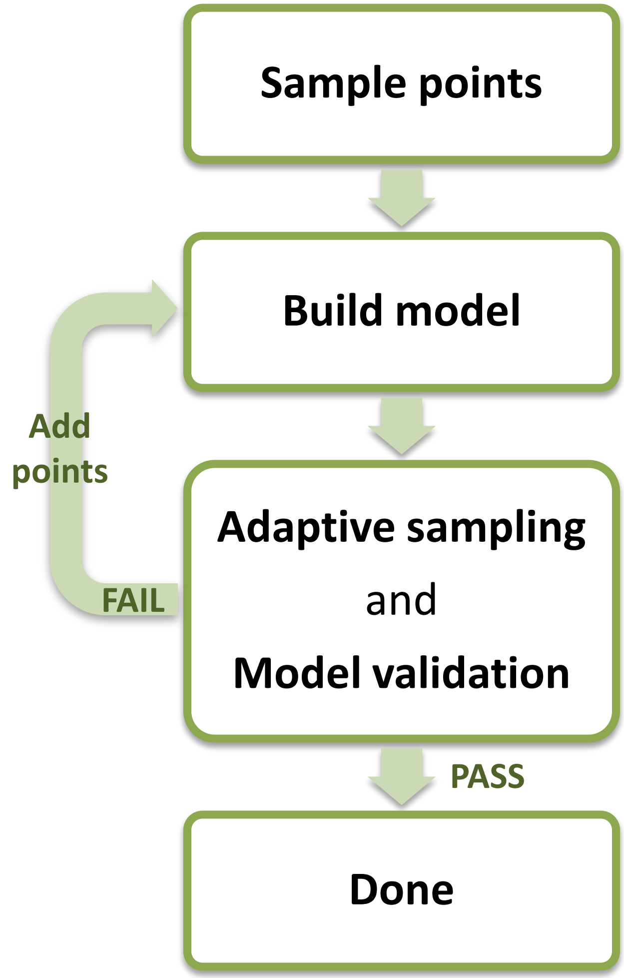
Independent variables, x

- Inlet conditions
  - Flow rates
  - Composition
  - Temperature
  - Pressure
- Operating conditions
- $x_i^l \leq x_i \leq x_i^u$

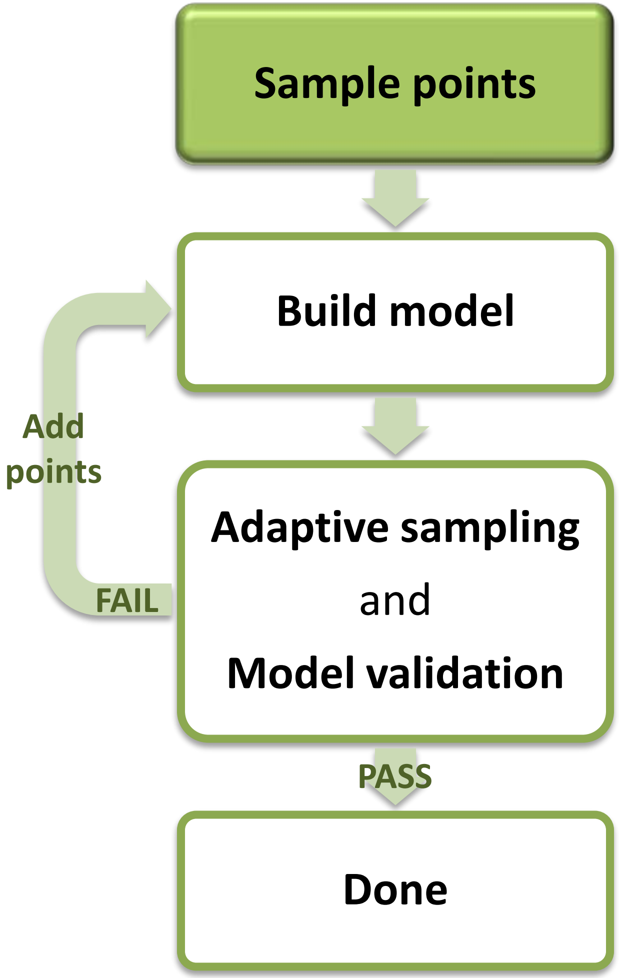
Dependent variables, z

- Outlet conditions
  - Flow rates
  - Composition
  - Temperature
  - Pressure
- Other relevant conditions

SURROGATE MODEL GENERATION

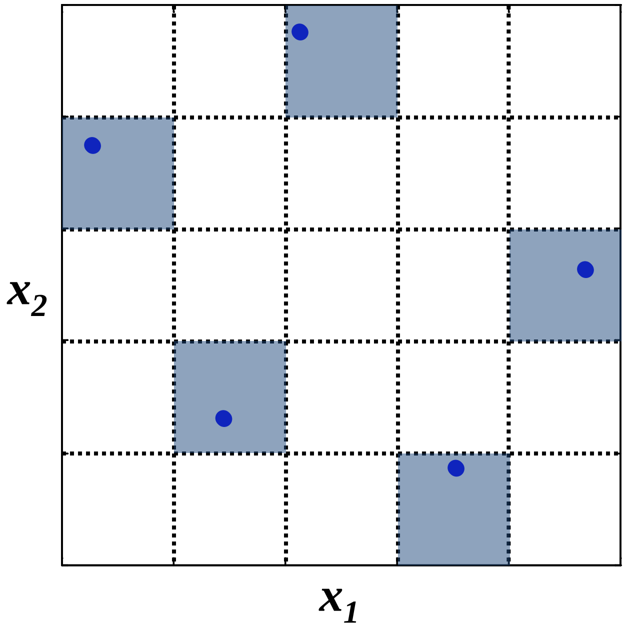


SAMPLE PROBLEM SPACE

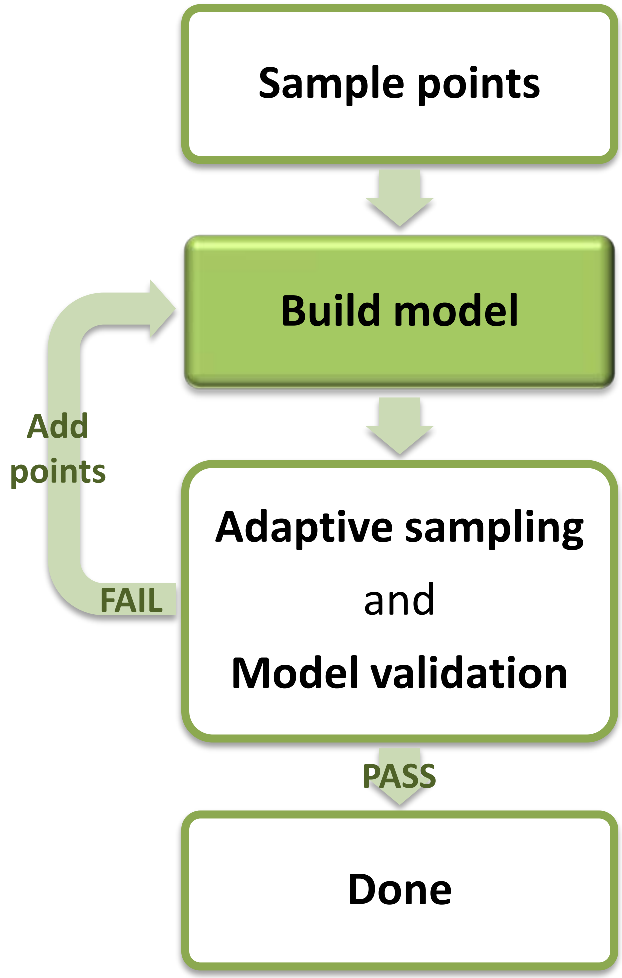


Design of experiments

1. Random points sampling
2. Factorial design
3. Latin hypercube design
   - *Space-filling design*



MODEL BUILDING

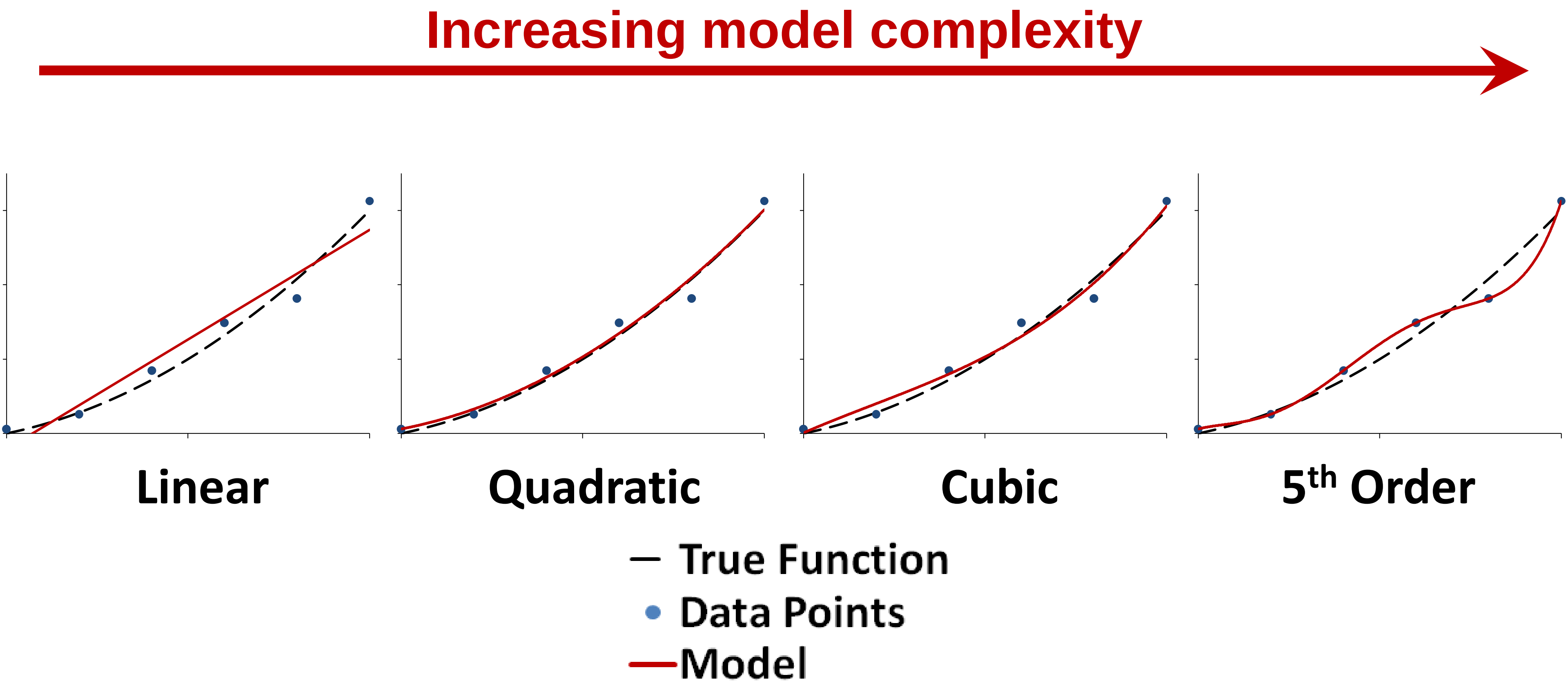


- **Build model for output z_k**

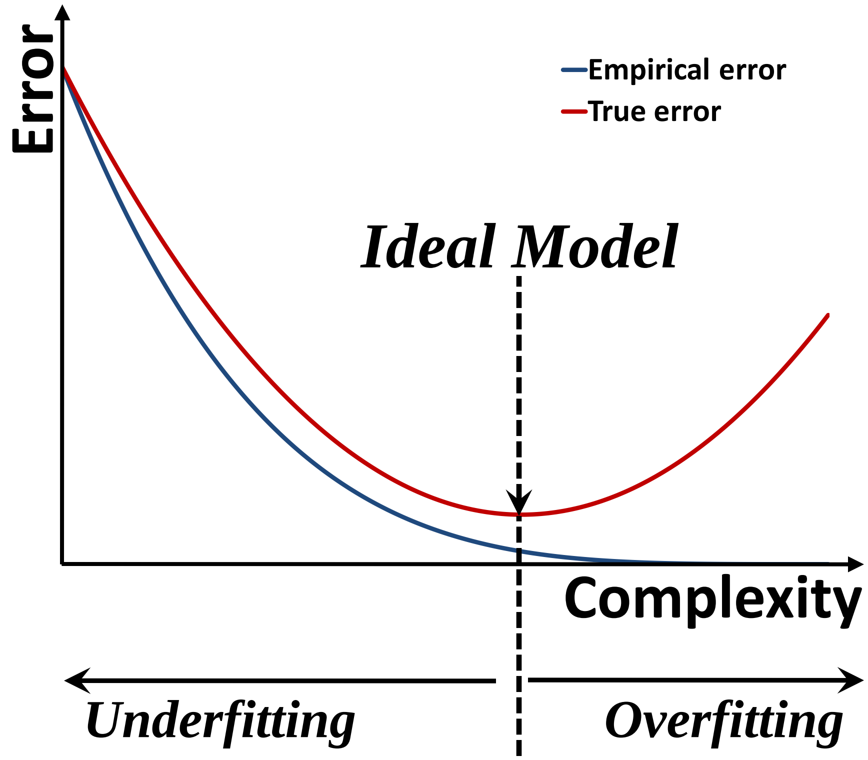
$$\hat{z}_k = \sum_{j=1}^{J} C_{kj} B_j(z,x) + C_{k0}$$

- **Basis functions $B_j(z,x)$**
  - **Explicit $B_j(x)$**
    - *Polymonial* x_i^{β}
    - *Pairwise polynomial* $x_i^{\beta} x_{i'}^{\beta}$ $\frac{x_i}{x_{i'}}$
    - *Exponential and logarithmic*
    - *Expected basis functions*
  - **Implicit $B_j(z,x)$**
    - *Ex: log mean temperature difference*

AVOID OVERFITTING THE DATA



EMPIRICAL VERSUS TRUE ERROR



- **Empirical error:**

  Error between the model and the sampled data points

- **True error:**

  Error between the model and the true function

BEST SUBSET METHOD

1. **Start with a liner combination of basis functions** ***d=4*****:** $\hat{y} = \alpha + \beta_1 x + \beta_2 x^2 + \beta_3 \sqrt{x}$

2. **Generate all possible subsets of basis functions**

One term	Two terms	Three terms	Four terms
$\hat{y} = \alpha$	$\hat{y} = \beta_1 x + \alpha$	$\hat{y} = \beta_1 x + \beta_2 x^2 + \beta_3 \sqrt{x}$	$\hat{y} = \alpha + \beta_1 x + \beta_2 x^2 + \beta_3 \sqrt{x}$
$\hat{y} = \beta_1 x$	$\hat{y} = \beta_2 x^2 + \alpha$	$\hat{y} = \alpha + \beta_2 x^2 + \beta_3 \sqrt{x}$	
$\hat{y} = \beta_2 x^2$	$\hat{y} = \beta_3 \sqrt{x} + \alpha$	$\hat{y} = \alpha + \beta_1 x + \beta_3 \sqrt{x}$	
$\hat{y} = \beta_3 \sqrt{x}$	$\hat{y} = \beta_2 x^2 + \beta_1 x$	$\hat{y} = \alpha + \beta_1 x + \beta_2 x^2$	
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3. **Pick the best**

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2^d-1
subsets!

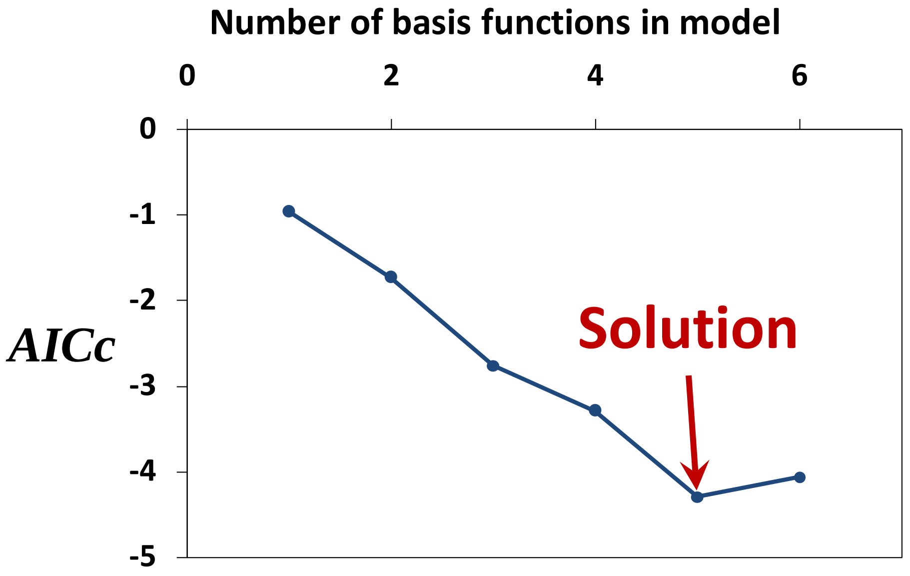
3. **Pick the best**

HOW TO PICK THE BEST SUBSET

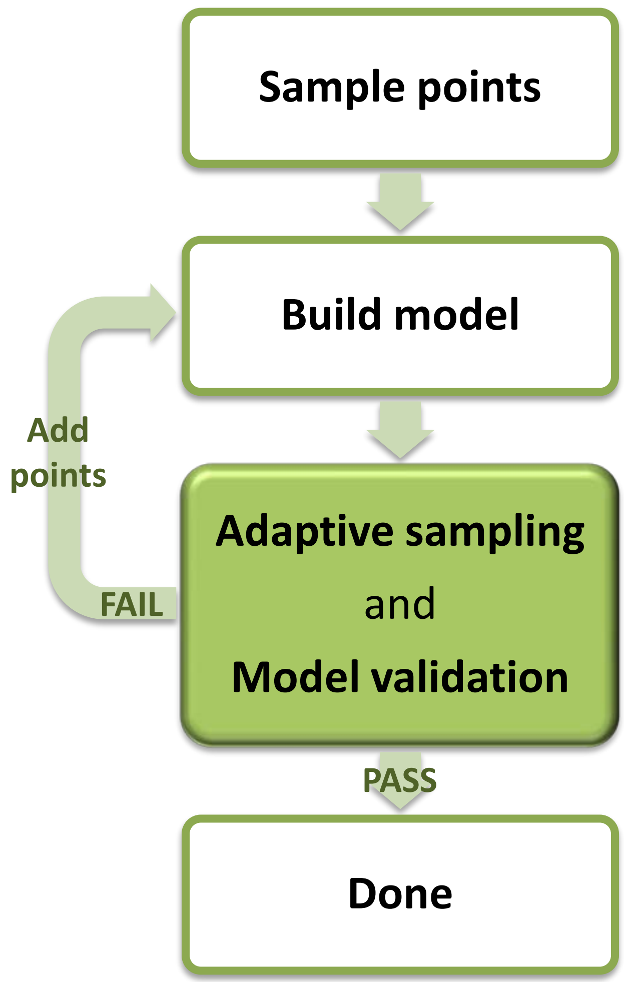
- **Corrected Akaike Information Criterion (AICc)**
  - Gives an estimate of the difference between a model and the true function

$$AICc = \underbrace{n \log\left(\frac{SSE}{n}\right)}_{\text{Accuracy}} + \underbrace{2p + \frac{2p(p+1)}{n-p-1}}_{\text{Complexity}}$$

Accuracy + Complexity

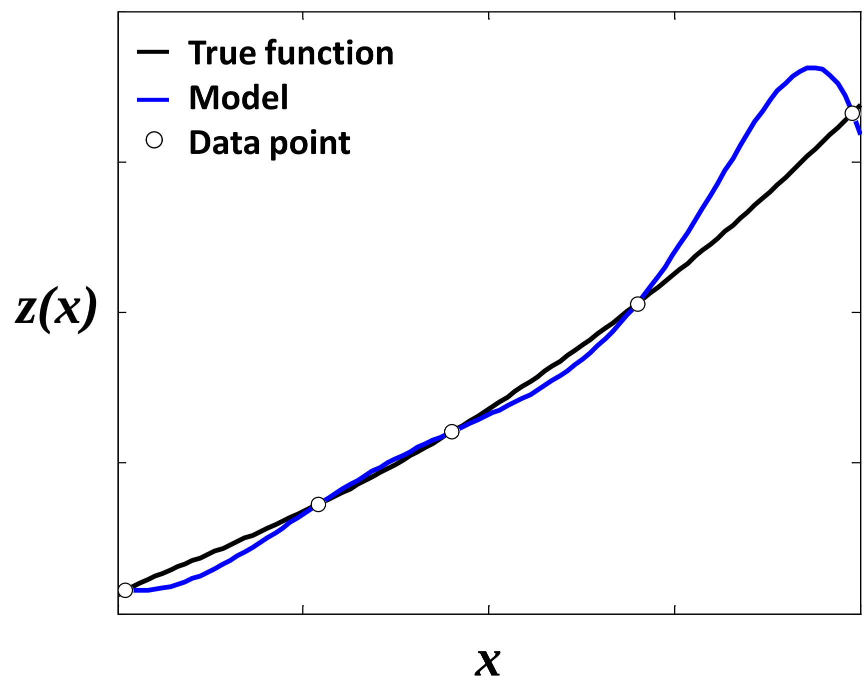


ADAPTIVE SAMPLING



- **Find values of x where the model is inconsistent**
  - **Maximize the relative model error using a black-box solver:**

$$\max_{x} \left(\frac{z(x) - \hat{z}(x)}{z(x)} \right)^2$$



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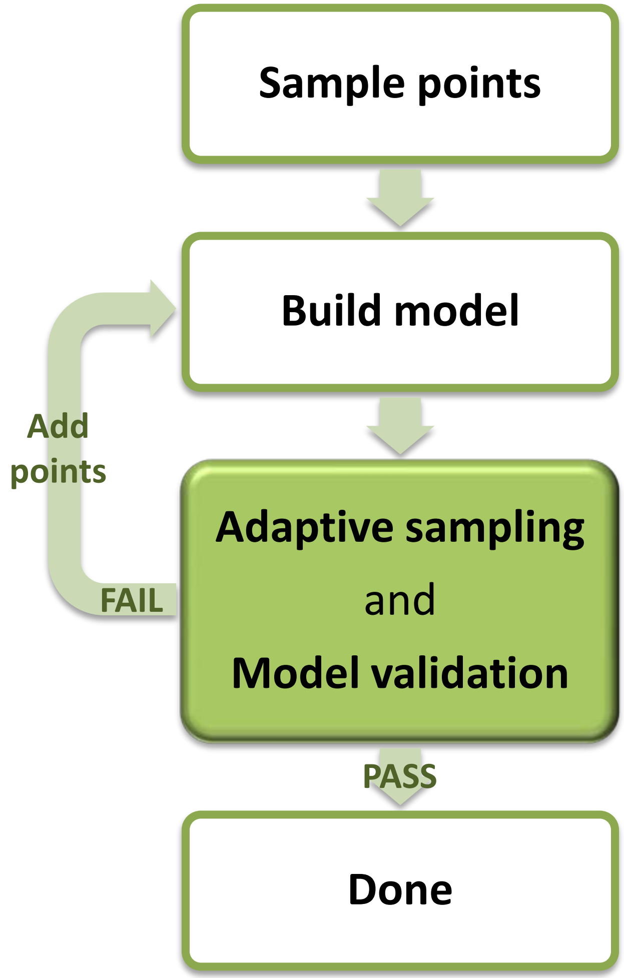

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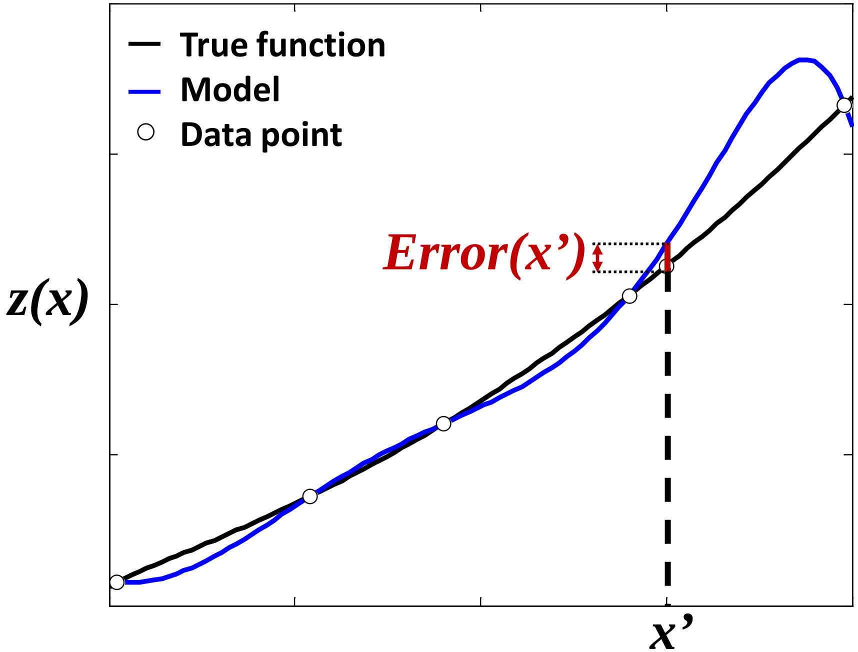

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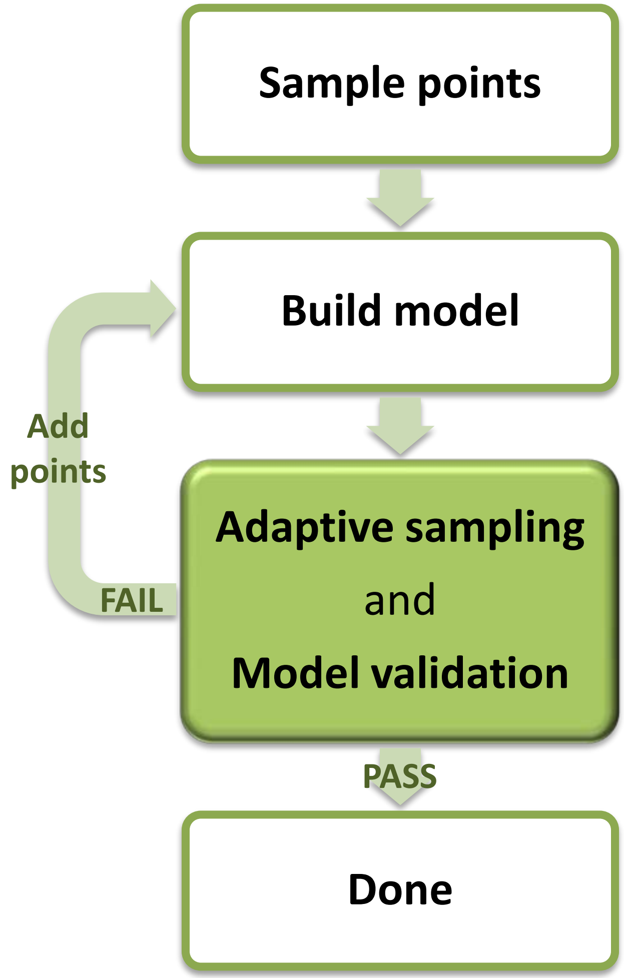

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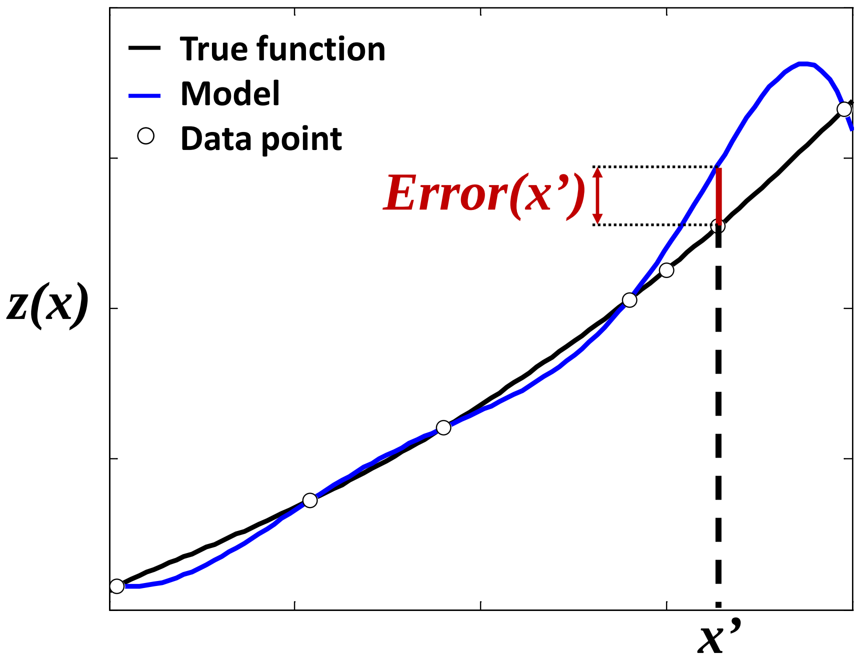

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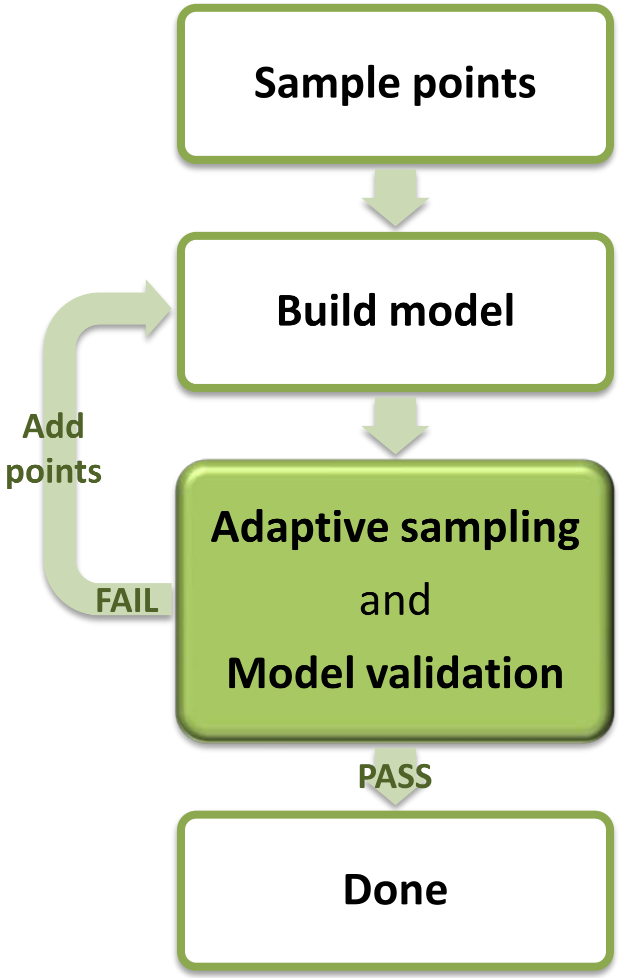

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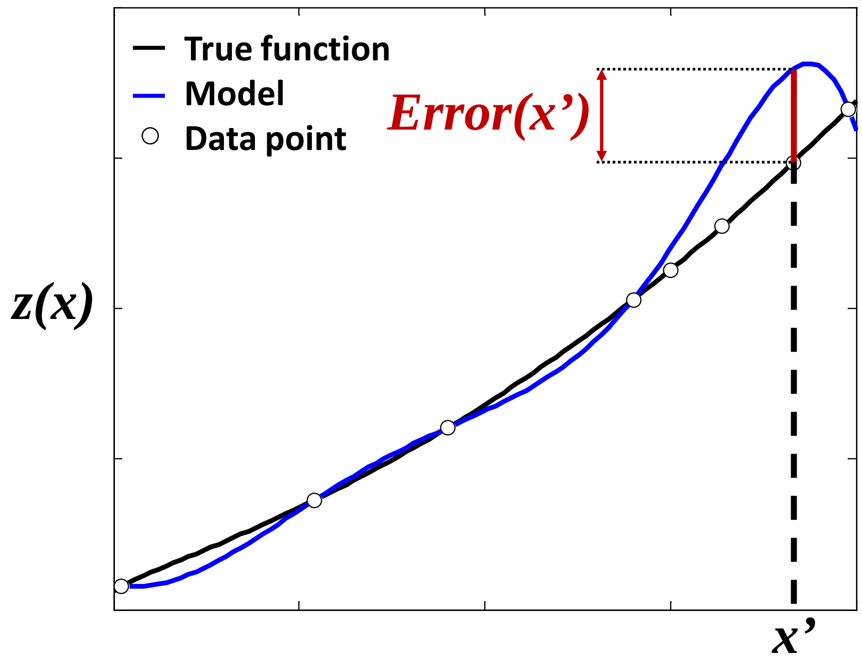
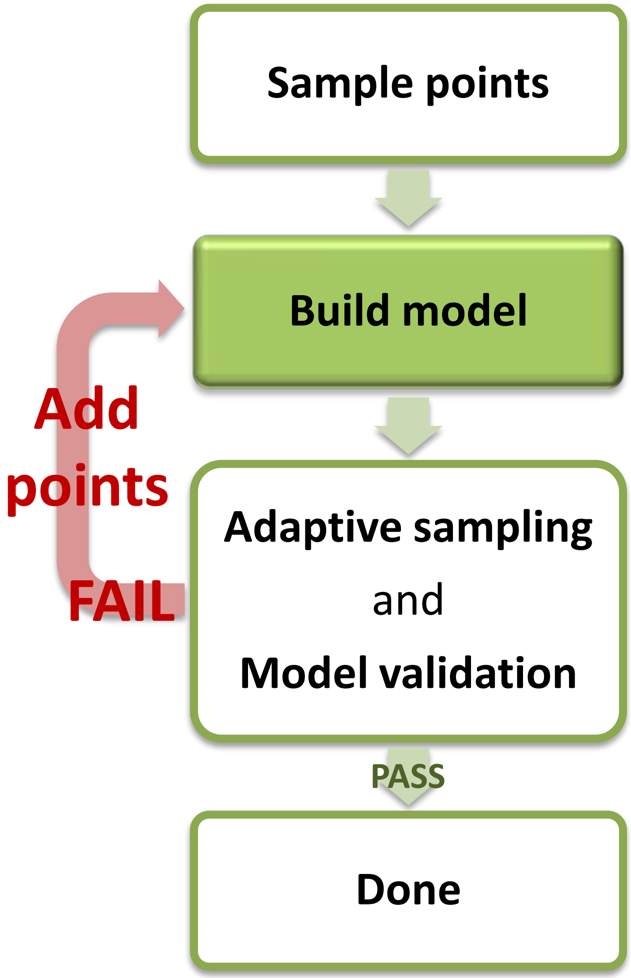
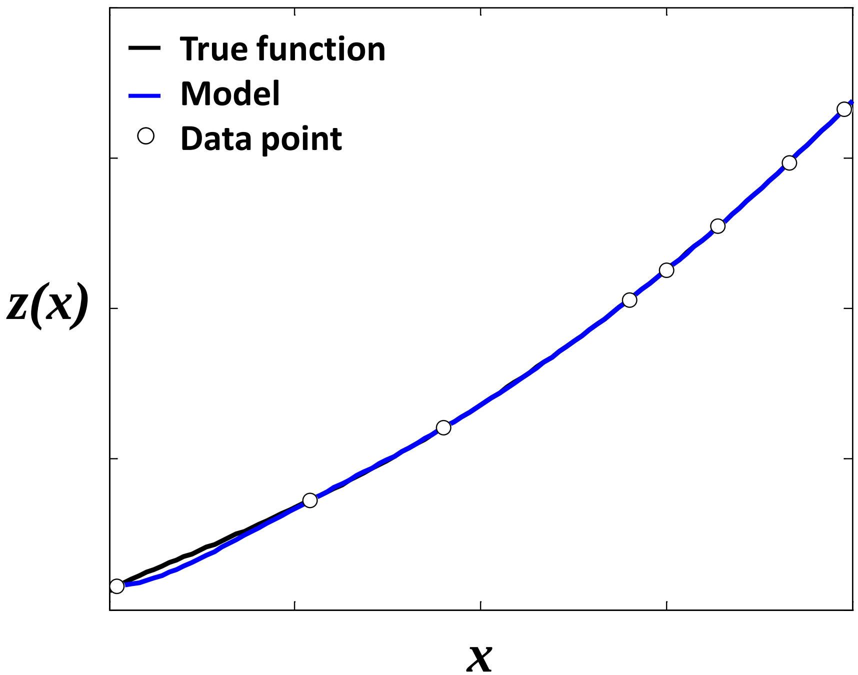


REBUILD THE MODEL



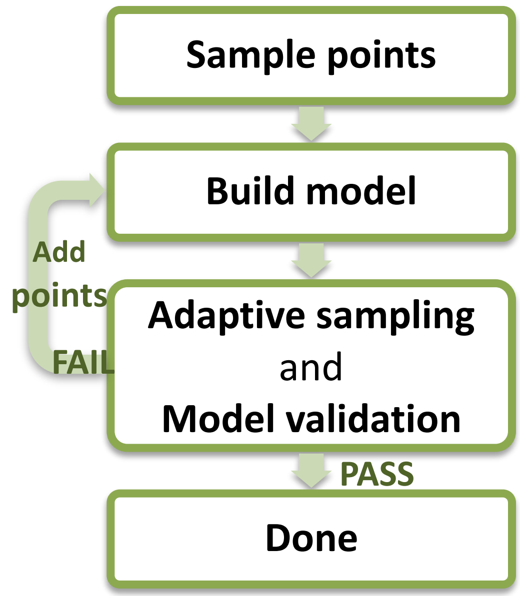
- **Add the data points found during adaptive sampling to the training set**
- **Rebuild the model**



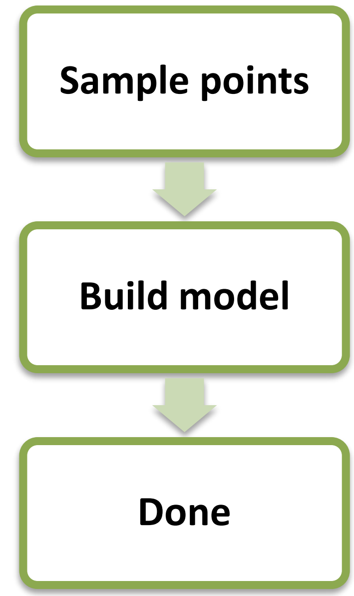
TESTING MODEL GENERATION

- Compare the method with and without adaptive sampling:

Full algorithm:



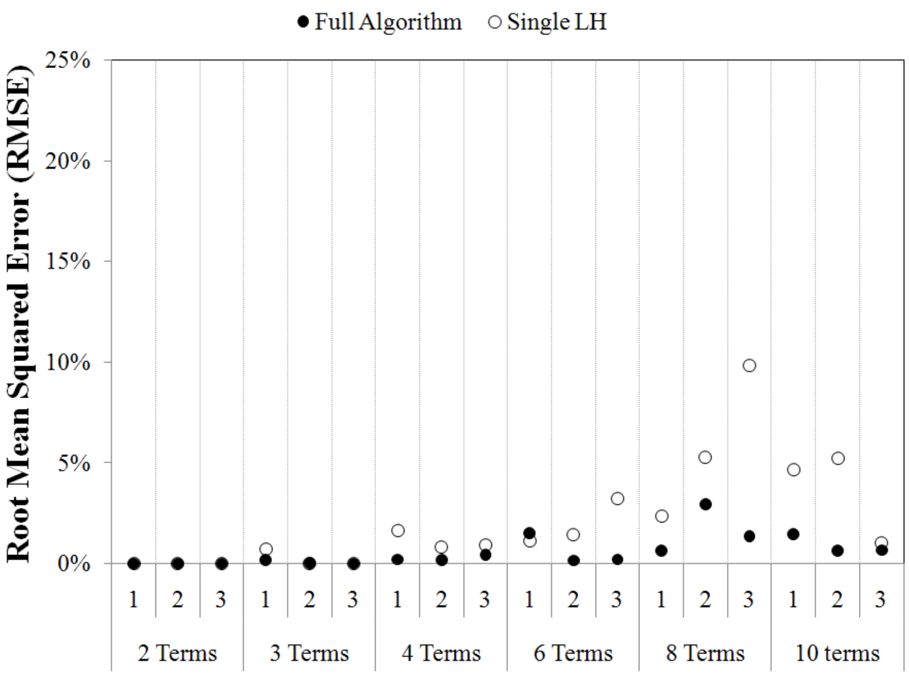
Single Latin hypercube:



- Two sets of known equations made up of functions
  - Present in the algorithm's basis set
  - Not present in the algorithm's basis set

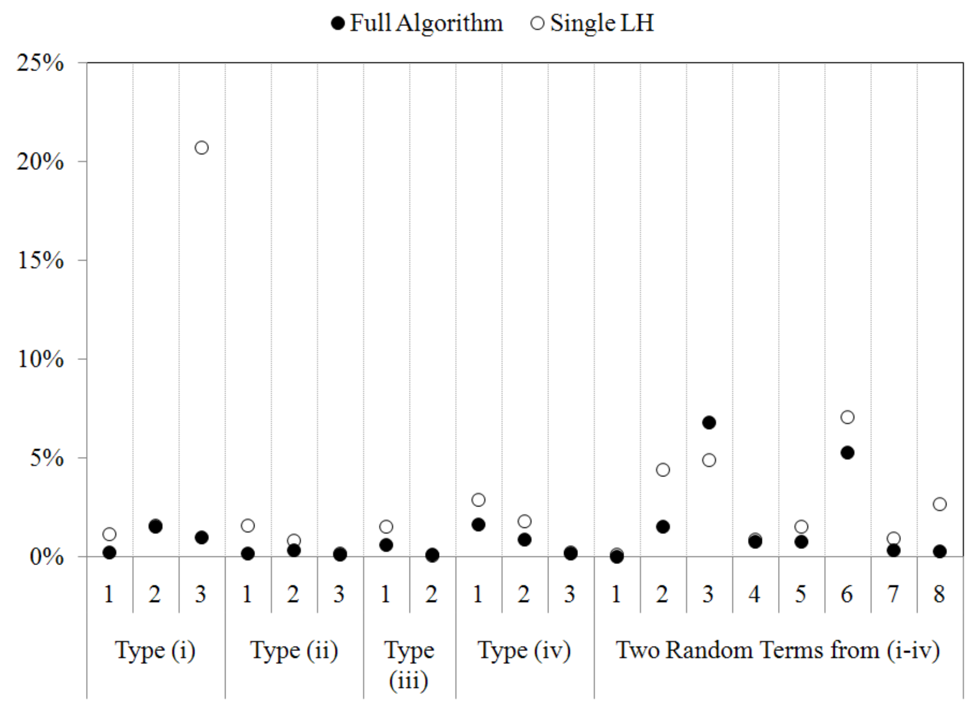
TESTING MODEL GENERATION

Functions present in the basis set



Averaged over three runs for every equation

Functions NOT present in the basis set



- ***i.*** ***Pairwise polynomial with unequal exponents***
- ***ii.*** ***Complex, unavailable, fractional forms***
- ***iii.*** $x_i^{\beta} e^{x_i}$
- ***iv.*** $x_i^{\beta} \log x_i$

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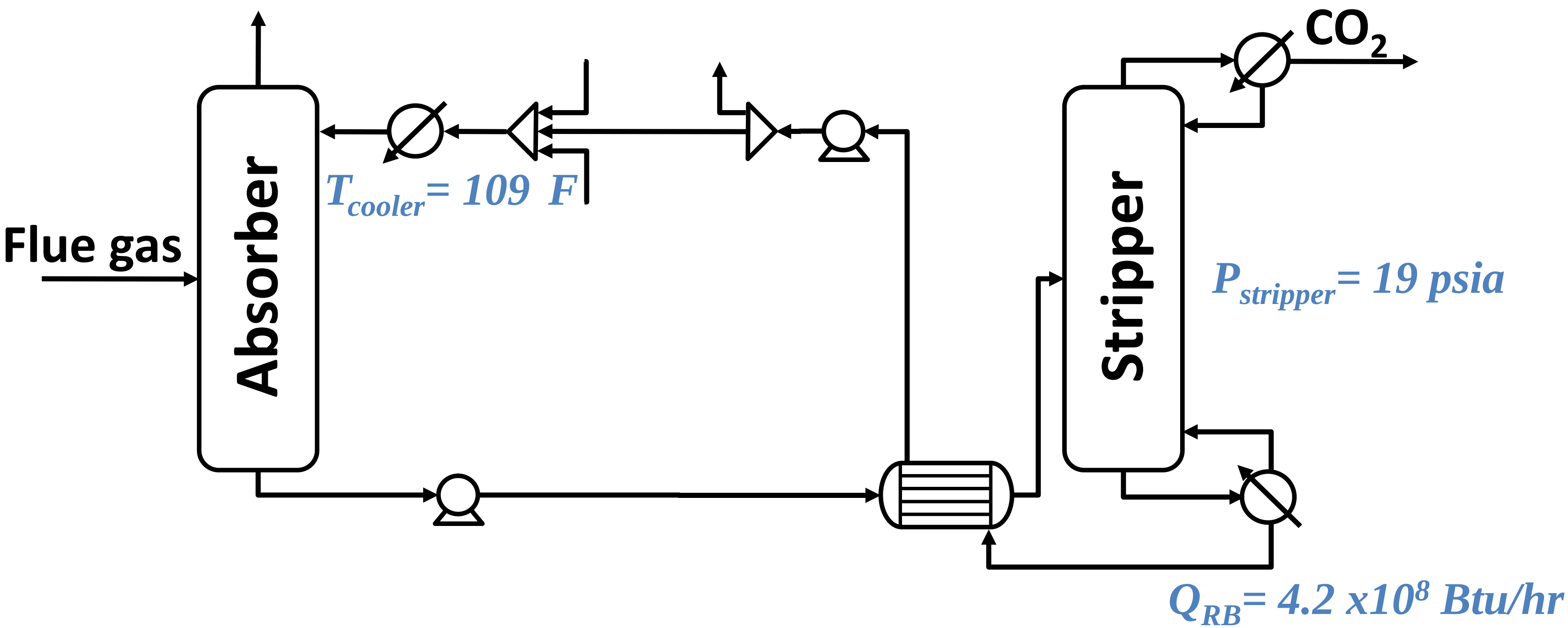
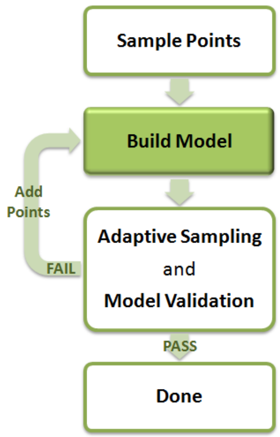
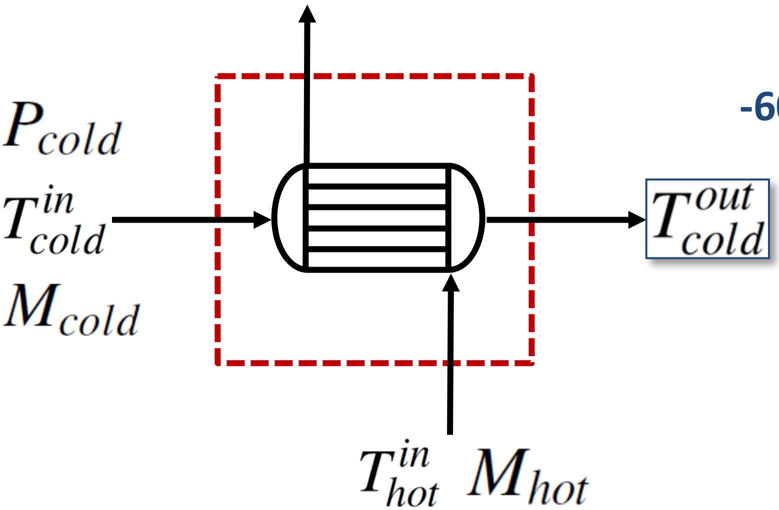
PRELIMINARY RESULTS

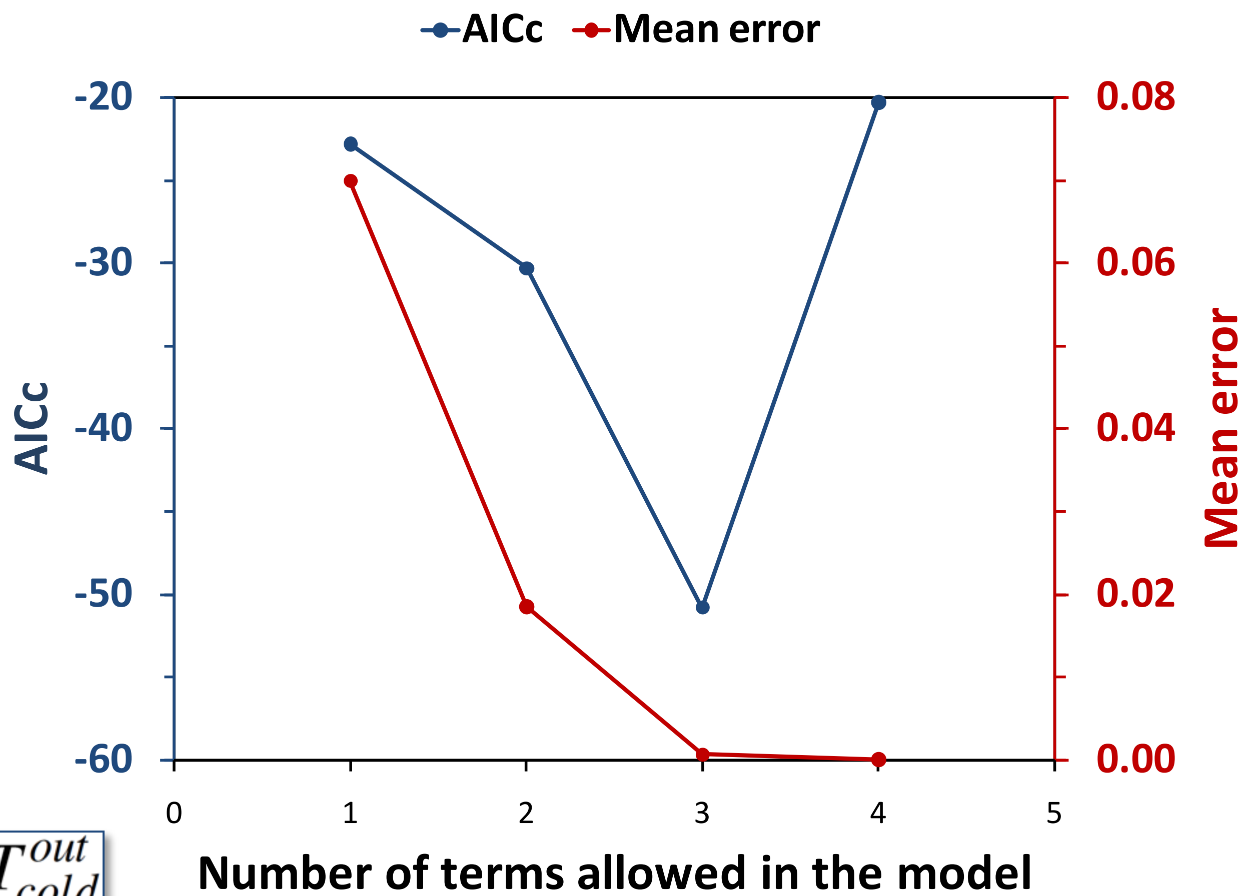


- **Minimize stripper reboiler duty (Q_{RB}) with 90% CO_2 capture**
- **Base case (blue)**

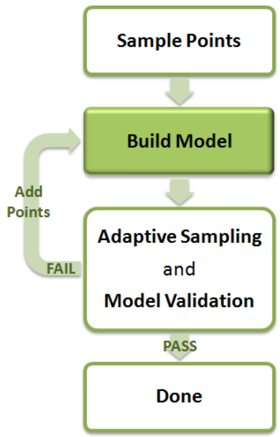
BUILDING THE CC MODEL

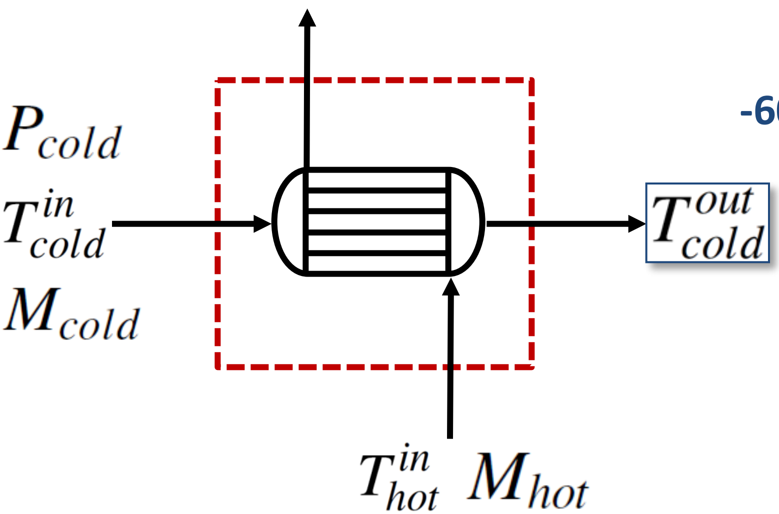


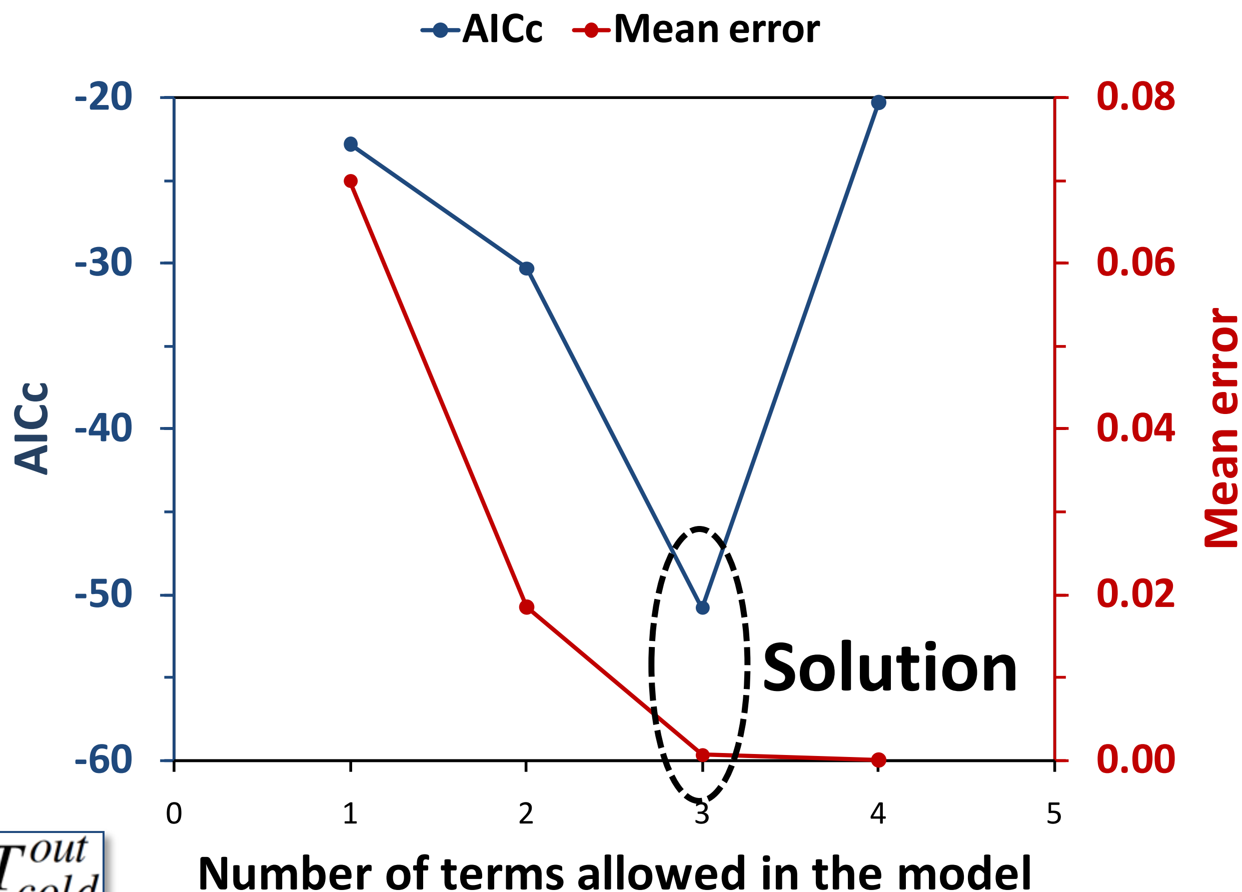




BUILDING THE CC MODEL



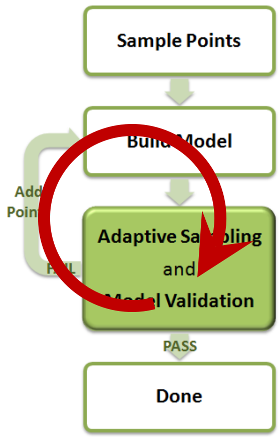


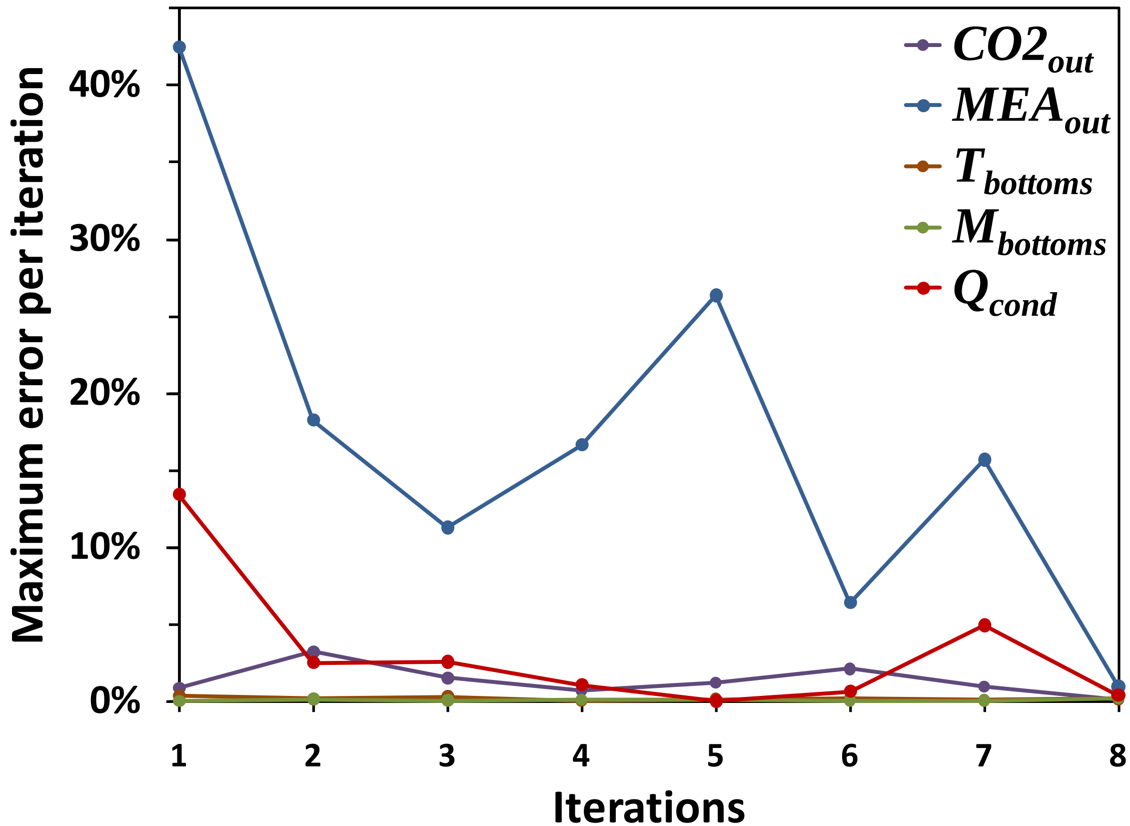


BUILDING THE CC MODEL

Terms Allowed	Model for T_{cold}^{out}, $^\circ F$
1	$0.017\left(\frac{T_{hot}^{in}}{242}\right)\left(\frac{M_{cold}}{2.3\cdot 10^6}\right)^{-1}$
2	$0.020\left(\frac{T_{hot}^{in}}{242}\right)\left(\frac{M_{hot}}{2.0\cdot 10^6}\right)^{-1} - 0.0021\left(\frac{P_{cold}}{22}\right)\left(\frac{M_{hot}}{2.0\cdot 10^6}\right)^{-1}$
3	$-0.0077\left(\frac{T_{hot}^{in}}{242}\right)^2 + 0.013\left(\frac{T_{cold}^{in}}{131}\right)\left(\frac{T_{hot}^{in}}{242}\right)^{-1} + 0.018\Delta T_{LM}$
4	$0.011\left(\frac{T_{hot}^{in}}{242}\right)^2 - 0.052\left(\frac{T_{cold}^{in}}{131}\right)\left(\frac{T_{hot}^{in}}{242}\right)^{-1} + 0.018\Delta T_{LM} + 0.046\left(\frac{T_{cold}^{in}}{131}\right)^{-1}$

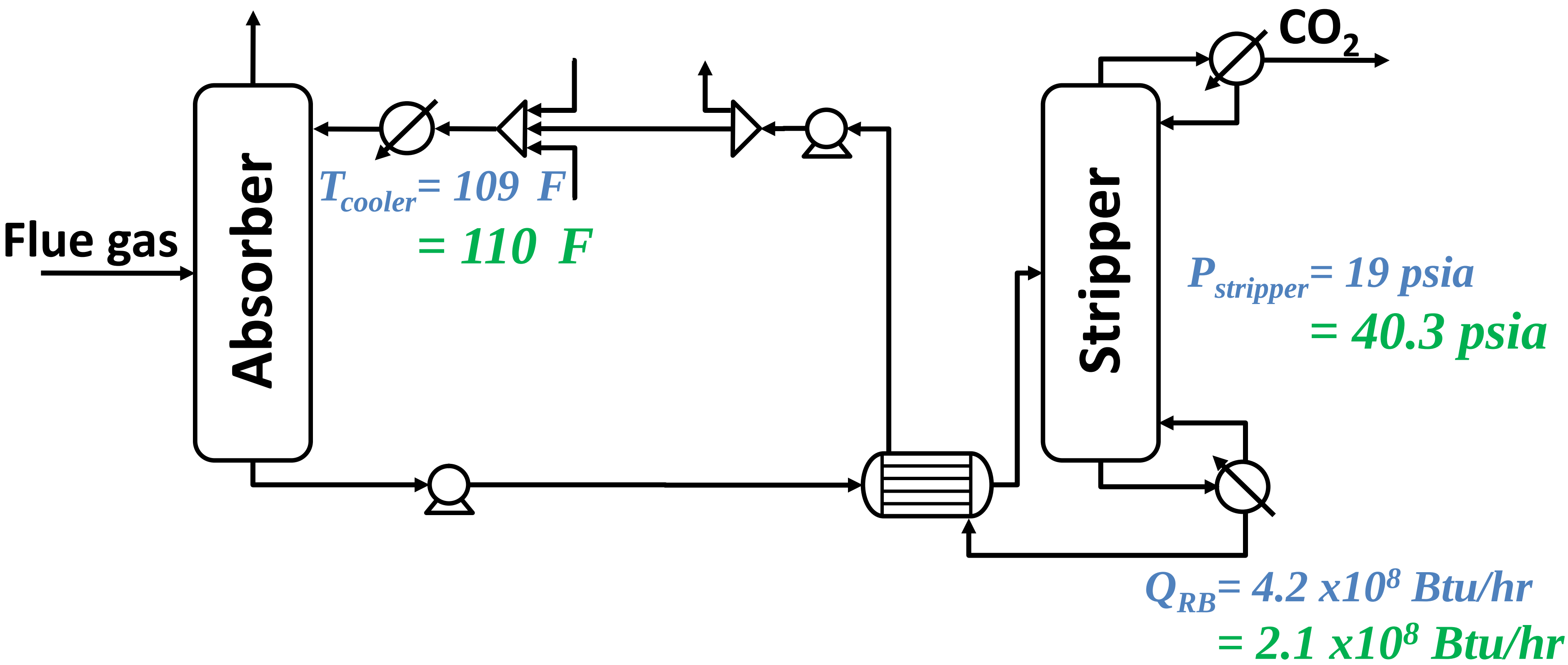
ADAPTIVE SAMPLING





- Progression through algorithm for Block 3
- Maximum error found can increase because the derivative-free solver "gets smarter" after each iteration

PRELIMINARY RESULTS



- **Minimize stripper reboiler duty (Q_{RB}) with 90% CO_2 capture**
- **Base case (blue)**
- **Optimized results (green)**

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CONCLUSIONS

- We developed a method to generate surrogate models of process simulations that
  - Are highly accurate
  - Have low complexity
  - Use minimal function evaluations
- We optimized a carbon capture process with two primary decision variables that showed a 50% reduction in reboiler heat over the base case
- Future work includes optimizing a carbon capture process integrated with a pulverized coal plant