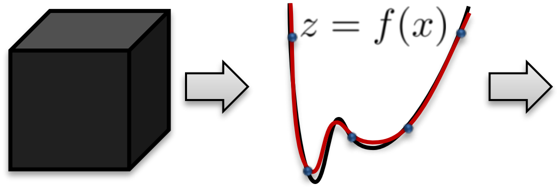

$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & g(x) = 0 \end{aligned}$$

DERIVATIVE-FREE OPTIMIZATION ENHANCED-SURROGATE MODEL DEVELOPMENT FOR OPTIMIZATION

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CAPD CENTER

Carnegie Mellon University

NETL NATIONAL ENERGY TECHNOLOGY LABORATORY

CCSI™

Carbon Capture Challenge

- **The traditional pathway from discovery to commercialization of energy technologies can be quite long, i.e., ~ 2-3 decades**
- **President's plan requires that barriers to the widespread, safe, and cost-effective deployment of CCS be overcome within 10 years**
- **To help realize the President's objectives, new approaches are needed for taking carbon capture concepts from lab to power plant, quickly, and at low cost and risk**
- **CCSI will accelerate the development of carbon capture technology, from discovery through deployment, with the help of science-based simulations**

Bench Research
~ 1 kWe

↓

Small pilot
< 1 MWe

↓

Medium pilot
1 – 5 MWe

↓

Semi-works pilot
20-35 MWe

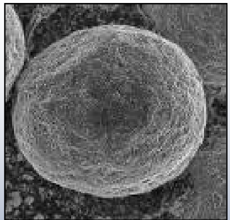
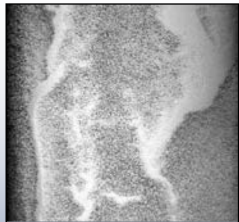
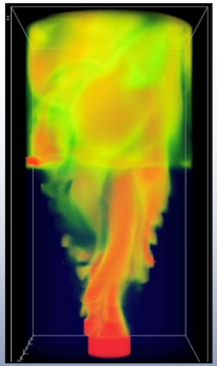
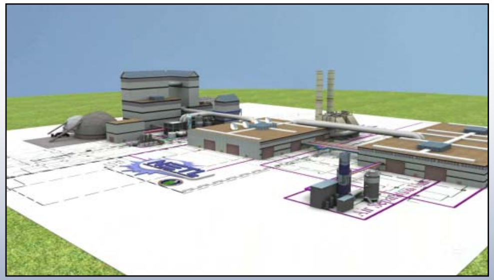
↓

First commercial plant, 100 MWe

↓

Deployment, >500 MWe, >300 plants

Carbon Capture Simulation Initiative
www.acceleratecarboncapture.org

Identify promising concepts → **Reduce the time for design & troubleshooting** → **Quantify the technical risk, to enable reaching larger scales, earlier** → **Stabilize the cost during commercial deployment**

National Labs

- Berkeley Lab
- Pacific Northwest National Laboratory
- NETL
- Los Alamos National Laboratory EST. 1943
- Lawrence Livermore National Laboratory

Academia

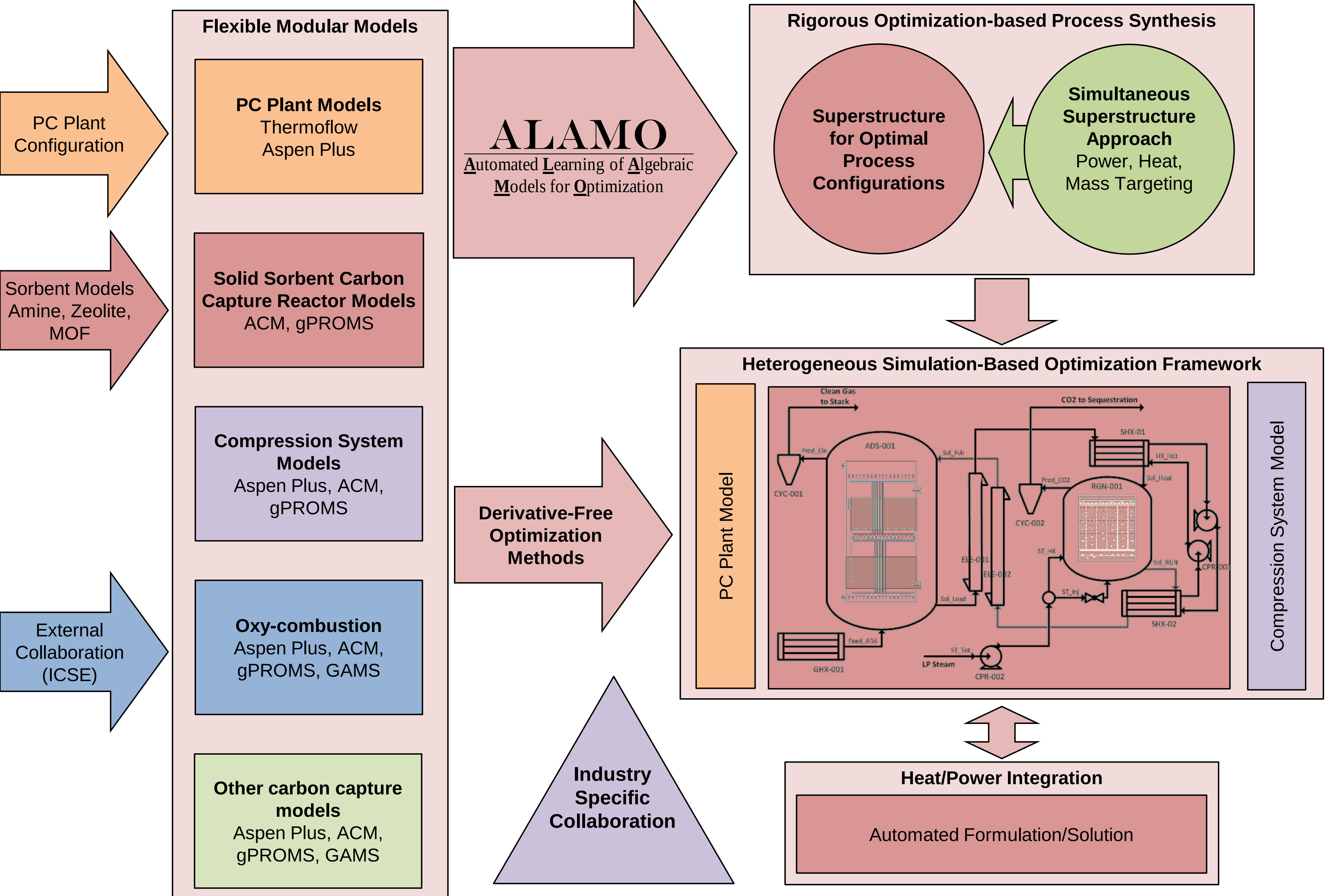
- Carnegie Mellon
- Princeton University
- West Virginia University
- Boston University
- Institute for Clean and Secure Energy, The University of Utah

Industry

- Fluor
- ADA Environmental Solutions
- B&W the babcock & wilcox company
- GE
- EPRI Electric Power Research Institute
- Air Products
- Burns & McDonnell Since 1898
- Southern California Edison An EDISON INTERNATIONAL Company San Onofre Nuclear Generating Station
- Alstom
- Southern Company
- Duke Energy
- URS
- Boeing
- DuPont
- ExxonMobil
- Chevron
- Phillips 66
- WorleyParsons resources & energy
- Eastman

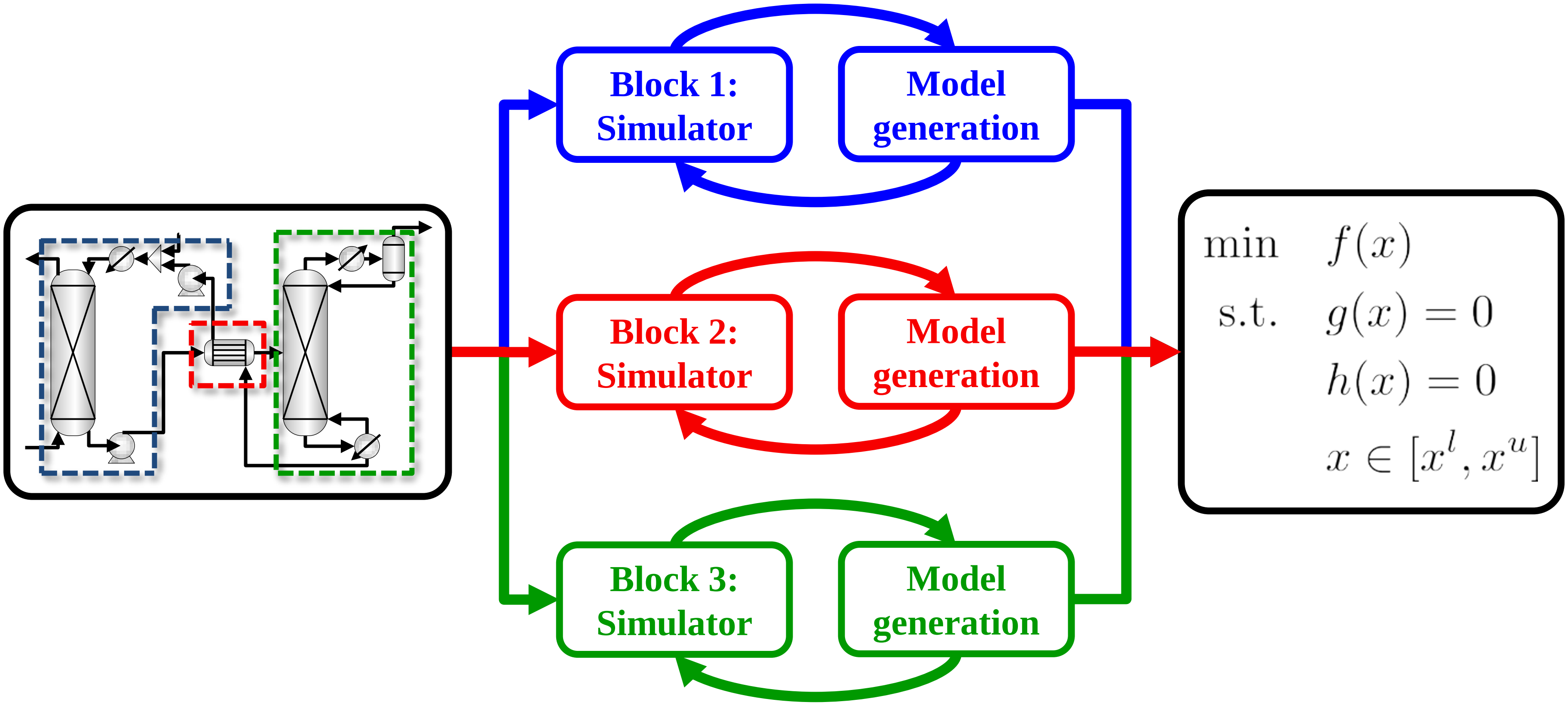
CCSI Carbon Capture Simulation Initiative

NETL · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory EST. 1943 · Pacific Northwest National Laboratory · U.S. Department of Energy



CCSI Carbon Capture Simulation Initiative · NETL · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · Pacific Northwest National Laboratory · U.S. Department of Energy

PROCESS DISAGGREGATION



Process Simulation

Disaggregate process into process blocks

Surrogate Models

Build simple and accurate models with a functional form tailored for an optimization framework

Optimization Model

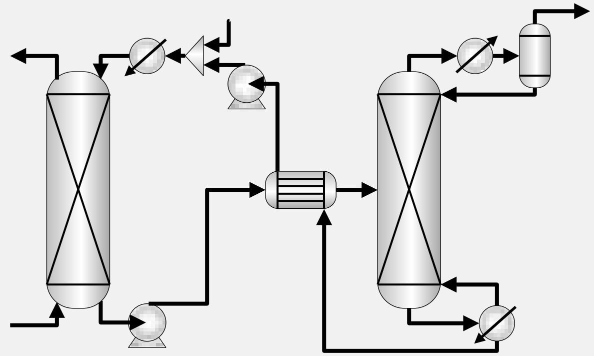
Add algebraic constraints *h(x)*=0: design specs, heat/mass balances, and logic constraints

MODELING PROBLEM STATEMENT

- **Build a model of output variables z as a function of input variables x over a specified interval**

$$x \in \mathbb{R}^D \qquad x^l \le x \le x^u \qquad \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \\ \vdots \\ x_D \end{pmatrix}$$

Process simulation

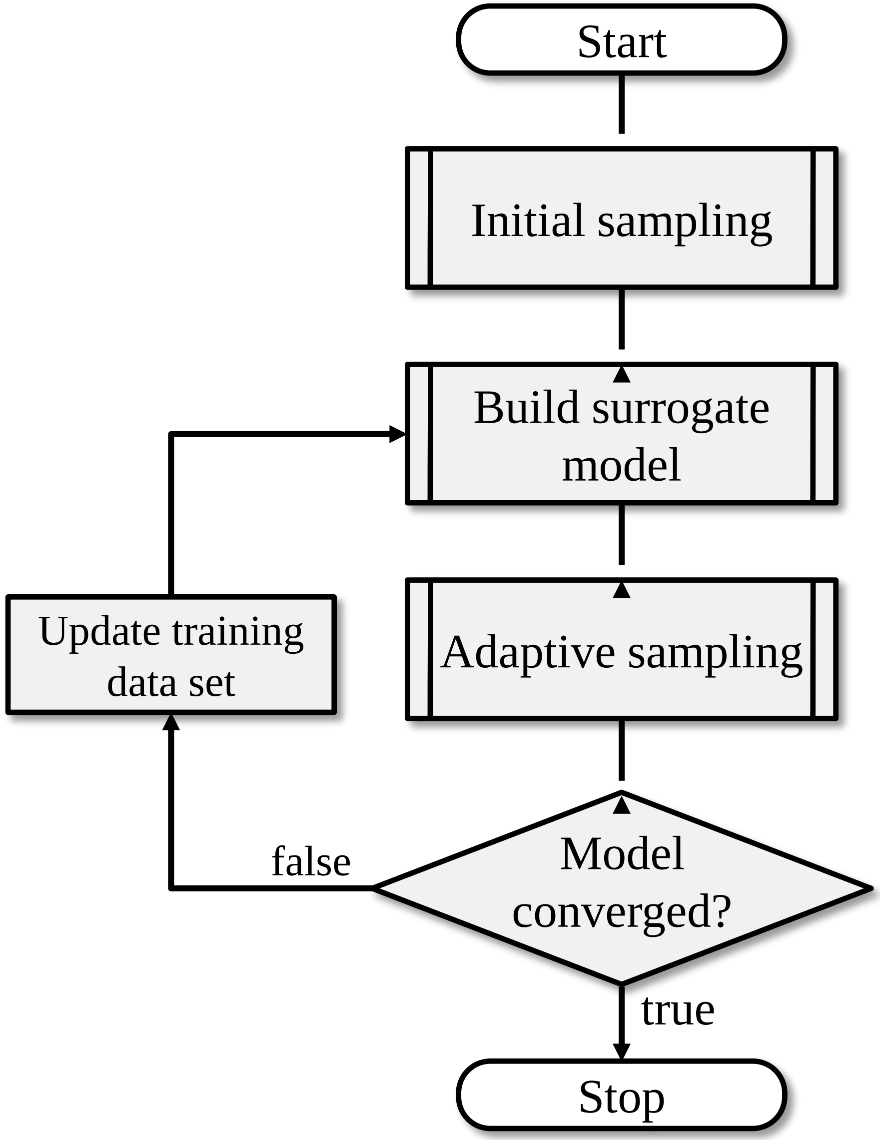


$$\begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_k \\ \vdots \\ z_K \end{pmatrix} \qquad z \in \mathbb{R}^K \qquad z = f(x)$$

Independent variables:
Operating conditions, inlet flow properties, unit geometry

Dependent variables:
Efficiency, outlet flow conditions, conversions, heat flow, etc.

ALGORITHMIC FLOWSHEET

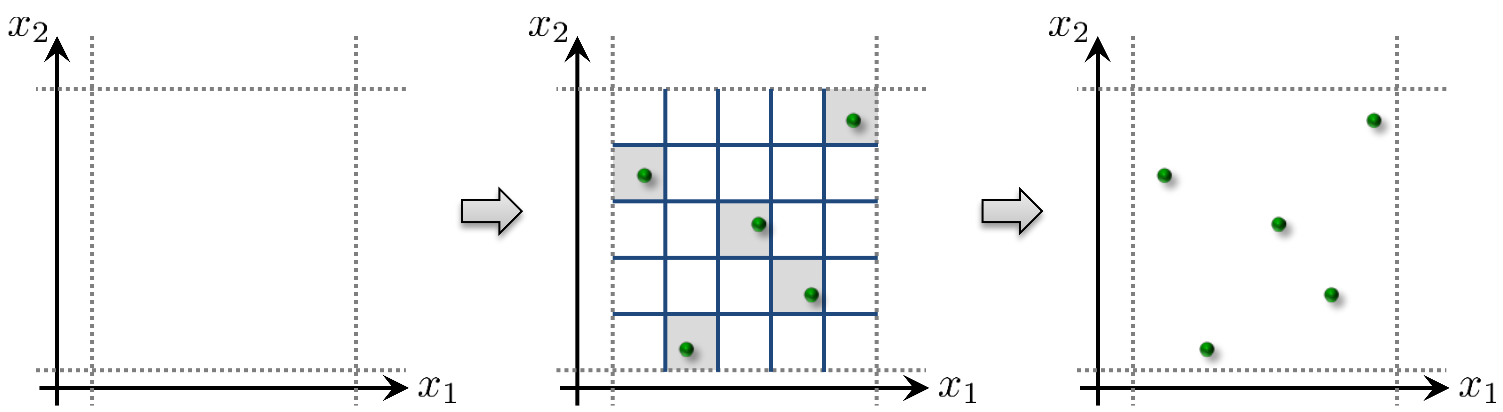


DESIGN OF EXPERIMENTS

- **Goal: To generate an initial set of input variables to evenly sample the problem space**

$$x = \begin{pmatrix} x^1 & x^2 & \cdots & x^i & \cdots & x^N \end{pmatrix} \qquad x^i = \begin{pmatrix} x_1^i \\ x_2^i \\ \vdots \\ x_d^i \\ \vdots \\ x_D^i \end{pmatrix}$$

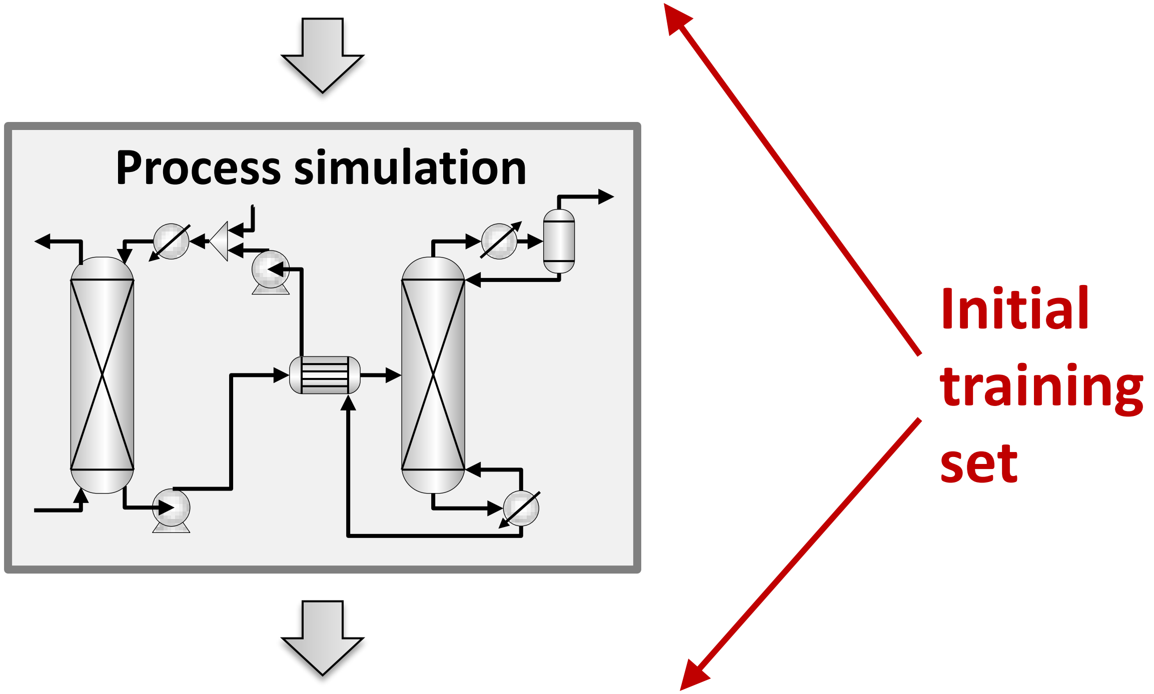
- **Latin hypercube design of experiments** [McKay et al., 79]



INITIAL SAMPLING

- **After running the design of experiments, we will evaluate the black-box function to determine each z^i**

$$x = \begin{pmatrix} x^1 & x^2 & \cdots & x^i & \cdots & x^N \end{pmatrix}$$



$$z = \begin{pmatrix} z^1 & z^2 & \cdots & z^i & \cdots & z^N \end{pmatrix}$$

MODEL IDENTIFICATION

- **Goal: Identify the functional form and complexity of the surrogate models**

$$z = f(x)$$

- **Functional form:**
  - **General functional form is unknown: Our method will identify models with combinations of simple basis functions**

Category		$X_j(x)$
I.	Polynomial	$(x_d)^\alpha$
II.	Multinomial	$\prod_{d \in \mathcal{D}' \subseteq \mathcal{D}} (x_d)^{\alpha_d}$
III.	Exponential and logarithmic forms	$\exp\left(\frac{x_d}{\gamma}\right)^\alpha$, $\log\left(\frac{x_d}{\gamma}\right)^\alpha$
IV.	Expected bases	From experience, simple inspection, physical phenomena, etc.

BEST SUBSET METHOD

- **Surrogate subset model:**

$$\hat{z}(x) = \sum_{j \in \mathcal{S}} \beta_j X_j(x)$$

- **Mixed-integer surrogate subset model:**

$$\hat{z}(x) = \sum_{j \in \mathcal{B}} (y_j \beta_j) X_j(x) \quad \text{such that} \quad \begin{array}{ll} y_j = 1 & j \in \mathcal{S} \\ y_j = 0 & j \notin \mathcal{S} \end{array}$$

- **Generalized best subset problem mixed-integer formulation:**

$$\begin{array}{ll} \min\limits_{\beta, y} & \Phi(\beta, y) \\ \text{s.t.} & y_j = \{0, 1\} \end{array}$$

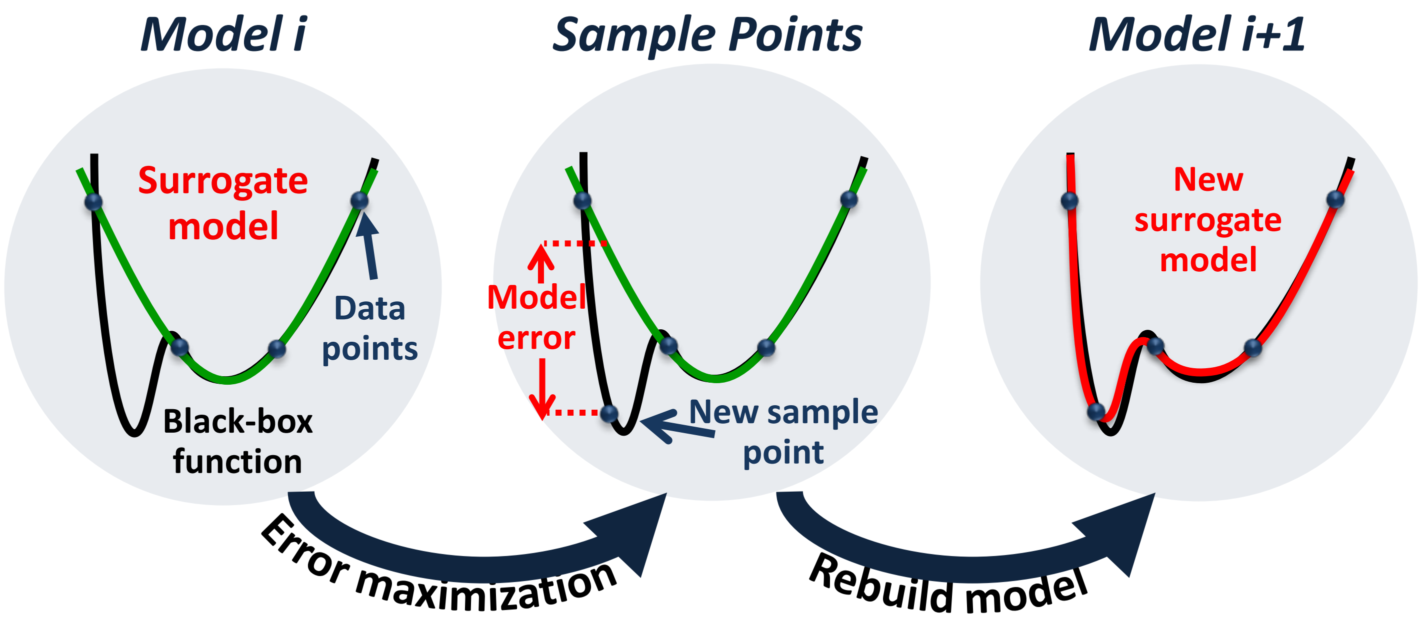
FINAL BEST SUBSET MODEL

$$
\begin{aligned}
\min \quad & SE = \sum_{i=1}^{N} \left| z_i - \sum_{j \in \mathcal{B}} \beta_j X_{ij} \right| \\
\text{s.t.} \quad & \sum_{j \in \mathcal{B}} y_j = T \\
& -U(1 - y_j) \leq \sum_{i=1}^{N} X_{ij} \left(z_i - \sum_{j \in \mathcal{B}} \beta_j X_{ij} \right) \leq U(1 - y_j) && j \in \mathcal{B} \\
& \beta^l y_j \leq \beta_j \leq \beta^u y_j && j \in \mathcal{B} \\
& y_j \in \{0, 1\} && j \in \mathcal{B} \\
& \beta_j \in \left[\beta_j^l, \beta_j^u\right] && j \in \mathcal{B}
\end{aligned}
$$

- **This model is solved for increasing values of *T* until the *AICc* worsens**

ADAPTIVE SAMPLING

- **Goal: Choose new locations to sample that can best be used to improve the model**
- **Solution: Search the problem space for areas of model inconsistency or model mismatch**



ADAPTIVE SAMPLING

- **Goal: Search the problem space for areas of model inconsistency or model mismatch**

- **More succinctly, we are trying to find points that maximizes the model error with respect to the independent variables**

Surrogate model

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

  – **Optimized using a black-box or derivative-free solver (SNOBFIT)** [Huyer and Neumaier, 08]

COMPUTATIONAL TESTING

- **Surrogate generation methods have been implemented into a package:**

ALAMO

(Automated Learning of Algebraic Models for Optimization)

- **Modeling methods compared**
  - **MIP – Proposed methodology**
  - **EBS – Exhaustive best subset method**
    - ***Note: due to high CPU times this was only tested on smaller problems***
  - **LASSO – The lasso regularization**
  - **OLR – Ordinary least-squares regression**

- **Sampling methods compared**
  - **DFO – Proposed error maximization technique**
  - **SLH – Single Latin hypercube (no feedback)**

DESCRIPTION – TEST SET A

- **Two and three input black-box functions randomly chosen basis functions available to the algorithms with varying complexity from 2 to 10 terms**

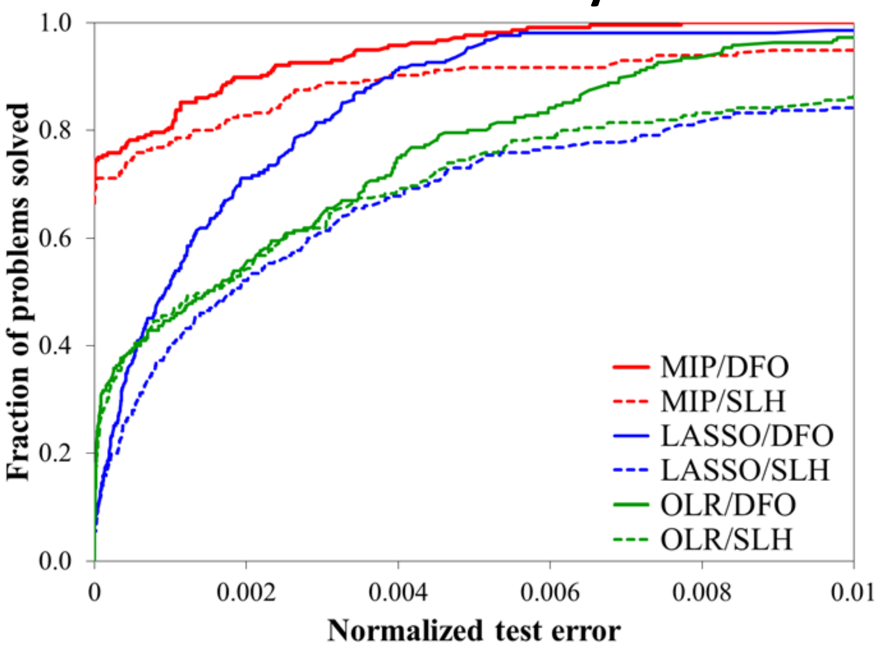
- **Basis functions allowed:**

Category		$X_j(x)$	Parameters used
I.	Polynomial	$(x_d)^\alpha$	$\alpha = \{\pm 3, \pm 2, \pm 1, \pm 0.5\}$
II.	Multinomial	$\prod_{d \in \mathcal{D}' \subseteq \mathcal{D}} (x_d)^{\alpha_d}$	for $\lvert\mathcal{D}'\rvert = 2 \quad \alpha = \{\pm 2, \pm 1, \pm 0.5\}$ for $\lvert\mathcal{D}'\rvert = 3 \quad \alpha = \{\pm 1\}$
III.	Exponential and logarithmic forms	$\exp\left(\frac{x_d}{\gamma}\right)^\alpha, \log\left(\frac{x_d}{\gamma}\right)^\alpha$	$\alpha = 1, \ \gamma = 1$

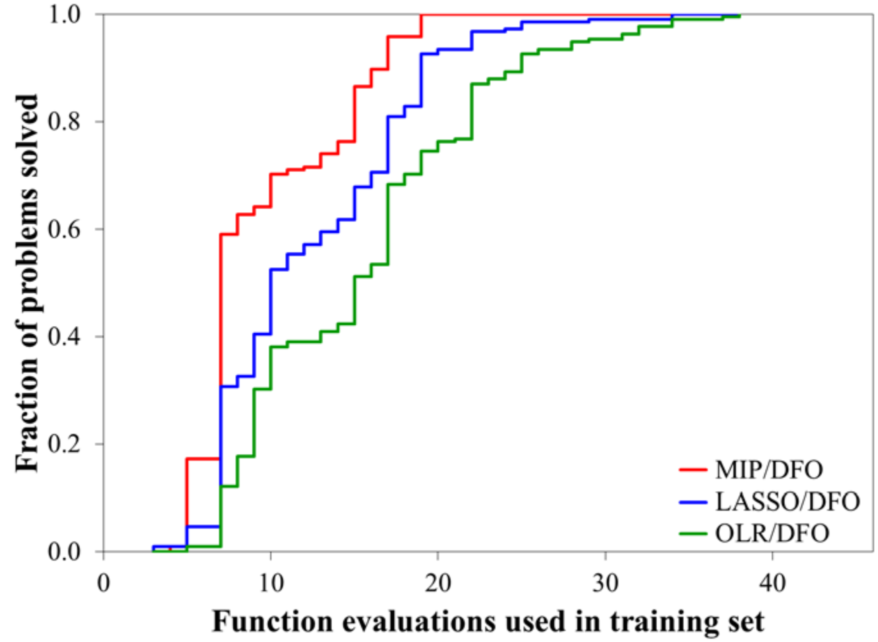
True basis function coefficients were randomly chosen from a uniform distribution where $\beta \in [-1, 1]$.

RESULTS – TEST SET A

Model accuracy



Function evaluations



45 test problems, repeated 5 times, tested against 1000 independent data points

MODEL COMPLEXITY – TEST SET A

No. inputs	No. true terms	MIP/ DFO	MIP/ SLH	EBS/ DFO	EBS/ SLH	LASSO/ DFO	LASSO/ SLH	OLR/ DFO	OLR/ SLH
2	2	2	[2, 2]	2	2	[6, 8]	[6, 11]	[12, 15]	[12, 15]
2	3	3	3	3	3	[5, 12]	[5, 10]	[12, 14]	[12, 14]
2	4	[3, 4]	[3, 4]	[3, 4]	[3, 4]	[8, 11]	[8, 10]	[11, 12]	[11, 12]
2	5	[2, 4]	[2, 4]	[2, 5]	[2, 5]	[3, 12]	[4, 11]	[10, 16]	[10, 16]
2	6	[5, 6]	[6, 6]	[5, 6]	[6, 6]	[7, 10]	[6, 7]	[11, 13]	[11, 13]
2	7	[4, 6]	[4, 6]	[4, 7]	[4, 7]	[7, 11]	[6, 12]	[8, 13]	[8, 13]
2	8	[4, 5]	[5, 6]	[4, 5]	[5, 6]	[6, 8]	[6, 9]	[10, 15]	[10, 15]
2	9	[4, 6]	[4, 6]	NA	NA	[6, 14]	[7, 12]	[10, 17]	[10, 17]
2	10	[4, 8]	[4, 8]	NA	NA	[5, 14]	[7, 14]	[10, 14]	[10, 14]
3	2	[2, 3]	[2, 3]	NA	NA	[6, 12]	[7, 13]	[27, 29]	[27, 29]
3	3	[3, 3]	[3, 3]	NA	NA	[8, 16]	[7, 15]	[19, 22]	[19, 22]
3	4	4	[3, 4]	NA	NA	[10, 13]	[9, 10]	[16, 21]	[16, 21]
3	5	5	5	NA	NA	[11, 17]	[9, 15]	[15, 23]	[15, 23]
3	6	[5, 6]	[6, 6]	NA	NA	[9, 18]	[10, 13]	[15, 26]	[15, 26]
3	7	7	[7, 8]	NA	NA	[10, 22]	[10, 22]	22	22

DESCRIPTION – TEST SET B

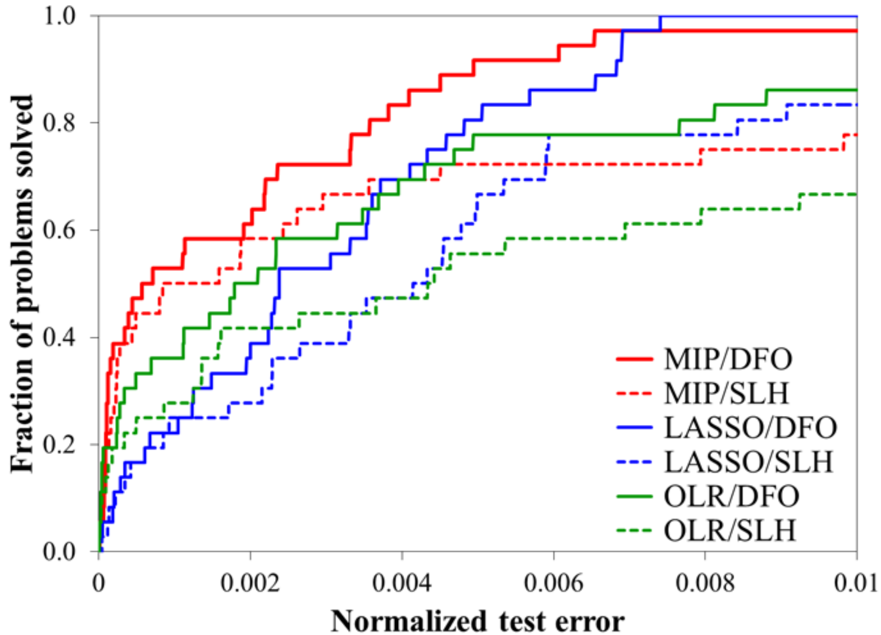
- **Two input black-box functions with basis functions unavailable to the algorithms with**

Function type	Functional form
I	$z(x) = \beta x_i^\alpha \exp(x_j)$
II	$z(x) = \beta x_i^\alpha \log(x_j)$
III	$z(x) = \beta x_1^\alpha x_2^\nu$
IV	$z(x) = \dfrac{\beta}{\gamma + x_i^\alpha}$

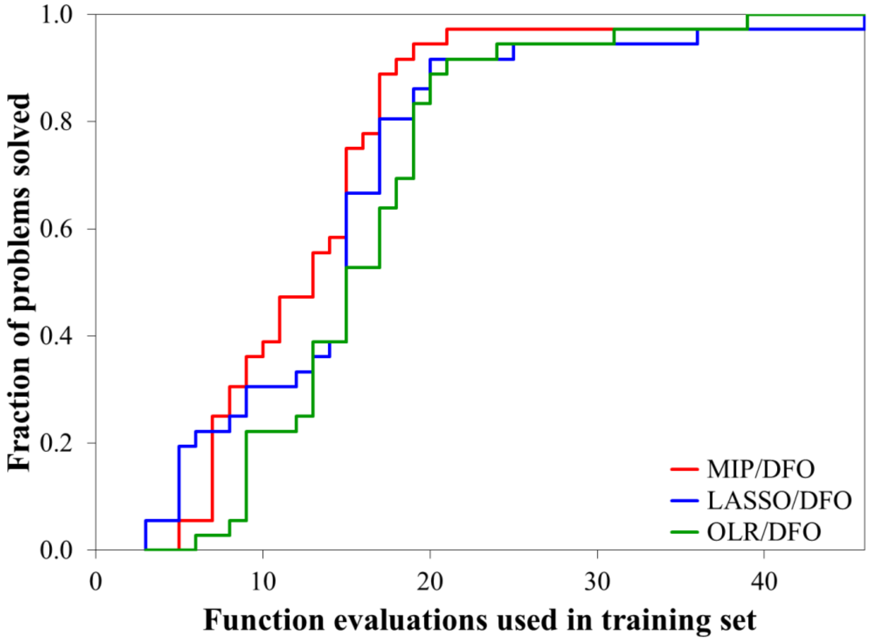
with true parameters chosen from a uniform distribution where $\beta \in [-1, 1]$, $\alpha, \nu \in [-3, 3]$, $\gamma \in [-5, 5]$, and $i, j \in \{1, 2\}$.

RESULTS – TEST SET B

Model accuracy



Function evaluations



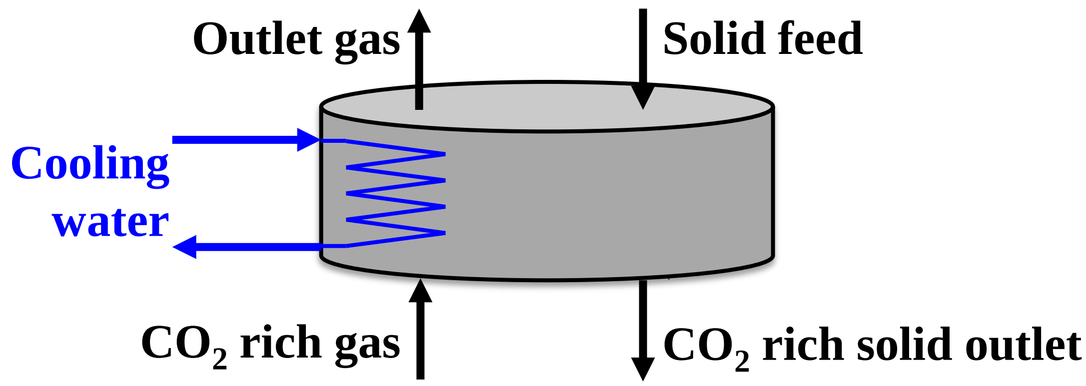
12 test problems, repeated 5 times, tested against 1000 independent data points

MODEL COMPLEXITY – TEST SET B

True function type	Function ID	MIP/ DFO	MIP/ SLH	LASSO/ DFO	LASSO/ SLH	OLR/ DFO	OLR/ SLH
I	a	5	5	[3, 5]	[4, 9]	[6, 17]	[6, 17]
I	b	[4, 10]	[4, 10]	[10, 14]	[5, 8]	[8, 17]	[8, 17]
I	c	[3, 10]	[6, 9]	[8, 9]	[4, 10]	[13, 17]	[13, 17]
II	a	[4, 6]	[4, 10]	[8, 15]	[7, 9]	[15, 19]	[15, 19]
II	b	[1, 7]	[1, 9]	[13, 16]	[11, 17]	[13, 30]	[13, 30]
II	c	[5, 12]	[5, 12]	[9, 13]	[9, 16]	[9, 19]	[9, 19]
III	a	[3, 4]	[1, 4]	[2, 5]	[2, 5]	[9, 20]	[9, 20]
III	b	4	[1, 4]	5	5	[9, 20]	[9, 20]
III	c	[3, 4]	[3, 4]	[5, 8]	[5, 9]	[18, 24]	[18, 24]
IV	a	[7, 8]	[4, 10]	[8, 17]	[11, 18]	[13, 19]	[13, 19]
IV	b	[8, 9]	[9, 10]	[8, 12]	[10, 14]	[9, 17]	[9, 17]
IV	c	[6, 9]	[9, 10]	[5, 13]	[4, 12]	[13, 15]	[13, 15]

BUBBLING FLUIDIZED BED

Bubbling fluidized bed adsorber diagram

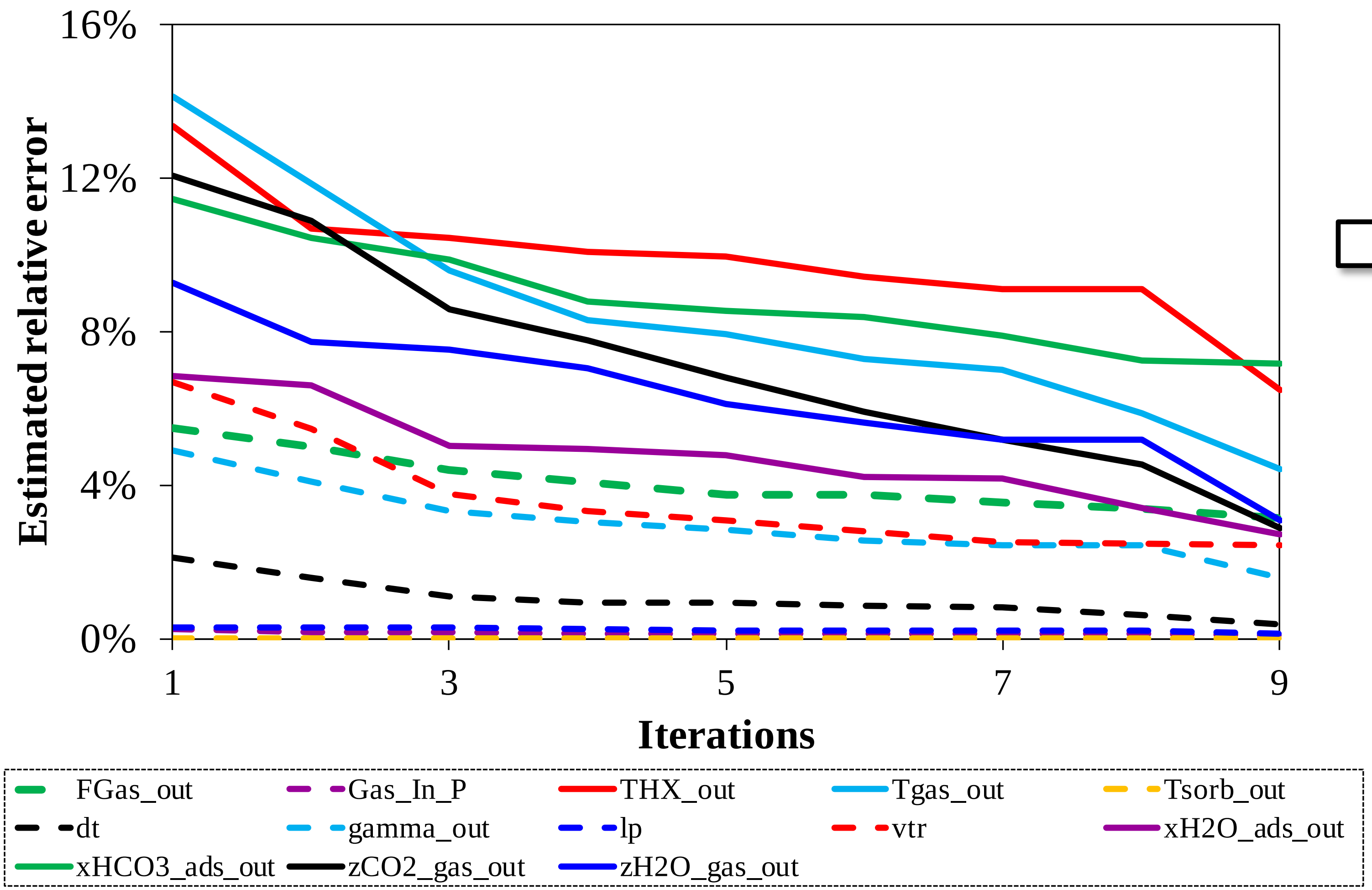


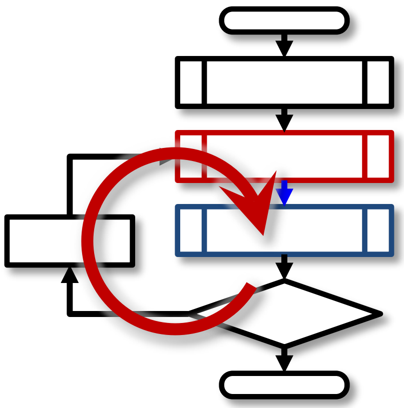
- **Model inputs (14 total)**
  - Geometry (3)
  - Operating conditions (4)
  - Gas mole fractions (2)
  - Solid compositions (2)
  - Flow rates (4)
- **Model outputs (13 total)**
  - Geometry required (2)
  - Operating condition required (1)
  - Gas mole fractions (2)
  - Solid compositions (2)
  - Flow rates (2)
  - Outlet temperatures (3)
  - Design constraint (1)

Model created by Andrew Lee at the National Energy and Technology Laboratory

ADAPTIVE SAMPLING

Progression of mean error through the algorithm

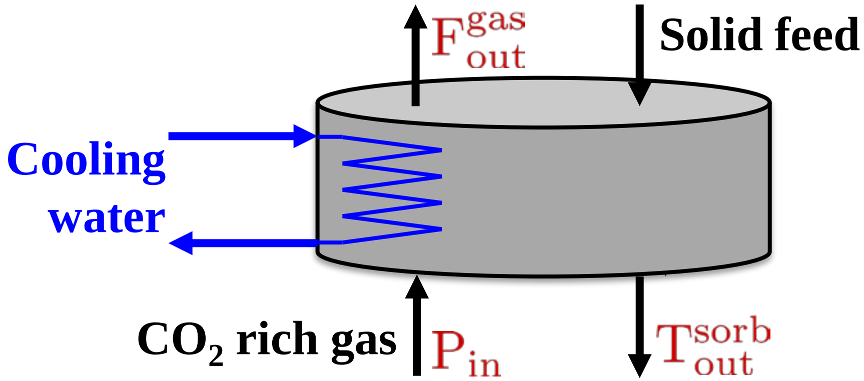




Initial data set: 137 pts

Final data set: 261

EXAMPLE MODELS



$$\mathrm{P_{in}} = 1.0\,\mathrm{P_{out}} + 0.0231\,L_b - 0.0187\,\ln(0.167\,L_b) - 0.00626\,\ln(0.667\,\mathrm{v_{gi}}) - \frac{51.1\,\mathrm{xHCO3^{ads}_{in}}}{\mathrm{F^{gas}_{in}}}$$

$$T^{\mathrm{sorb}}_{\mathrm{out}} = 1.0\,\mathrm{T^{gas}_{in}} - \frac{\left(1.77\cdot 10^{-10}\right)\,\mathrm{NX}^2}{\gamma^2} - \frac{3.46}{\mathrm{NX\,T^{gas}_{in}\,T^{sorb}_{in}}} + \frac{1.17\cdot 10^4}{\mathrm{F^{sorb}\,NX\,xH2O^{ads}_{in}}}$$

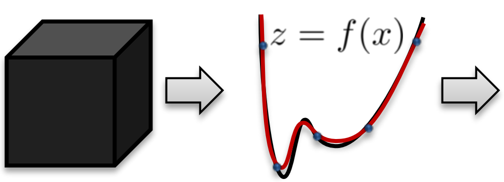
$$F^{\mathrm{gas}}_{\mathrm{out}} = 0.797\,\mathrm{F^{gas}_{in}} - \frac{9.75\,\mathrm{T^{sorb}_{in}}}{\gamma} - 0.77\,\mathrm{F^{gas}_{in}\,xCO2^{gas}_{in}} + 0.00465\,\mathrm{F^{gas}_{in}\,T^{sorb}_{in}} - 0.0181\,\mathrm{F^{gas}_{in}\,T^{sorb}_{in}\,xH2O^{gas}_{in}}$$

CONCLUSIONS

- **The algorithm we developed is able to model black-box functions for use in optimization such that the models are**
  - ✓ **Accurate**
  - ✓ **Tractable in an optimization framework (low-complexity models)**
  - ✓ **Generated from a minimal number of function evaluations**
- **Surrogate models can then be incorporated within a optimization framework with global objective functions and additional constraints**
- **http://archimedes.cheme.cmu.edu/?q=alamo**

ALAMO

Automated **L**earning of **A**lgebraic **M**odels for **O**ptimization



$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & g(x) = 0 \end{aligned}$$

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