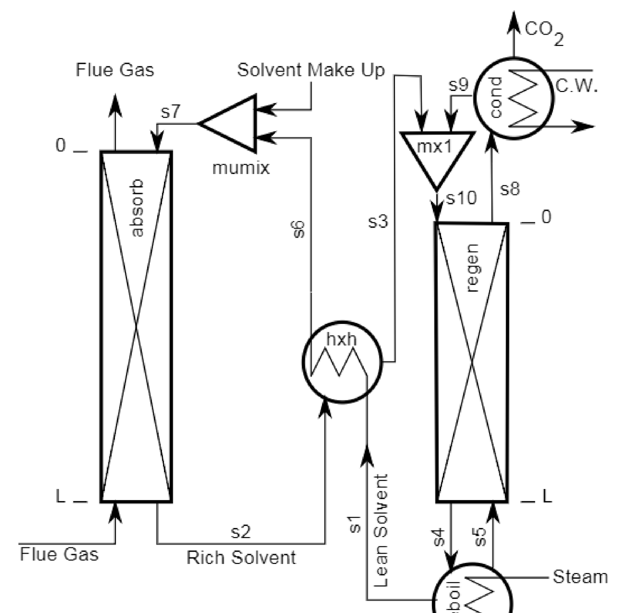
# A General Approach for Robust Process Design: Application to a $CO_2$ Capture Flowsheet

**Natalie M. Isenberg**[a], Paul Akula[b], Debangsu Bhattacharyya[b], David C. Miller[c], Chrysanthos E. Gounaris[a]
[a]Carnegie Mellon University, [b]West Virginia University, [c]National Energy Technology Laboratory

## Motivation: MEA-$CO_2$ Capture System

### Property Uncertainty in Sub-Models[1]

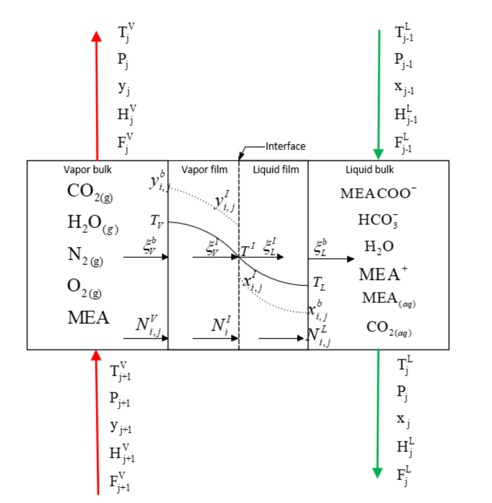
- Parameters describing thermodynamics, kinetics, and/or transport phenomena are not known with certainty
- Many properties are obtained via data regression, leading to confidence intervals




Process flowsheet

### Operational Uncertainty

- Feedstock quality varies over time
- Process economics and market conditions vary over time



Two-film based vapor-liquid interface

**Key Objective:**
To develop IDAES capability to apply robust optimization methodologies during the optimization of advanced energy systems under uncertainty

## Robust Optimization

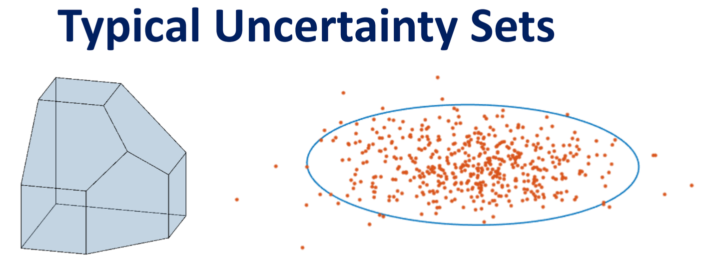
### Robust Optimization (RO)[2,3,4]

- Rigorous uncertainty mitigation framework for mathematical optimization models
- Seeks the **best possible solution** that **remains feasible** for every possible realization of the uncertainty from within a specified **uncertainty set**

**RO Counterpart Formulation**

$$\begin{aligned} \min_{x \in \mathbb{R}} \ \max_{q \in \mathcal{Q}} \ & f(x,q) \\ \text{s.t.} \ & g(x,q) \le 0 \quad \forall q \in \mathcal{Q} \end{aligned}$$

**Typical Uncertainty Sets**



Polyhedral　　Ellipsoidal

- The uncertainty set can be constructed based on historical data, i.e., probability densities, confidence intervals

### Standard RO Approach

Epigraph Reformulation

$$\begin{aligned} \min_{x \in \mathbb{R}} \ & x_0 \\ \text{s.t.} \ & \max_{q \in \mathcal{Q}} f(x,q) \le x_0 \\ & \max_{q \in \mathcal{Q}} g(x,q) \le 0 \end{aligned}$$

Duality-based Reformulation

$$\begin{aligned} \min_{x \in \mathbb{R}} \ & x_0 \\ \text{s.t.} \ & \min_{p \in \mathcal{P}^f} f^D(x,p) \le x_0 \\ & \min_{p \in \mathcal{P}^g} g^D(x,p) \le 0 \end{aligned}$$

Single-level Equivalent

$$\begin{aligned} \min_{x, p^f, p^g \in \mathbb{R}} \ & x_0 \\ \text{s.t.} \ & f^D(x,p^f) \le x_0 \\ & p^f \in \mathcal{P}^f \\ & g^D(x,p^g) \le 0 \\ & p^g \in \mathcal{P}^g \end{aligned}$$

## Generalized Robust Cutting Set Method

### Challenges with Non-Linear Robust Optimization (NLRO)

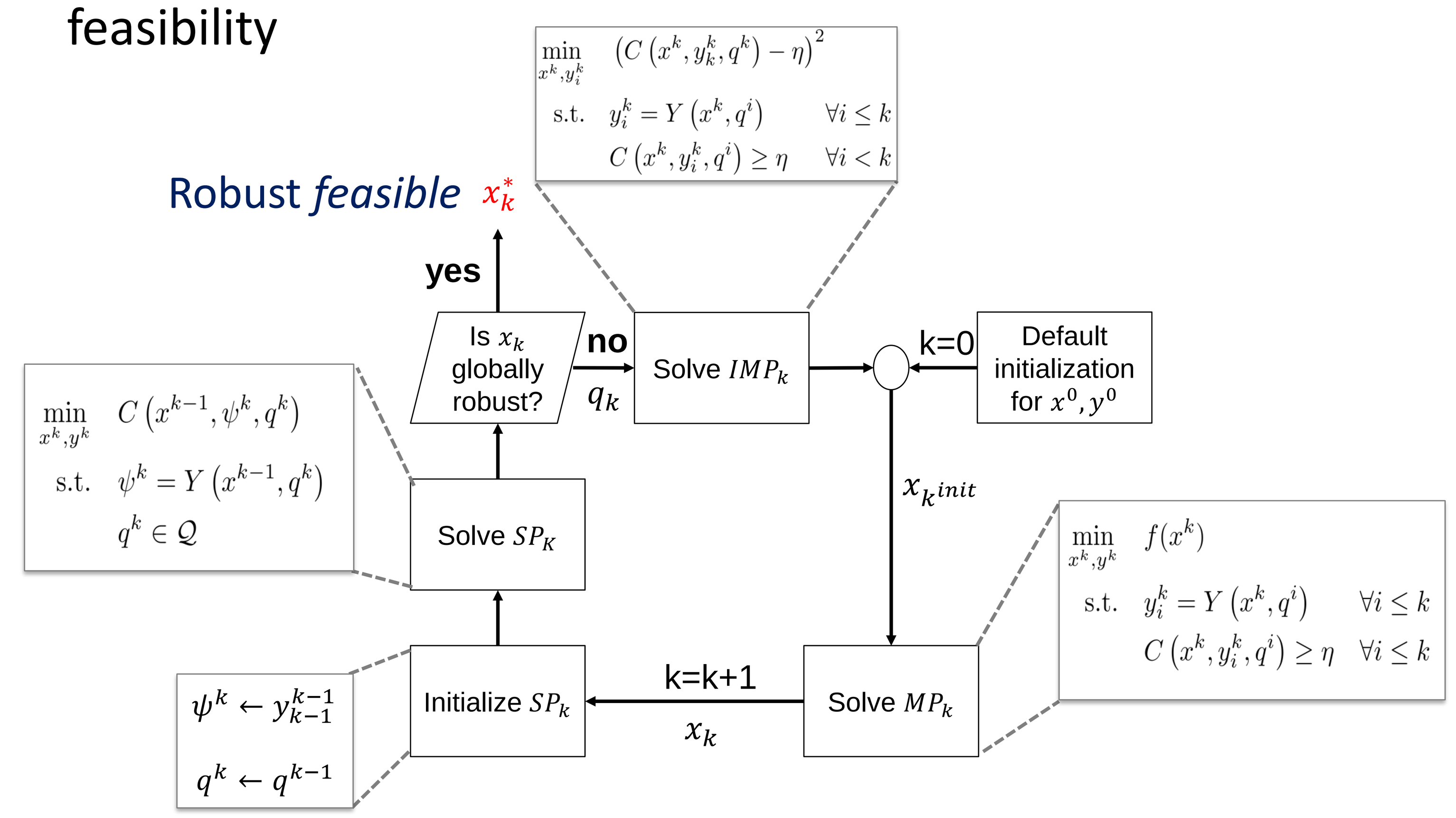
- The duality gap present in non-convex models gives rise to **overly conservative, and hence suboptimal, solutions**
- The presence of **state-equations** requires special treatment

### Robust Cutting Set Approach (RCS)[5]

- Utilizes the primal deterministic model
- Sequentially hedges against uncertainty set by separating uncertainty realizations that violate one or more constraints, until no more violations are found

### Generalized RCS (GRCS) Algorithm

- State variables are copied for realizations of uncertain parameters found to violate inequality constraints
- Utilizes local and global NLP solvers to guarantee robust feasibility




**Potential Issues:**

1. Linear growth of master problem size may not be practical for large models.
2. We need to investigate if the use of local NLP solvers yields iterations that do indeed increase robustness monotonically, thus ensuring convergence.

## Generalized RCS Method with Decision Rules

### Adjustable Robust Optimization

- Treats state variables as second-stage decision variables
- Postulates nonlinear decision rule (relationship) between second-stage variables and uncertain parameters, and substitute
- **Eliminates state variables from robust counterpart formulation**

$$\begin{aligned} \min_{x \in \mathbb{R}^p} \ \max_{q \in \mathcal{Q}} \ \min_{y \in \mathbb{R}^n} \ & y_0 \\ \text{s.t.} \ & g_j(x,y,q) \le 0 \quad \forall j \in J \\ & h_i(x,y,q) = 0 \quad \forall i \in I \end{aligned}$$

$$y = \bar{y}(d,q)$$

$$\begin{aligned} \min_{x,d \in \mathbb{R}^p} \ \max_{q \in \mathcal{Q}} \ & y_0 \\ \text{s.t.} \ & g_j(x,\bar{y}(d,q),q) \le 0 \quad \forall j \in J, \forall q \in \mathcal{Q} \\ & h_i(x,\bar{y}(d,q),q) = 0 \quad \forall i \in I, \forall q \in \mathcal{Q} \end{aligned}$$

**Coefficient matching**

$$\begin{aligned} \min_{x,d \in \mathbb{R}^p} \ \max_{q \in \mathcal{Q}} \ & y_0 \\ \text{s.t.} \ & \bar{g}_j(x,d,q) \le 0 \quad \forall j \in J, \forall q \in \mathcal{Q} \\ & \bar{h}_i(x,d) = 0 \quad \forall i \in I \end{aligned}$$

## GRCS Implementation and Results

### Uncertainty In MEA-$CO_2$ Flowsheet

- Goal: optimize economics while achieving 90% capture
- Uncertainty in equilibrium constant parameters $b_1, b_2$

$$K_{eq,i} = e^{\left(a_i + \frac{b_i}{T} + c_i \log(T)\right)} \qquad i = 1,2$$

- $K_{eq,i}$ implicitly relate to capture performance constraint
- Postulate ellipsoidal uncertainty set, 95% confidence interval

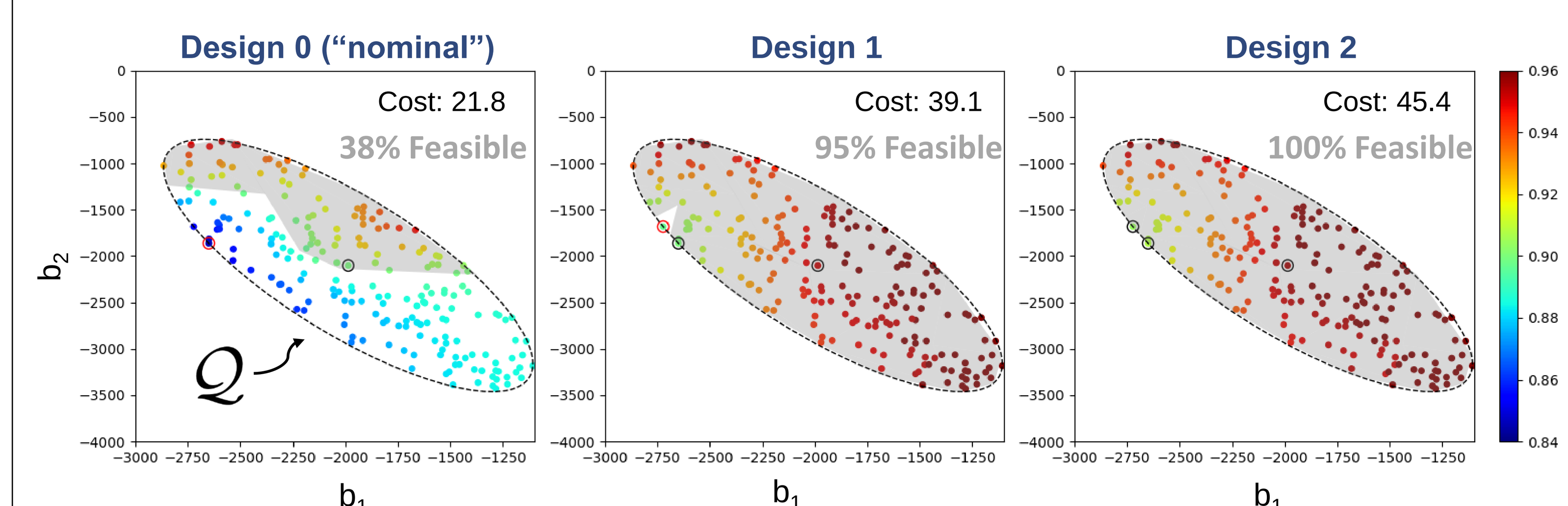
$$q = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \qquad \mathcal{Q} \ : \ (q - q_0)^T \Sigma^{-1} (q - q_0) \le s$$

### GRCS Algorithm Implementation in Pyomo

- **Heat maps** below show relative robustness and cost of solutions at each iteration

Legend:
○ Explicitly robust against
○ Violation identified in separation

: shaded regions = feasible region for given design




- Utilizing the GCRS approach, we **can identify designs that are proven to be robust feasible** against the whole uncertainty set

## Conclusions

- ➢ Process systems models inherently contain parametric uncertainty
- ➢ NLRO capabilities within IDAES will allow users to design processes that remain robust against such uncertainty

## References

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## Contacts

Natalie M. Isenberg, nisenberg@cmu.edu; Chrysanthos E. Gounaris, gounaris@cmu.edu