

# A General Approach for Robust Process Design: Application to a CO<sub>2</sub> Capture Flowsheet

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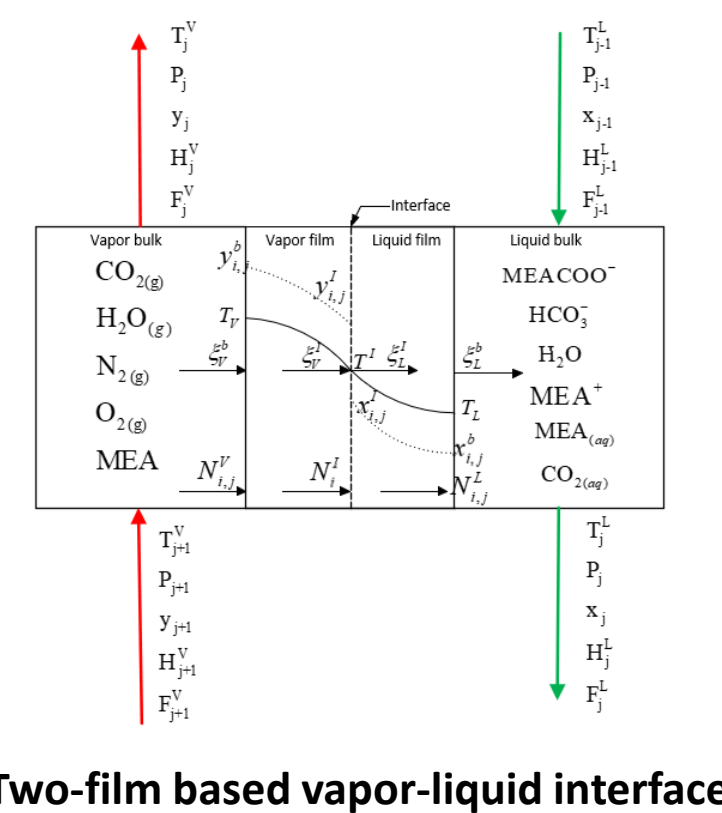
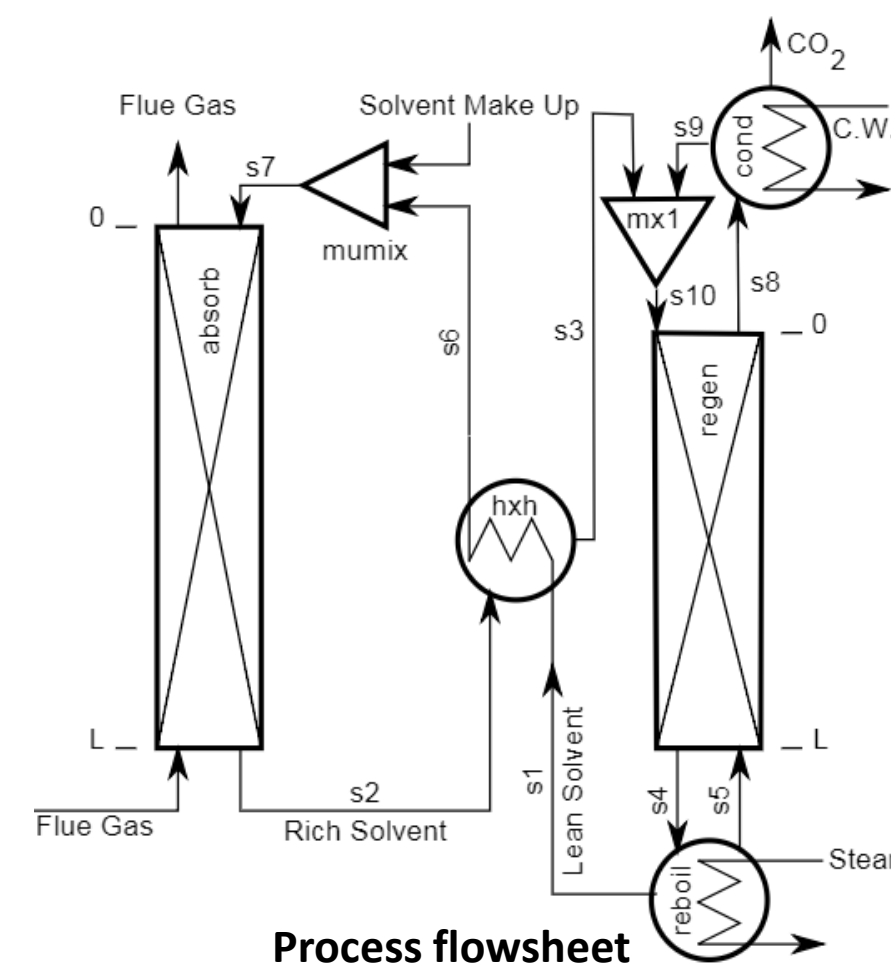
## MOTIVATION: MEA-CO<sub>2</sub> CAPTURE SYSTEM

### Property Uncertainty in Sub-Models<sup>[1]</sup>

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

### Operational Uncertainty

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



### Key Objective:

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

## ROBUST OPTIMIZATION

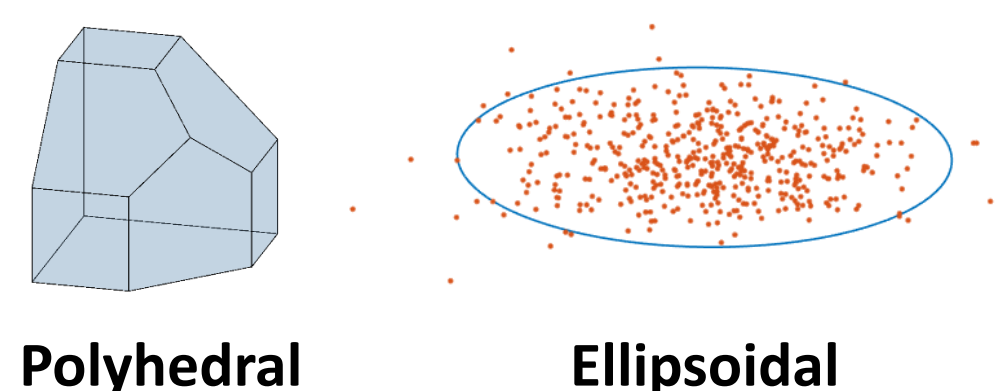
### Robust Optimization (RO)<sup>[2,3,4]</sup>

- 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

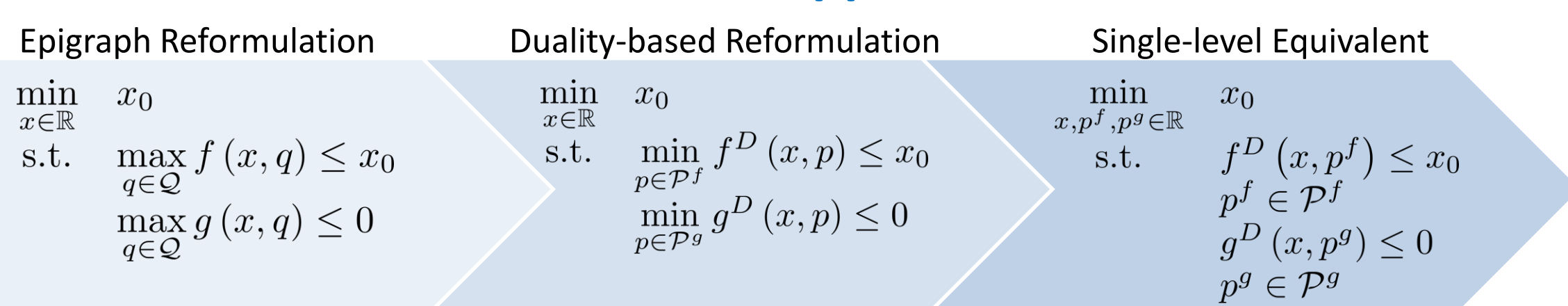
$$\begin{aligned} \min_{x \in \mathbb{R}} \quad & \max_{q \in \mathcal{Q}} f(x, q) \\ \text{s.t.} \quad & g(x, q) \leq 0 \quad \forall q \in \mathcal{Q} \end{aligned}$$

### Typical Uncertainty Sets



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

### Standard RO Approach



## GENERALIZED ROBUST CUTTING SET METHOD

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

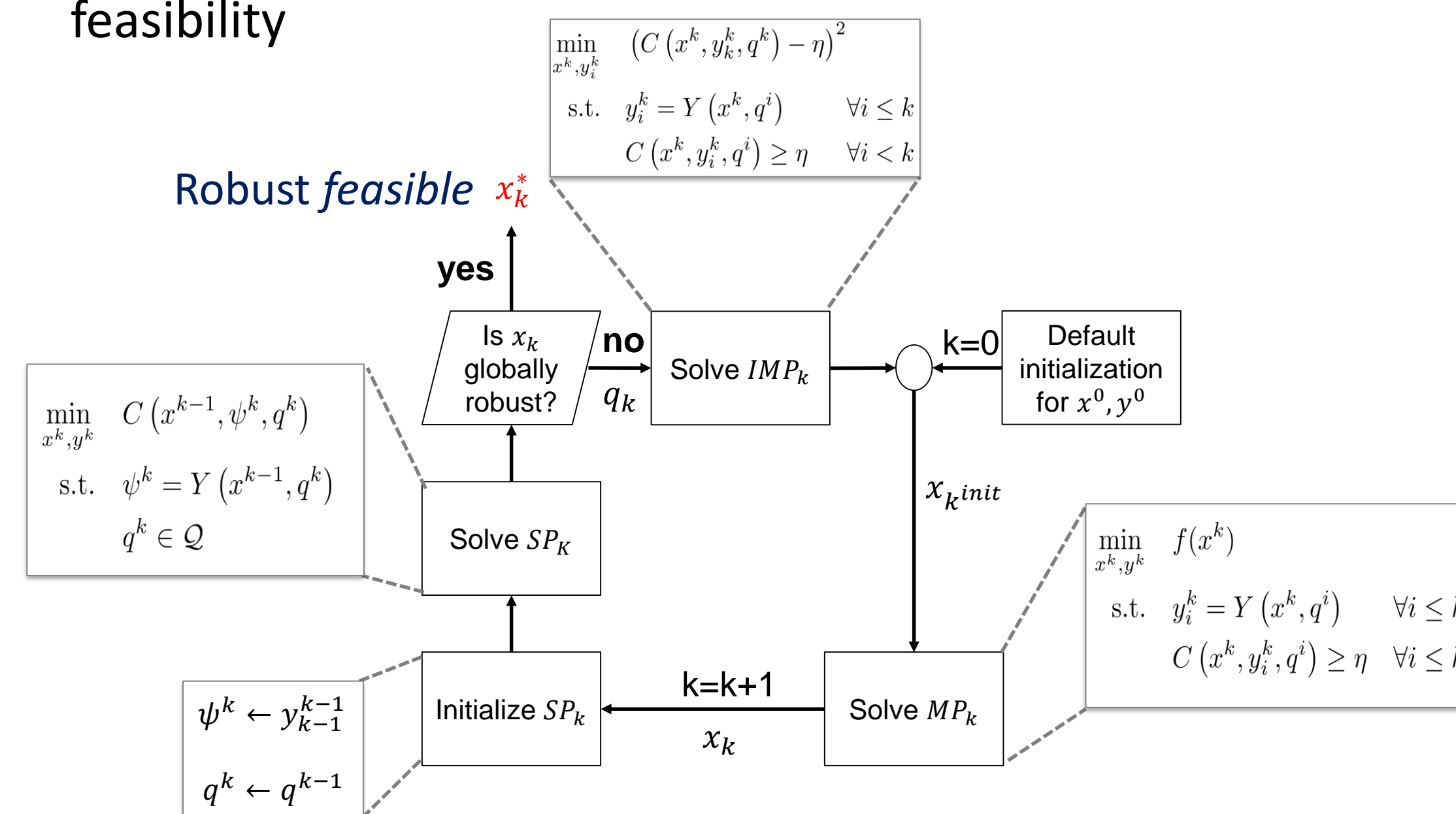
- The duality gap present in non-convex models gives rise to **overly conservative, and hence suboptimal, solutions**
- The presence of **state-equations** requires special treatment

### Robust Cutting Set Approach (RCS)<sup>[5]</sup>

- 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



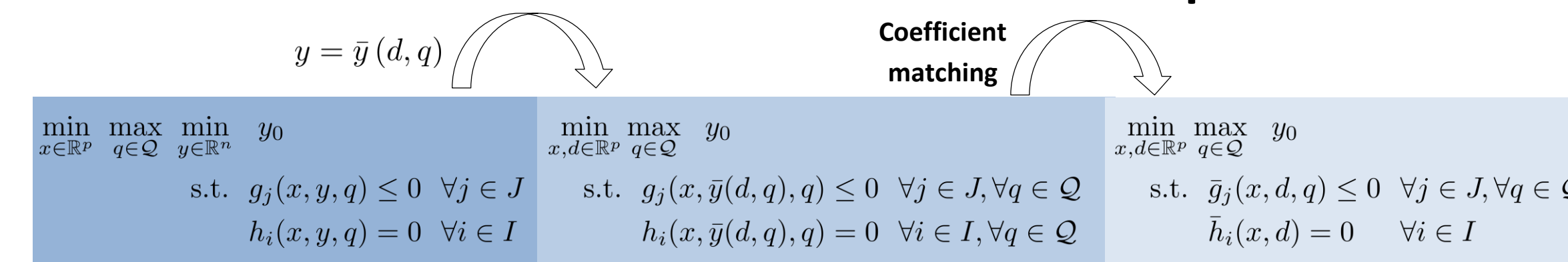
### Potential Issues:

- Linear growth of master problem size may not be practical for large models.
- 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**



## GRCS IMPLEMENTATION AND RESULTS

### Uncertainty In MEA-CO<sub>2</sub> Flowsheet

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

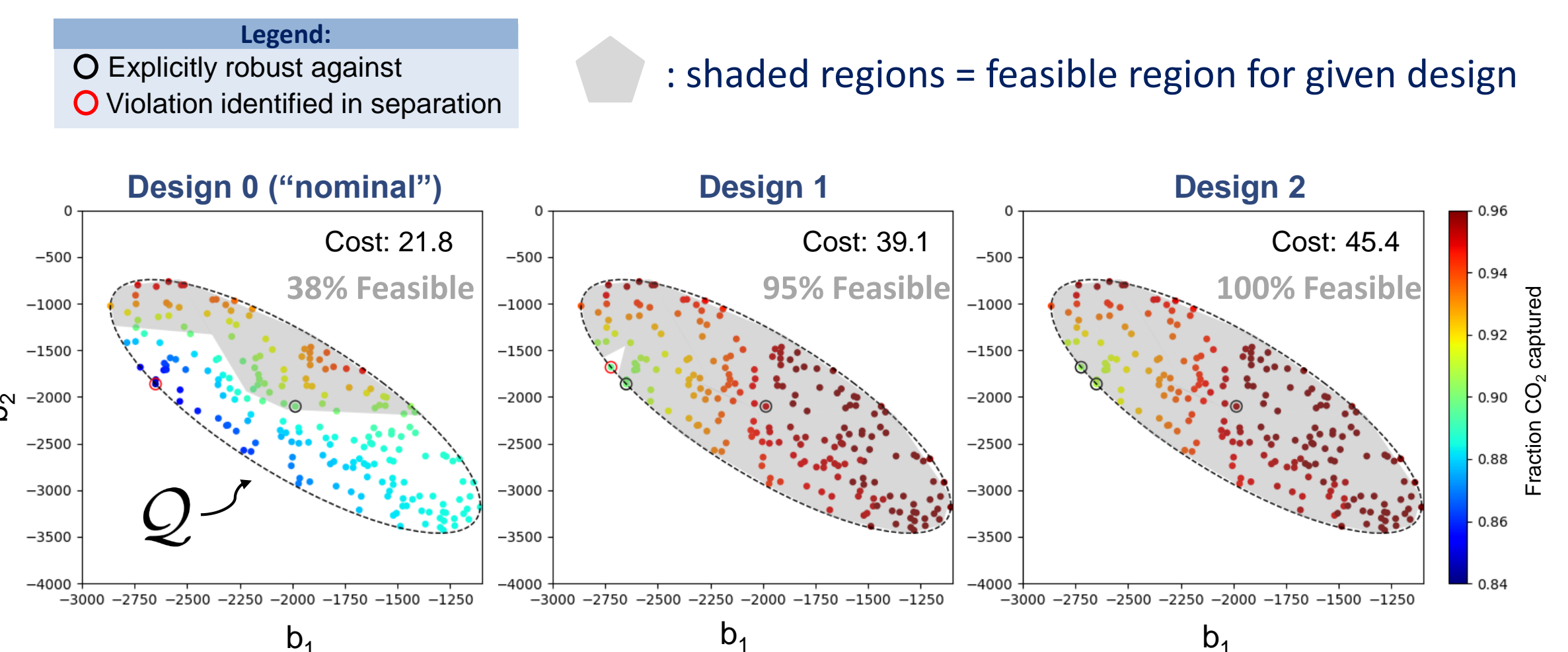
$$K_{eq,i} = e^{(a_i + \frac{b_i}{T} + c_i \log(T))} \quad i = 1, 2$$

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

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

### GRCS Algorithm Implementation in Pyomo

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



- Utilizing the GRCS 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

- Morgan, J.C., Bhattacharyya, D., Tong, C. Miller, D.C. (2015). Uncertainty quantification of property models: Methodology and its application to CO<sub>2</sub>-loaded aqueous MEA solutions. *AIChE Journal*, 61(6):1822-1839
- D. Bertsimas, D.B. Brown and C. Caramanis (2011). *Theory and Applications of Robust Optimization*. SIAM Review, 53(3):464
- B.L. Gorissen, I. Yanikoglu and D. den Hertog (2015). A Practical Guide to Robust Optimization. *Omega*, 53:124
- C.E. Gounaris (2017). Advances in Robust Optimization and Opportunities for Process Operations. In: *Proceedings of FOCAPO 2017/CPC IX*, Paper ID IF110
- A. Mutapcic and S. Boyd, (2009). "Cutting-set methods for robust convex optimization with pessimizing oracles." *Optimization Methods & Software* 24.3 (2009): 381-406.

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