Designing an Amine-Based CO_2 Absorption System in Light of Epistemic Uncertainty

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Background

- Amine-based CO_2 absorption systems are considered important for CO_2 emissions reduction pathways
- Models for amine-based absorption are highly sensitive to epistemic uncertainty in their thermodynamic and physical property submodels

Objectives

- Development of a rate-based optimization model for an MEA-based absorption column for CO_2 removal from NGCC flue gas
- Uncertainty quantification (UQ) studies to assess the robustness of deterministically optimal designs
- Two-stage robust optimization (RO) with the recently developed PyROS solver for technical risk reduction

Absorption Column Model

Degrees of Freedom:

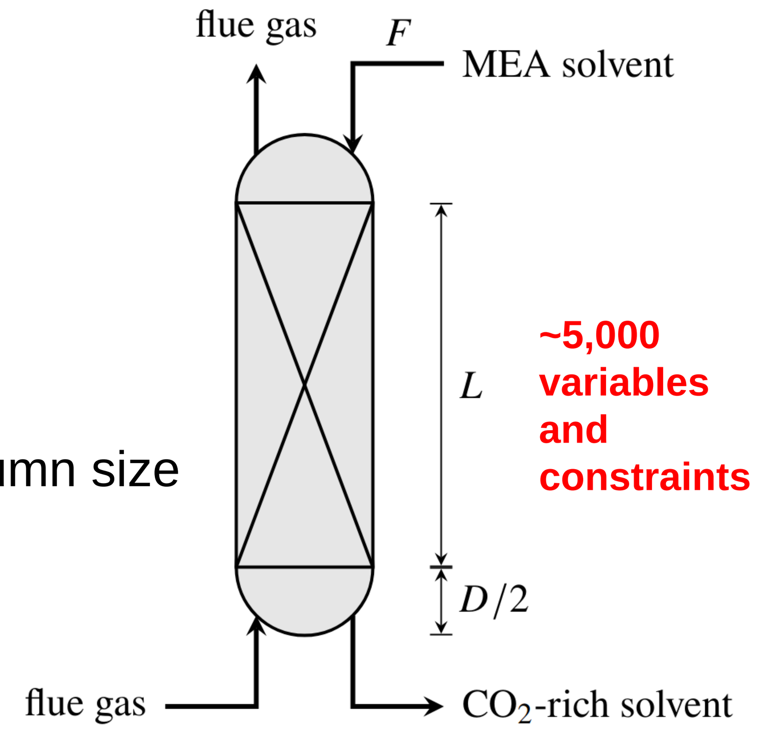
- **Column length (L)**
- **Column diameter (D)**
- **Solvent recirculation rate (F)**
  - adjustable during operation

Minimize:

- **Proxy cost objective** combining column size (CAPEX) and MEA flowrate (OPEX)

Subject to:

- **Process equality constraints**
  - thermodynamic and transport equations
- **Sizing constraints**
  - bounds on the L/D ratio (1.2–30 used)
- **Performance constraints**
  - CO_2 capture rate requirement
  - Flooding fraction bound constraints (simplified after rigorous analysis)

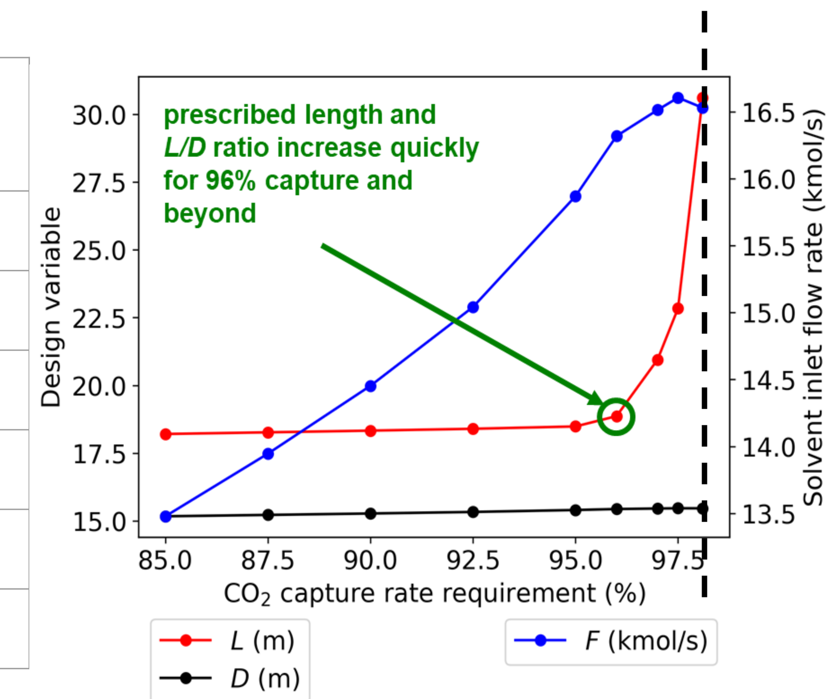


~5,000 variables and constraints

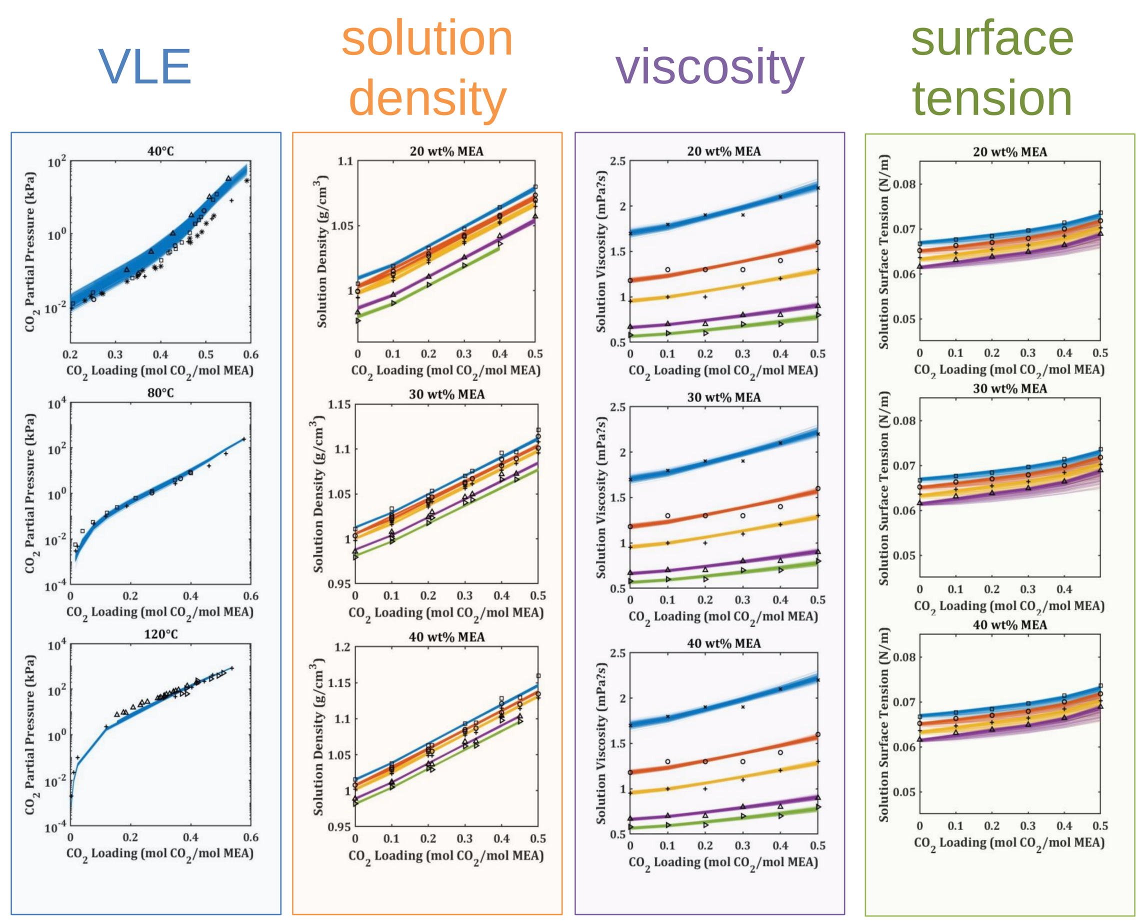
Deterministic Optimization

- Gives **minimal cost designs** for different capture targets
- Model predicts maximum possible CO_2 capture rate of 98.2% (dashed line), we were able to obtain designs for targets up to 98.1%

% Capture Target	Cost
85.0	13.69
87.5	14.00
90.0	14.32
92.5	14.70
95.0	15.21
97.0	16.06



Parameter Estimation and UQ



Used **parmest**[1] to identify **point estimates** and **covariances** in:

- vapor-liquid equilibrium (VLE),
- solution density,
- viscosity, and
- surface tension

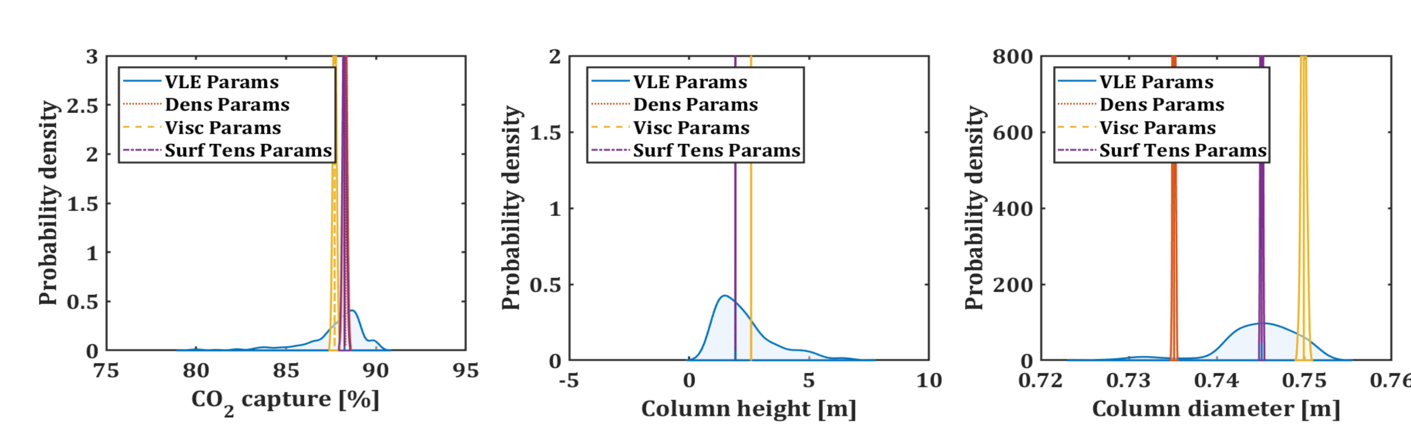
parameters.

Outcomes:

(1) Model predictions most affected by uncertainty in **VLE parameters**

(2) Insignificant response to uncertainty in the remaining property model parameters

Uncertainty Propagation through absorption column model:



Non-Robustness of Nominal Designs

- **Nominal designs are non-robust and less likely to adapt to increased capture targets**
- **A significant level of over-design required to establish guarantees**

Nominally optimal for increasing % capture

Deterministic Solution for Min. % CO_2 Capture	Objective (10^3 m^3)	Total % Gaussian Probability Mass (and number of realizations out of 200) Feasible Subject to Capture Rate % Requirement of					
		85.0	**87.5**	**90.0**	**92.5**	**95.0**	**97.0**
85.0	13.69	48.1 (81)	1.2 (8)	0.0 (0)	0.0 (0)	0.0 (0)	0.0 (0)
87.5	14.00	90.3 (143)	46.9 (75)	3.9 (10)	0.0 (0)	0.0 (0)	0.0 (0)
90.0	14.32	98.5 (180)	81.1 (136)	48.1 (83)	6.0 (23)	0.0 (0)	0.0 (0)
92.5	14.70	99.3 (189)	97.6 (170)	80.8 (132)	48.5 (87)	6.4 (26)	0.1 (3)
95.0	15.21	99.8 (190)	99.3 (186)	97.5 (166)	81.9 (132)	48.2 (82)	11.9 (45)
97.0	16.06	99.6 (189)	99.5 (185)	99.5 (184)	98.2 (172)	81.5 (127)	48.2 (82)

Evaluating robustness for increasing capture rate requirement

Two-Stage Robust Optimization with the PyROS Solver

- **PyROS**[2, 3]: a nonconvex two-stage RO solver based on the Pyomo modeling language. Documentation at: https://pyomo.readthedocs.io/en/stable/contributed_packages/pyros.html
- Robust designs are **more expensive** than their deterministic counterparts
- Cost increases **only as necessary for increased feasibility guarantees** (more scenarios factored in)
- Such robust design hierarchies establish an upper limit on the **$ worth spending to reduce uncertainty**
  - *e.g., shall we do more "science" to improve our property models?*

Minimum Capture Rate (%)	Robust Column Proxy Cost and DOF (L, D, F) Values [m, m, kmol/s] for different Confidence Levels			
	0% (deterministic)	**90%**	**95%**	**99%**
90.0	14.32 (18.33, 15.28, 14.45)	17.19 (25.09, 15.51, 17.08)	17.57 (26.43, 15.52, 17.29)	18.37 (29.24, 15.55, 17.76)
92.5	14.70 (18.40, 15.33, 15.04)	18.05 (27.94, 15.54, 17.62)	18.48 (29.50, 15.56, 17.85)	19.40 (32.81, 15.59, 18.33)
95.0	15.21 (18.49, 15.41, 15.87)	19.37 (33.17, 15.58, 18.17)	19.92 (35.33, 15.60, 18.40)	21.14 (40.22, 15.63, 18.87)

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