Robust Design of a Carbon Capture Flowsheet Using PyROS

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Objectives

- **Present recent algorithmic and implementation advances of the Pyomo Robust Optimization Solver (PyROS)**, a Python package for solving nonconvex problems under uncertainty through two-stage robust optimization
- **Demonstrate utility of PyROS for large-scale process systems optimization** through a case study on optimization of an amine-based CO_2 capture system under epistemic uncertainty

Robust Optimization with the PyROS Solver

Two-Stage Decision-Making Framework

Commit upon **first-stage decisions** (i.e., design) → Observe **uncertain parameters** (directly or via system response) → Adjust system with **second-stage decisions** (i.e., control)

Goal of Two-Stage Robust Optimization (RO)

GIVEN

- **Deterministic model** (NLP model)
- **Degree-of-freedom partitioning** into 1st-stage and 2nd-stage
- **Quantification of uncertainty** in form of uncertainty set
  - e.g., 95% confidence ellipsoid

DETERMINE

- System **design that is guaranteed to remain feasible** under all scenarios
- Accompanying control policy to perform any **operating adjustments** needed for system to achieve feasibility
- Optimality in light of a **combined economic objective** (CapEx+OpEx)

Recent Updates to the PyROS Solver

- **Overhauled the preprocessing subroutine and subproblem formulations** to make the solver substantially more efficient and reliable
- **Updated the uncertainty set interfaces** to allow for more careful tracking and initialization of auxiliary uncertain parameters
- **Made the automated testing suite more comprehensive** to establish stronger guarantees that PyROS works as intended
- **Implemented minor documentation and bug fixes**

References

[1] Isenberg, Natalie M., et al. "A generalized cutting-set approach for nonlinear robust optimization in process systems engineering." *AIChE Journal* 67.5 (2021): e17175.

[2] N.M. Isenberg, J. Sherman, J.D. Siirola, C.E. Gounaris, "PyROS: Nonlinear Robust Optimization in Pyomo," Forthcoming, 2024.

Acknowledgements

The authors graciously acknowledge funding from the U.S. Department of Energy, Office of Fossil Energy and Carbon Management, through the Carbon Capture Program and Simulation-based Engineering/Crosscutting Research Program. JS and CEG also graciously acknowledge funding from the Carbon Capture Simulation for Industry Impact (CCSI²) program.

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Computational Benchmarking Study

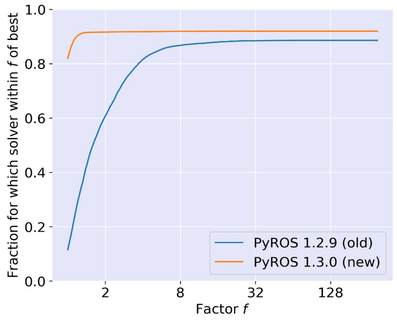
Generated a library of 8,591 two-stage RO model benchmark instances:

- 10 deterministic NLP models (from GAMS and PrincetonLib model libraries)
- 3–5 partionings of the degrees of freedom into first-stage and second-stage variables
- 71 uncertainty set types of varying geometry, size, and dimension
- 3 polynomial decision rule approximation schemes

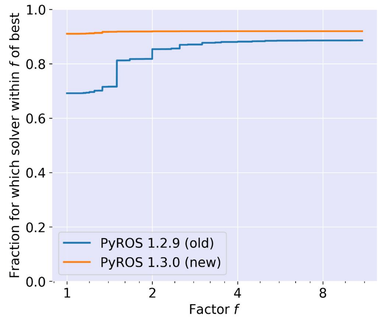
Solver Settings: Pyomo 6.7.4dev0/PyROS 1.3.0, with BARON 23.6.23/CPLEX 22.1.0 as the subordinate global solver

Results: 92.0% of instances solved successfully (vs. 88.6% solved successfully with Pyomo 6.7.1dev0/PyROS 1.2.9)

Solve Time Performance Profile



Iterations Performance Profile



Amine-Based Absorption Flowsheet Model

Degrees of Freedom:

- **Absorber and stripper column dimensions**
- **Cross heat exchanger, reboiler, and condenser areas**
- **Design capacities for** CO_2 capture mass flow rate, rich and lean solvent stream volumetric flow rates, reboiler duty, and initial solvent fill
- **Flow rates** (adjustable during operation):
  - Amine recirculation rate
  - Condenser cooling water flow rate
  - Reboiler steam flow rate

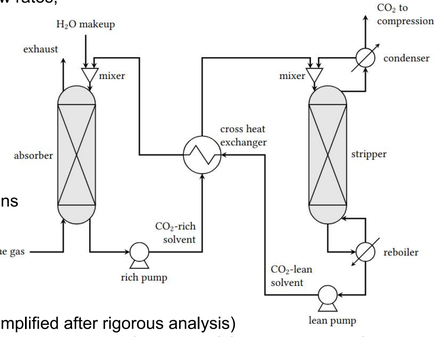
Minimize:

- **Total annualized cost*** of the flowsheet

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)
  - Operating limit constraints of solvent stream volumetric flow rates, CO2 capture mass flow, reboiler duty, and initial solvent fill
- **Uncertainty in six thermodynamic property model parameters**
  - Parameters downselected after rigorous uncertainty propagation studies
  - Confidence ellipsoidal uncertainty set
- **Fixed flue gas feed** flow rate (approximately 9300 mol/s) and composition (4.2 mol % CO_2). Flue gas is obtained from a natural gas combined cycle power plant

~10,000 variables and constraints

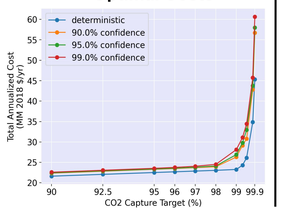


* To avoid solutions with negligible condenser areas, a penalty term proportional to the stripper vapor distillate H_2O mole fraction was added to the objective during the computational studies

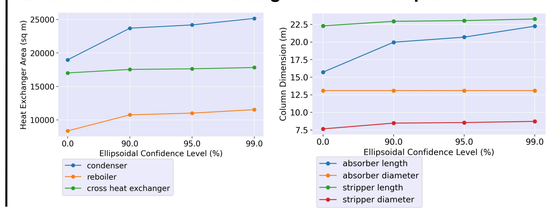
Robust Absorption Flowsheet Designs with PyROS

- Robust designs are **more expensive** and **generally require larger process units** than their deterministic counterparts
- Cost increases **only as necessary for increased feasibility guarantees** (more scenarios factored in)
- 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?*

Optimal Costs



Deterministic vs Robust Designs for 99.9% Capture

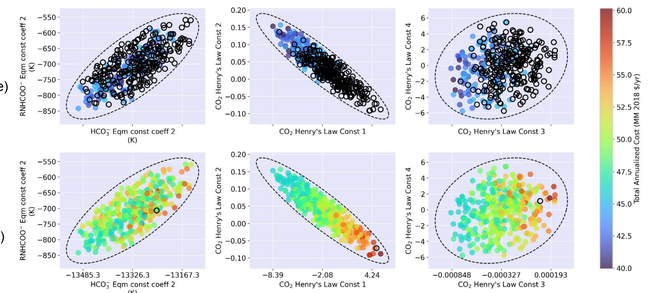


Visualizing feasibility and variations in cost of designs for 99.9% capture

- Generated 400 samples uniformly distributed over the 99% confidence ellipsoidal uncertainty set; the visualizations below show 2D coordinate plane projections
- Fixed the flowsheet design. For each sample, attempted to solve the resulting operational problem with the uncertain parameter values adjusted to the sample, noting the problem feasibility and, if applicable, re-optimized cost
- Calculated the total self-normalized Gaussian probability weight of the samples for which the operating problem was found to be feasible
  - infeasible

deterministic
26.27% feasible
(133/400 samples feasible)

99% confidence
98.99% feasible
(399/400 samples feasible)



Key Takeaways

- PyROS is designed to minimize the effort required to extend nonlinear deterministic optimization models to two-stage RO workflows
- Benchmarking results demonstrate the performance and reliability of PyROS on small-scale problem instances of varying problem size, nonconvexity, and uncertainty quantification
- PyROS is capable of obtaining robust solutions to large-scale CO_2 absorption process systems models, varied by CO_2 capture target and uncertainty quantification