

Optimal Design of a Distillation System for the Flexible Polygeneration of Dimethyl Ether and Methanol Under Uncertainty



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- Links to articles cited in the study
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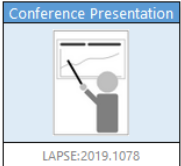
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Optimal Design of a Distillation System for the Flexible Polygeneration of Dimethyl Ether and Methanol Under Uncertainty

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October 18, 2019

Conference Presentation



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This presentation concerns the promising new area of flexible polygeneration, a chemical process design concept in which a chemical plant is able to change its product outputs throughout its lifetime in response to changing market conditions, business objectives, or other external factors. In this talk we present a new flexible polygeneration process system that can switch between dimethyl ether (DME) or methanol production, depending on need. Classic flexible polygeneration systems typically utilize separate process trains for each product, in which whole process trains are turned on or off (or up or down) depending on the current product. However, our proposed process combines the two process trains into one, in which most of the process equipment is always used during either mode of production, but with different operating conditions. In this work, we show how this significantly reduces capital expenditure, reduces the plant footprint, and ultimately is more economical than a traditional two-train approach. However, the optimal design problem is complicated because it requires both uncertainty considerations and a sufficiently high level of model rigour for the process equipment since the equipment will be utilized in different ways depending on the mode of operation. Therefore, we also present a novel optimization framework and accompanying methodology which can be used to solve the optimal design problem to global optimality without any loss of model rigour (in our case, rigorous Aspen Plus simulations with embedded Aspen Capital Cost Estimator economic predictions). This is achieved through a tabulation approach that exploits process structure for multicomponent distillation. The methodology allows for the rapid solution of many different kinds of optimization formulations, such as robust min-max formulations, scenario-based approaches, and other formulations, based on the amount of predictive knowledge about the future operations of the flexible polygeneration facility known at the conceptual process design stage.

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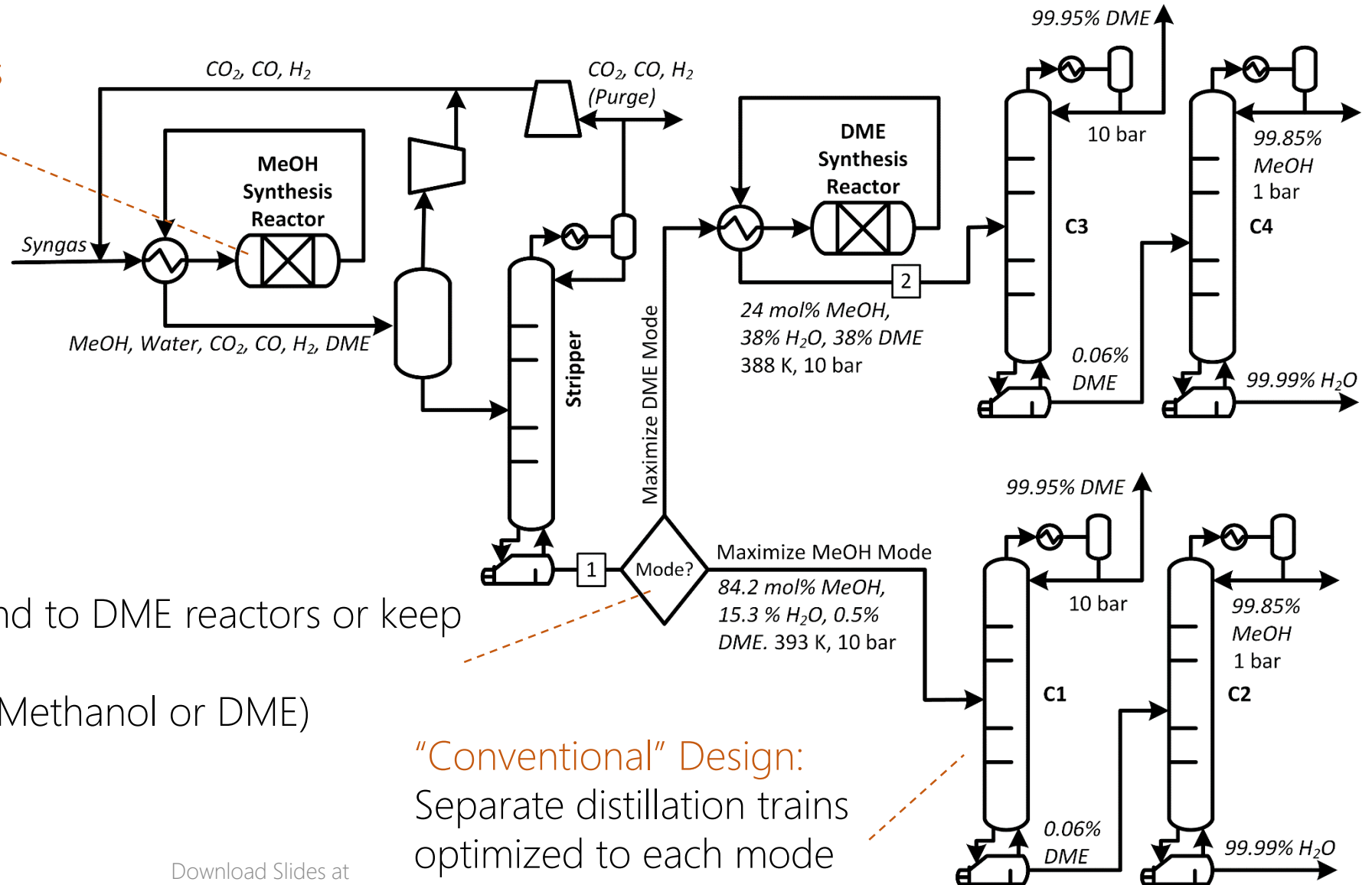
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Original Submitter
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Links to Related Works

Basic Premise: Flexible Production

Methanol synthesis from syngas



On-Demand Decision: Send to DME reactors or keep as product?

Two modes of operation (Methanol or DME)

"Conventional" Design: Separate distillation trains optimized to each mode

Design Under Uncertainty

- **Operating policy:** Operators will choose either DME or Methanol Mode depending on prevailing market conditions at that time.
- **Uncertainty:** Can only guess during the design phase what that proportion will be.
- **Design Implications:** If you think you will spend most of your time in Methanol Mode:
 - Invest in more capital to **ensure lower operating costs for the Methanol section**
 - Want **less efficient DME** section to save capital, since high energy costs will be brief

Optimization Strategy (Naïve Approach)

Decision variables are number of stages above and below feed for each column.

$$TAC_{BaseCase,Exp} = \sum_{c=C1..C4} Z_c$$

$$Z_c = \min_{N_{A,c}, N_{B,c}} TAC_{c,Exp}$$

$$s. t. \quad TAC_{c,Exp} = a_f TDC_c + AOC_{c,Exp}$$

$$AOC_{c,Exp} = h(Q_{H,c}U_{H,c} + Q_{C,c}U_{C,c})(1 - \phi_{Exp,D})(1 - \delta_c)$$

$$+ h(Q_{H,c}U_{H,c} + Q_{C,c}U_{C,c})(\phi_{Exp,D})\delta_c$$

$$\delta_c = \begin{cases} 0 & \text{for } c = C1, C2 \text{ (MeOH Mode)} \\ 1 & \text{for } c = C3, C4 \text{ (DME mode)} \end{cases}$$

$$TDC_c = f_1(A_{C,c}) + f_2(A_{H,c}) + f_3(N_{A,c} + N_{B,c}, D_c)$$

$$A_{C,c} = f_{4,c}(N_{A,c}, N_{B,c})$$

$$A_{H,c} = f_{5,c}(N_{A,c}, N_{B,c})$$

$$D_c = f_{6,c}(N_{A,c}, N_{B,c})$$

$$Q_{H,c} = f_{7,c}(N_{A,c}, N_{B,c})$$

$$Q_{C,c} = f_{8,c}(N_{A,c}, N_{B,c})$$

Minimize TAC of each column separately.

Because each column must meet a design spec by definition, they can be split into the sum of four minimization problems.

Key uncertainty parameter.

The amount of time we expect to operate in DME mode over the 15 year life time.

Surface area of condenser / reboiler for column c

Diameter of column c

Reboiler/condenser duties of column c

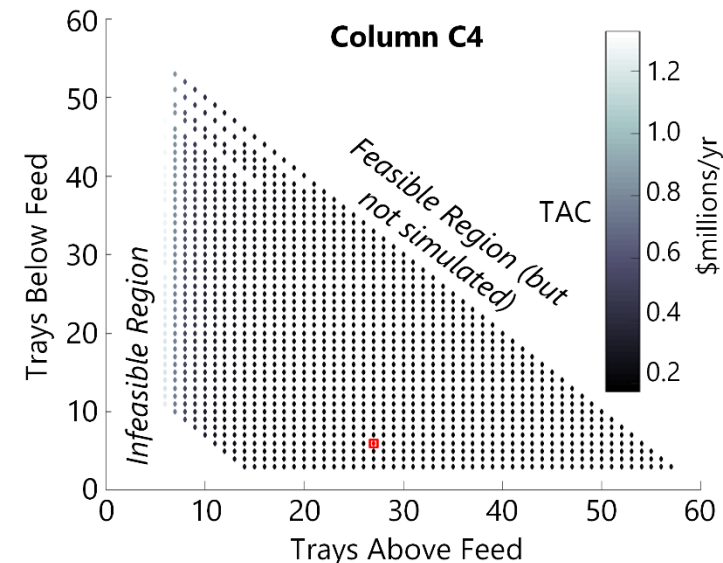
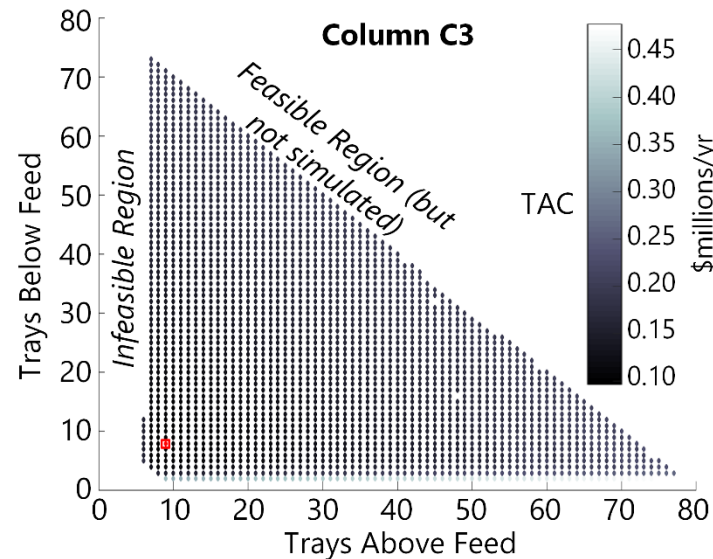
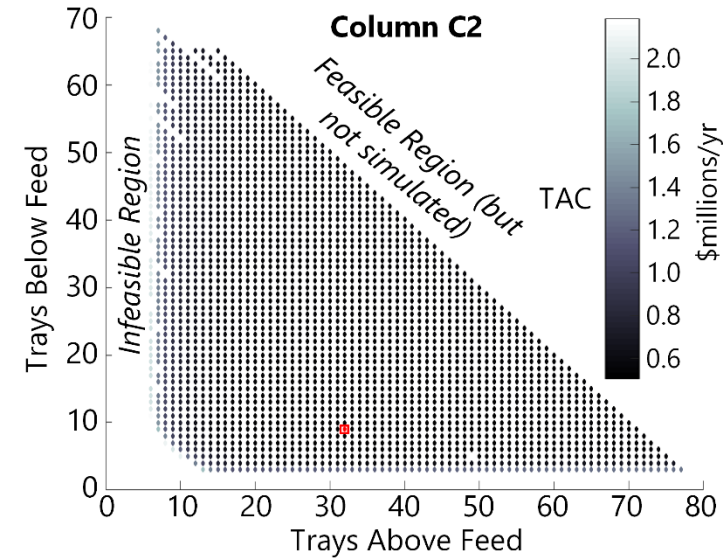
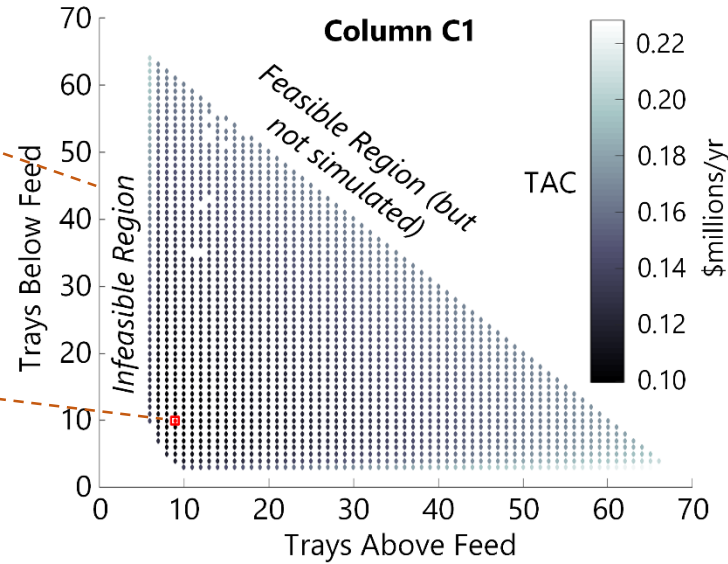
Capital cost models (can be equations or table lookups)

All of these can be exhaustively pre-tabulated with rigorous models in Aspen Plus. Implemented as table lookup.

Solve quickly through exhaustive search

Easy to identify infeasible regions.

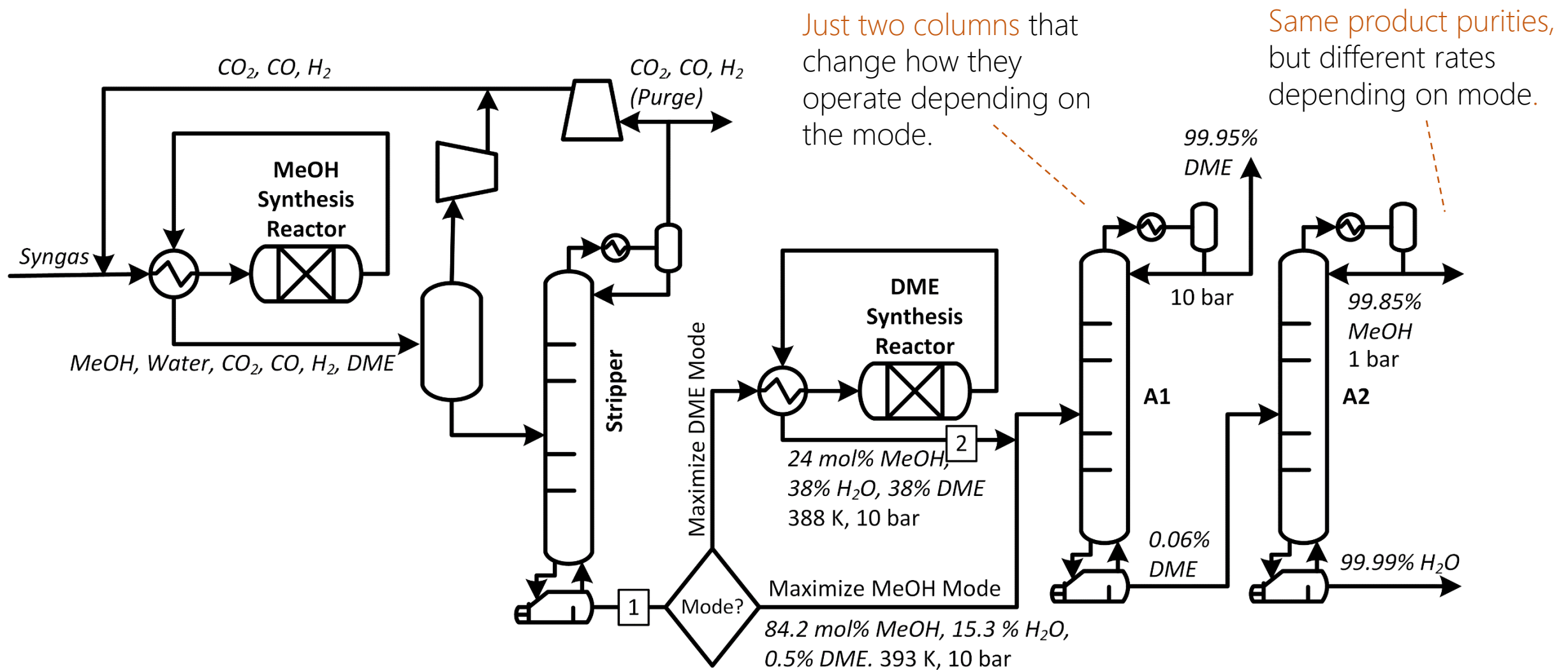
Minimum EXPECTED TAC for each column can be chosen by exhaustive search.



This example is for $\phi_{EXP,D} = 0.5$

Different optimums for different values of $\phi_{EXP,D}$

Alternative Design Strategy



Just two columns that change how they operate depending on the mode.

Same product purities, but different rates depending on mode.

Very quick optimization, trivial extra work

Only 4 decision variables instead of 8.

$$TAC_{CaseA,Exp} = \sum_{c=A1,A2} Z_c$$

$$Z_c = \min_{N_{A,c}, N_{B,c}} TAC_{c,Exp}$$

$$s. t. \quad TAC_{c,Exp} = a_f TDC_c + AOC_{c,Exp}$$

$$AOC_{c,Exp} = h(Q_{H,c,MeOH} U_{H,c} + Q_{C,c,MeOH} U_{C,c})(1 - \phi_{Exp,D}) + h(Q_{H,c,DME} U_{H,c} + Q_{C,c,DME} U_{C,c})(\phi_{Exp,D})$$

$$TDC_c = f_1(A_{C,c}) + f_2(A_{H,c}) + f_3(N_{A,c} + N_{B,c}, D_c)$$

$$A_{C,c} = \begin{cases} \max[f_{4,C1}(N_{A,c}, N_{B,c}), f_{4,C3}(N_{A,c}, N_{B,c})] & \text{for } c = A1 \\ \max[f_{4,C2}(N_{A,c}, N_{B,c}), f_{4,C4}(N_{A,c}, N_{B,c})] & \text{for } c = A2 \end{cases}$$

The max function ensures that the equipment is large enough to handle both modes.

Still have the uncertainty factor.

$$A_{H,c} = \begin{cases} \max[f_{5,C1}(N_{A,c}, N_{B,c}), f_{5,C3}(N_{A,c}, N_{B,c})] & \text{for } c = A1 \\ \max[f_{5,C2}(N_{A,c}, N_{B,c}), f_{5,C4}(N_{A,c}, N_{B,c})] & \text{for } c = A2 \end{cases}$$

$$D_c = \begin{cases} \max[f_{6,C1}(N_{A,c}, N_{B,c}), f_{6,C3}(N_{A,c}, N_{B,c})] & \text{for } c = A1 \\ \max[f_{6,C2}(N_{A,c}, N_{B,c}), f_{6,C4}(N_{A,c}, N_{B,c})] & \text{for } c = A2 \end{cases}$$

$$Q_{H,c,MeOH} = \begin{cases} f_{7,C1}(N_{A,c}, N_{B,c}) & \text{for } c = A1 \\ f_{7,C2}(N_{A,c}, N_{B,c}) & \text{for } c = A2 \end{cases}$$

$$Q_{H,c,DME} = \begin{cases} f_{7,C3}(N_{A,c}, N_{B,c}) & \text{for } c = A1 \\ f_{7,C4}(N_{A,c}, N_{B,c}) & \text{for } c = A2 \end{cases}$$

$$Q_{C,c,MeOH} = \begin{cases} f_{8,C1}(N_{A,c}, N_{B,c}) & \text{for } c = A1 \\ f_{8,C2}(N_{A,c}, N_{B,c}) & \text{for } c = A2 \end{cases}$$

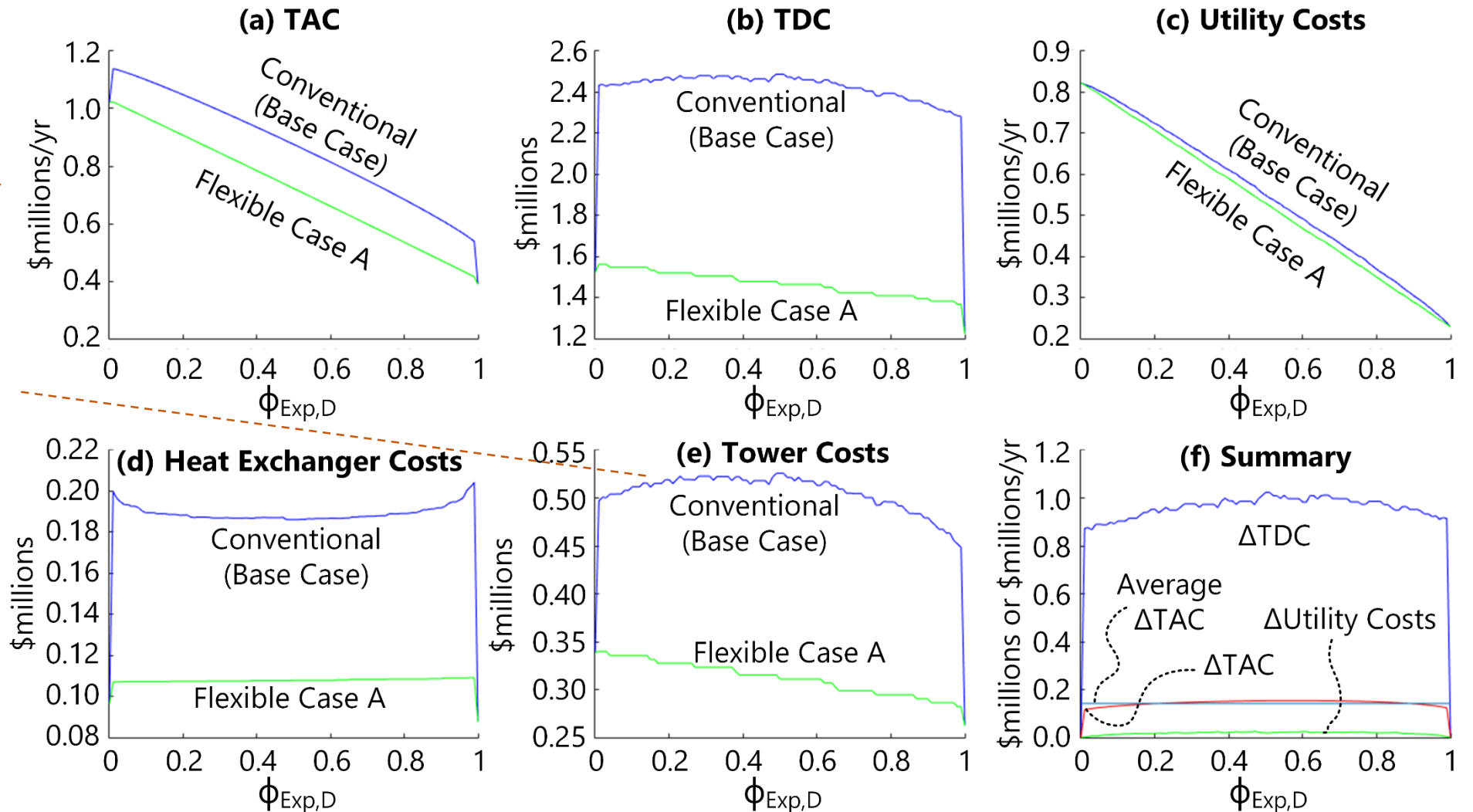
Can reuse the tabulated data from the Aspen Plus simulations without needing to rerun.

Quantify the Value of Flexibility.

Basically, my **EXPECTED TAC** is about 20% lower if I am flexible, regardless of what I expect.

“Noise” in equipment costs is expected and due to the impact of discrete decisions (# stages, discrete column diameters).

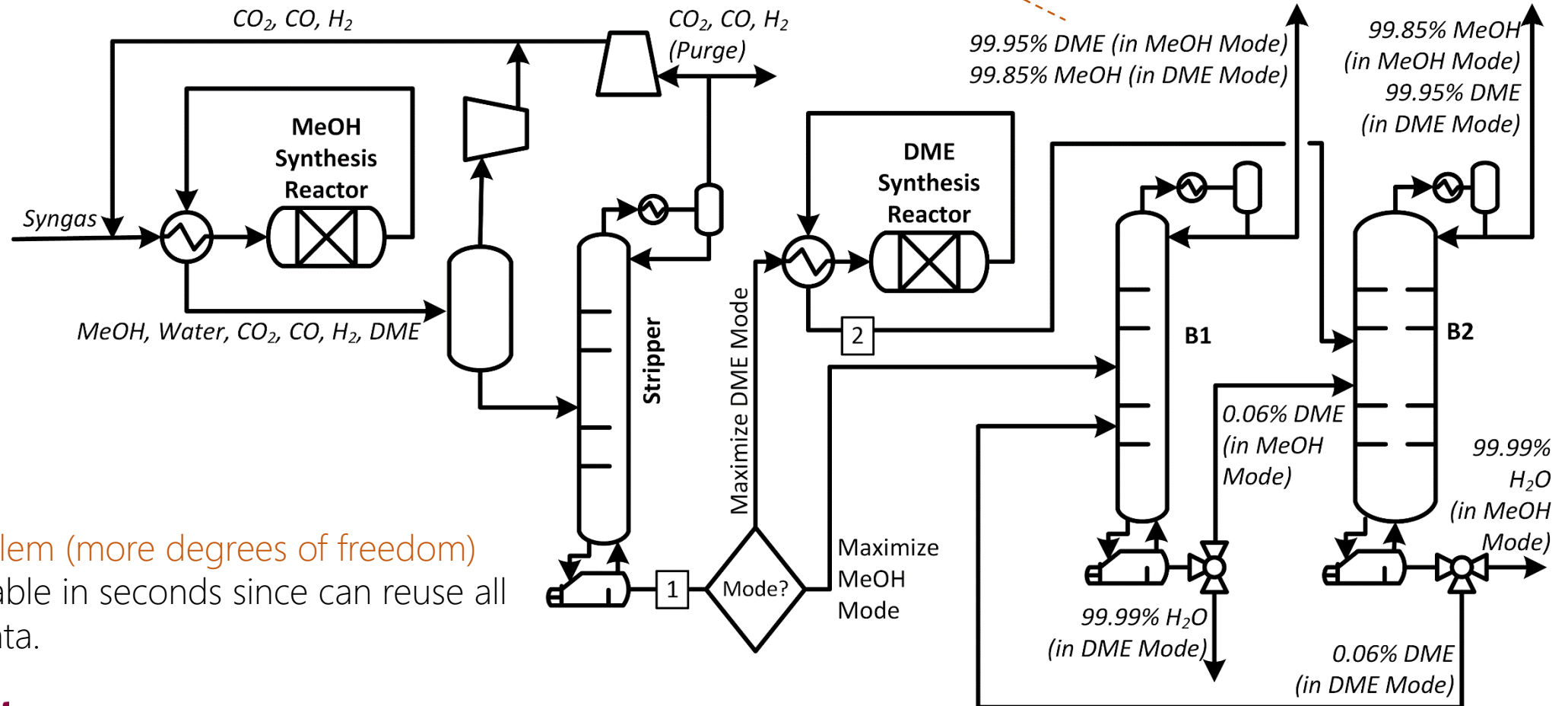
These are globally optimal.



Option B: "Fat / Skinny" columns

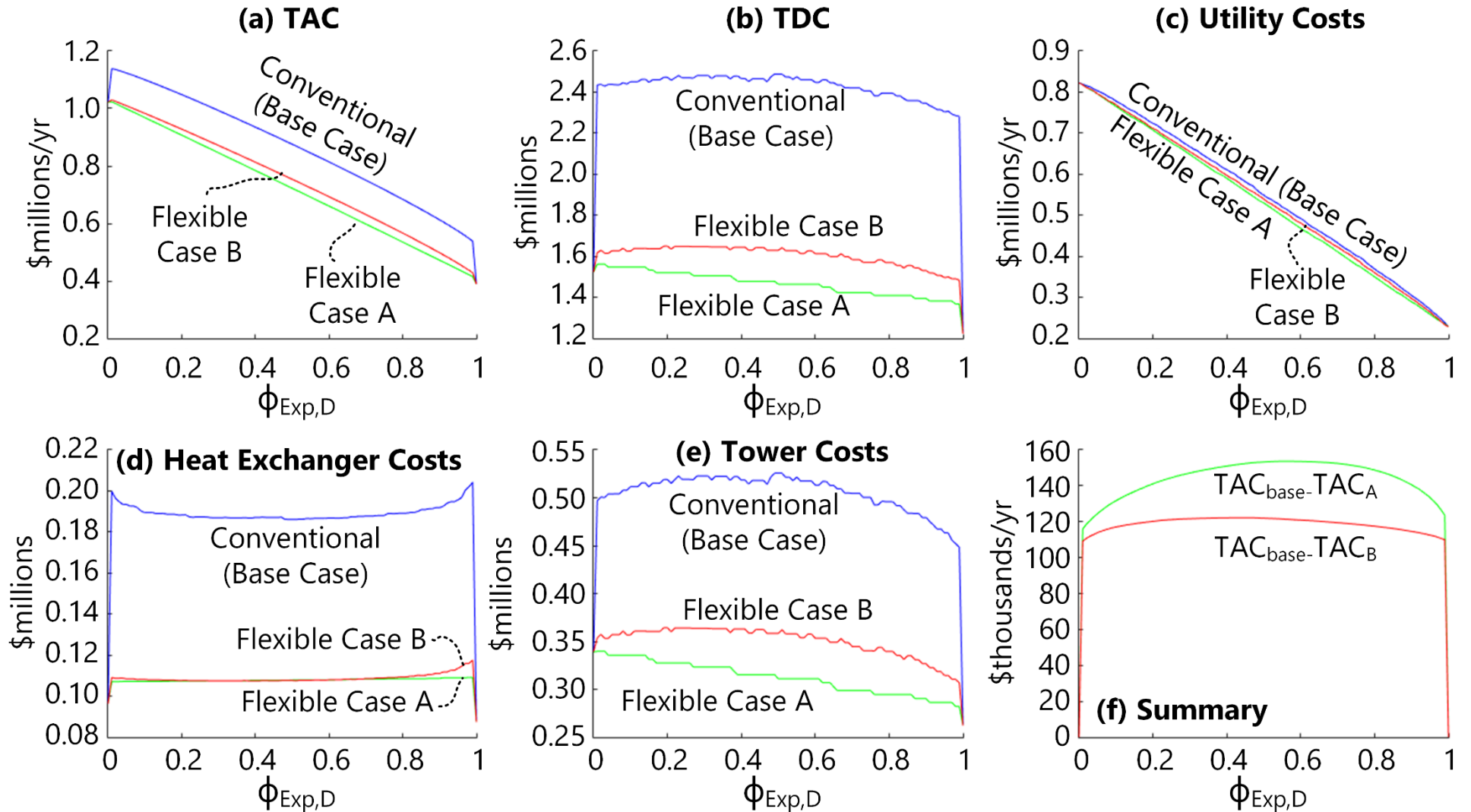
The column receiving the product feed, and the feed location changes with the mode.

Maybe I can save money by having one column for large loads and one column for small loads.



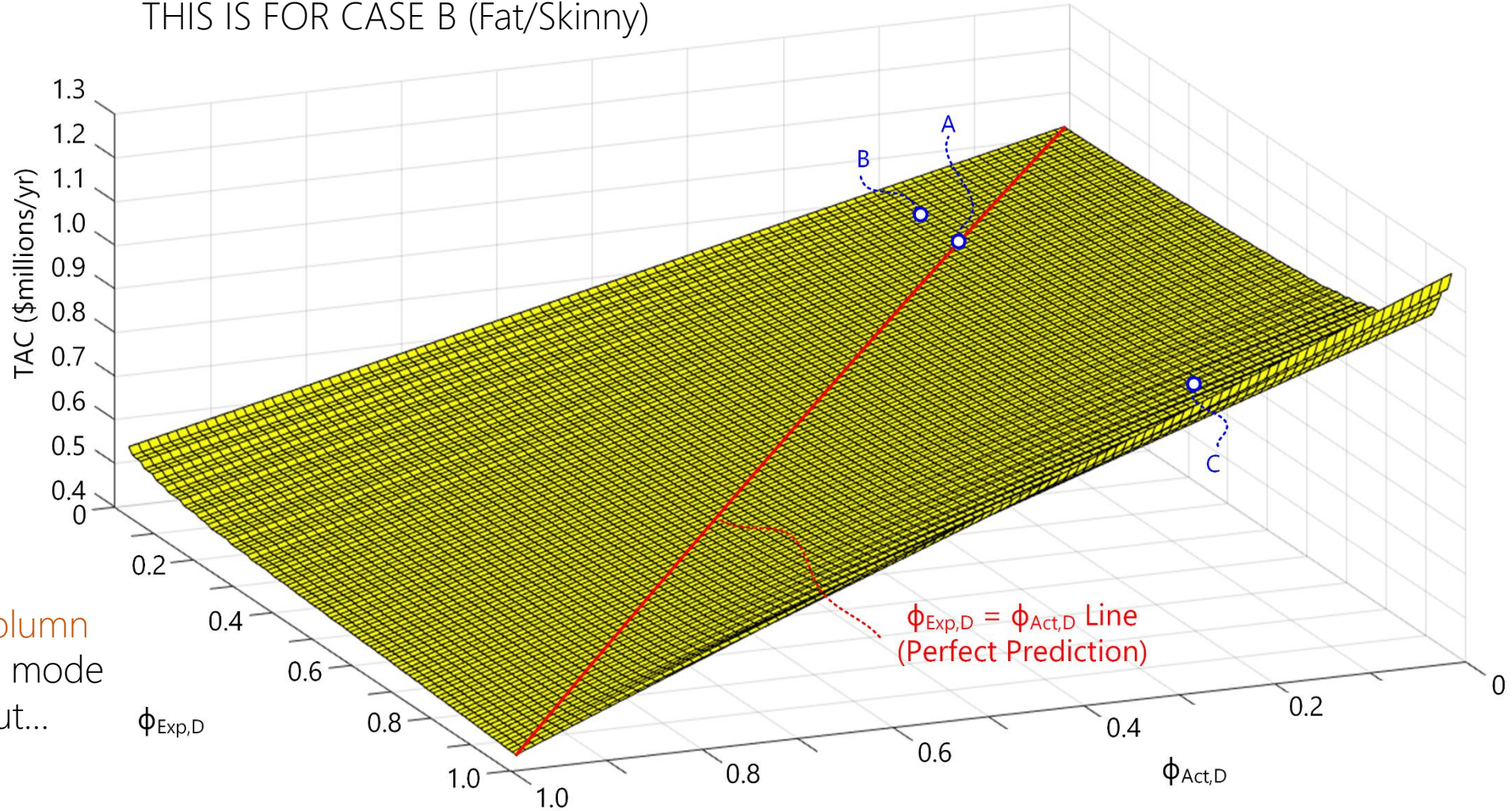
Harder problem (more degrees of freedom)
But still solvable in seconds since can reuse all tabulated data.

Well, ok, not as good.



Ok, but what if my predictions are wrong?

THIS IS FOR CASE B (Fat/Skinny)



This is the
ACTUAL TAC
if...

...I design a column
expecting this mode
distribution but...

...after 15 years of use we actually did
this.

Design Under Uncertainty Options

Probability Distribution Functions

Find the design that minimizes Expected TAC

$$TAC_{CaseB,Exp} = \sum_{c=B1,B2} Z_c$$

$$Z_c = \min_{N_{A,c,MeOH}, N_{B,c,MeOH}, N_{A,c,DME}} \sum_{i=1}^{i=S} P(\phi_{Exp,D,i}) TAC_{c,Exp,i}(\phi_{Exp,D,i})$$

Robust (Min Max) Formulation

Find the design that minimizes the worst case TAC of any outcome

$$TAC_{CaseB,Exp} = \sum_{c=B1,B2} Z_c$$

$$Z_c = \min_{N_{A,c,MeOH}, N_{B,c,MeOH}, N_{A,c,DME}} \max_{i=1..S} TAC_{c,Exp,i}(\phi_{Exp,D,i})$$

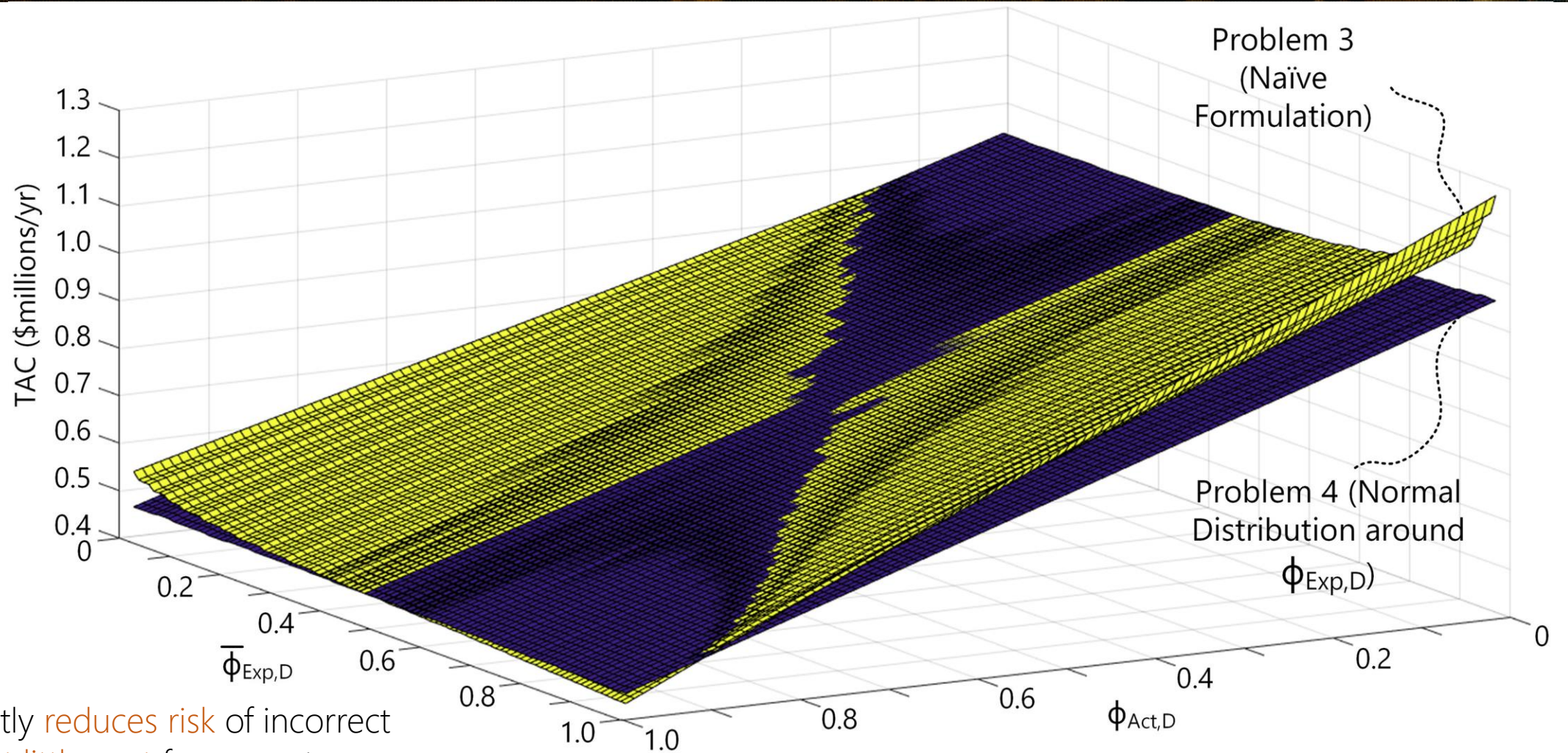
Example: Normal distribution around a guessed $\phi_{EXP, D}$

Example: Uniform distribution of $\phi_{EXP, D}$ (i.e. no predictive knowledge at all).

Example: Also useful with no predictive knowledge at all.

All of these can be solved to global optimality with no loss of fidelity in a few seconds.

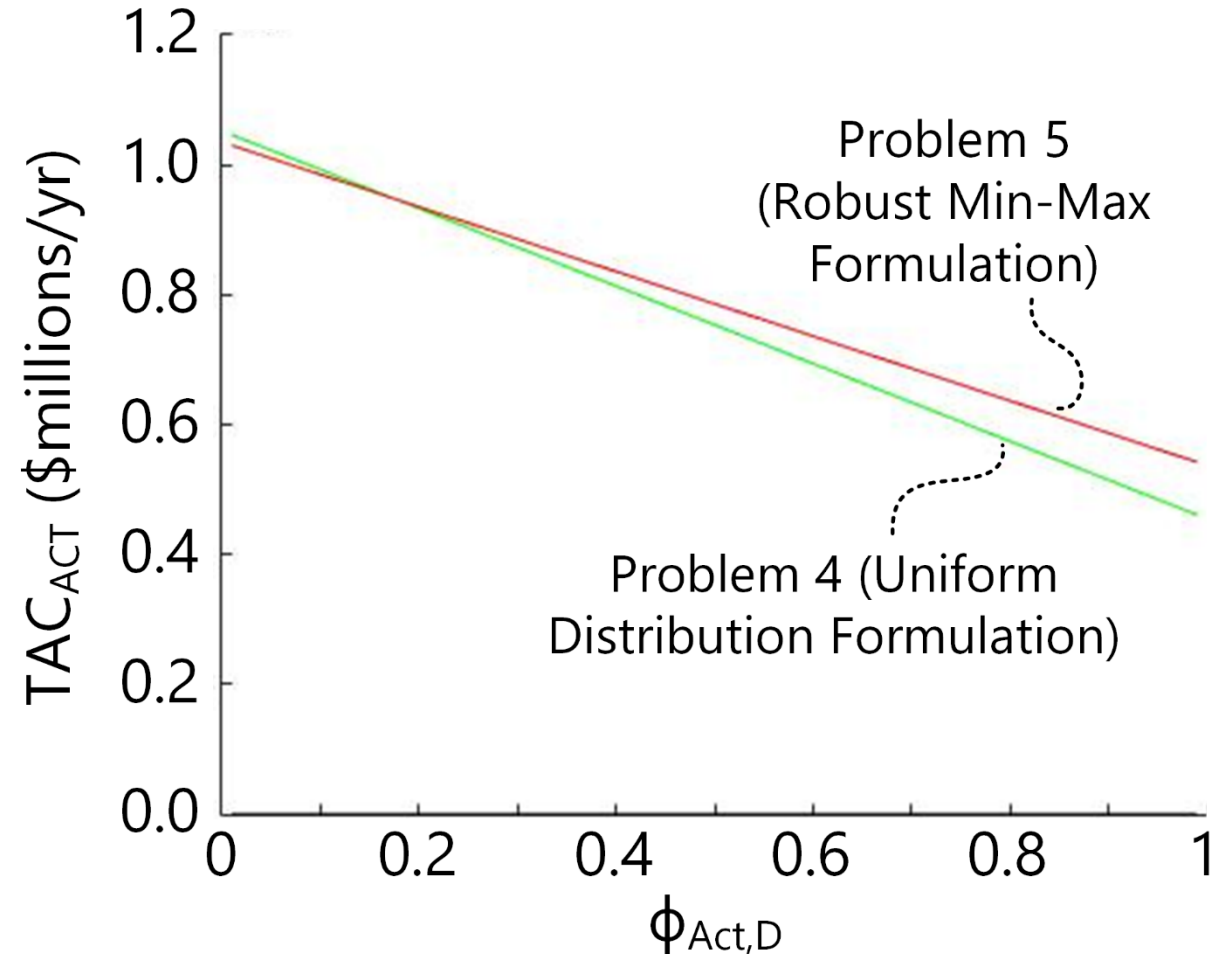
Uncertainty formulation comparison



Significantly **reduces risk** of incorrect guesses **at little cost** for correct guesses

Design Under Uncertainty with No Predictions

- Both methods result in a single design without making assumptions.
- This is the **Actual TAC** depending on the outcome.
- Neither is better in all cases, but uniform distribution happens to be better more often.
- Both are very good



Conclusions

- Strategic tabulation and **problem decoupling** makes for **very fast** optimal design under uncertainty solutions with many scenarios to **global optimality**
- Can **re-use design tables** for many case studies
- **Uniform distribution recommended** (requires no knowledge of the final outcomes) to minimize overall risk at little cost

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