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
- Links to data sets and simulations used in cited studies

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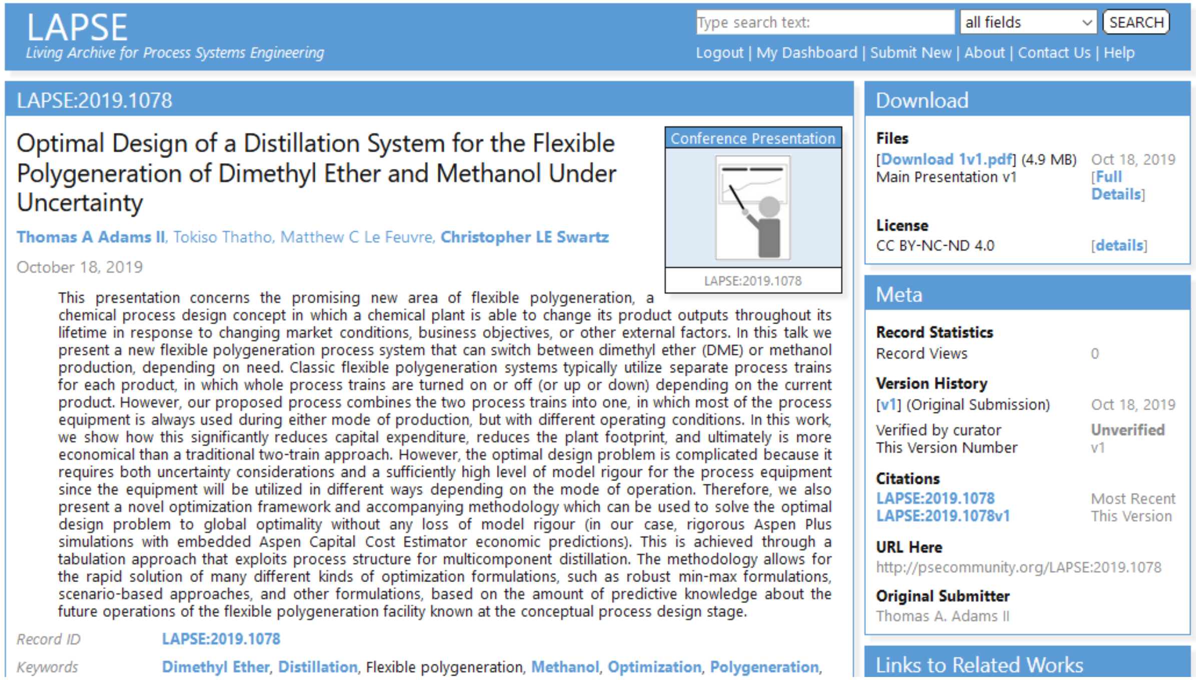

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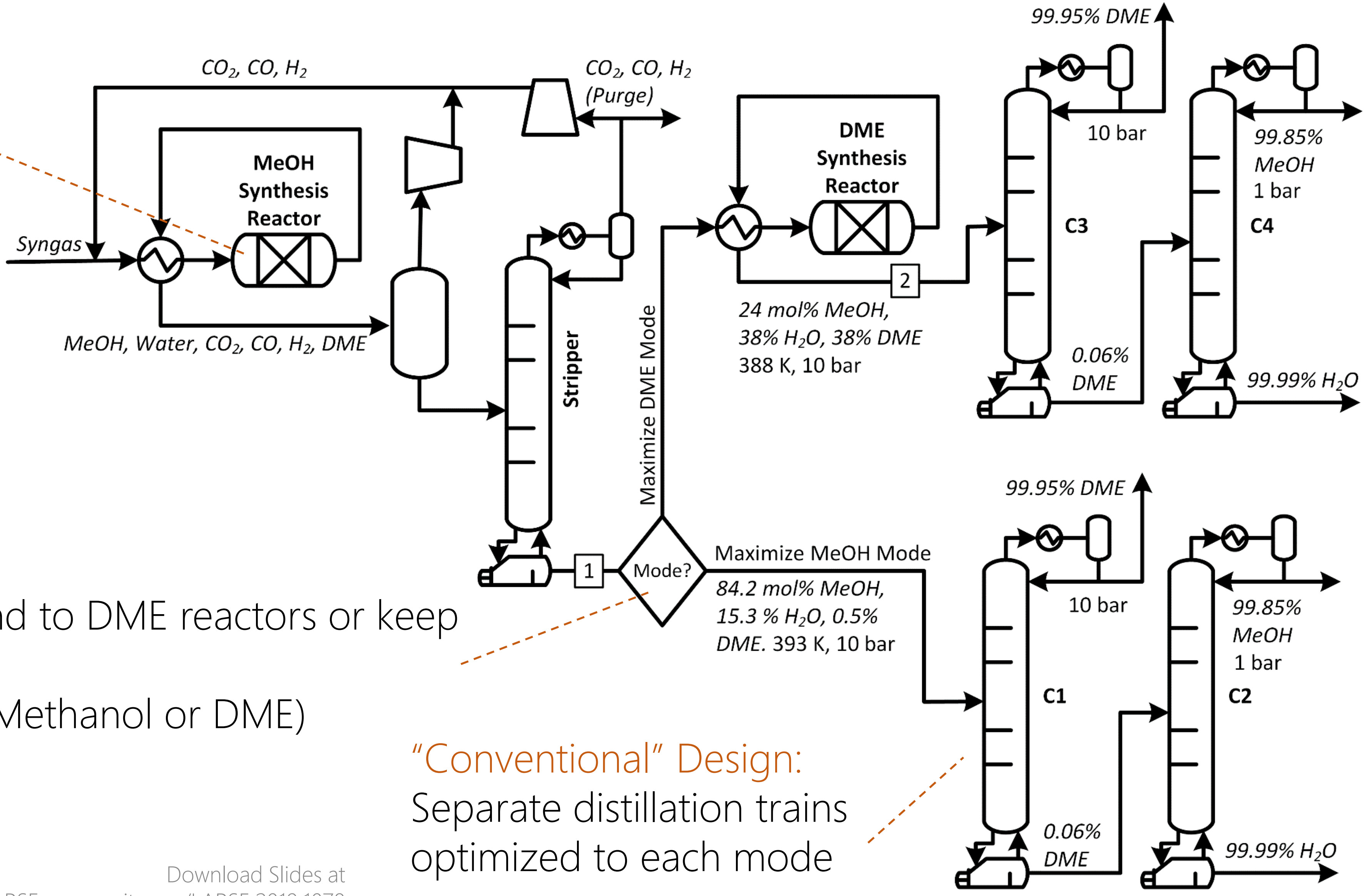
Basic Premise: Flexible Production

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

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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

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Optimization Strategy (Naïve Approach)

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

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

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

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

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

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

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

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

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

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

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

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

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

Capital cost models (can be equations or table lookups)

Diameter of column c

Reboiler/condenser duties of column c

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

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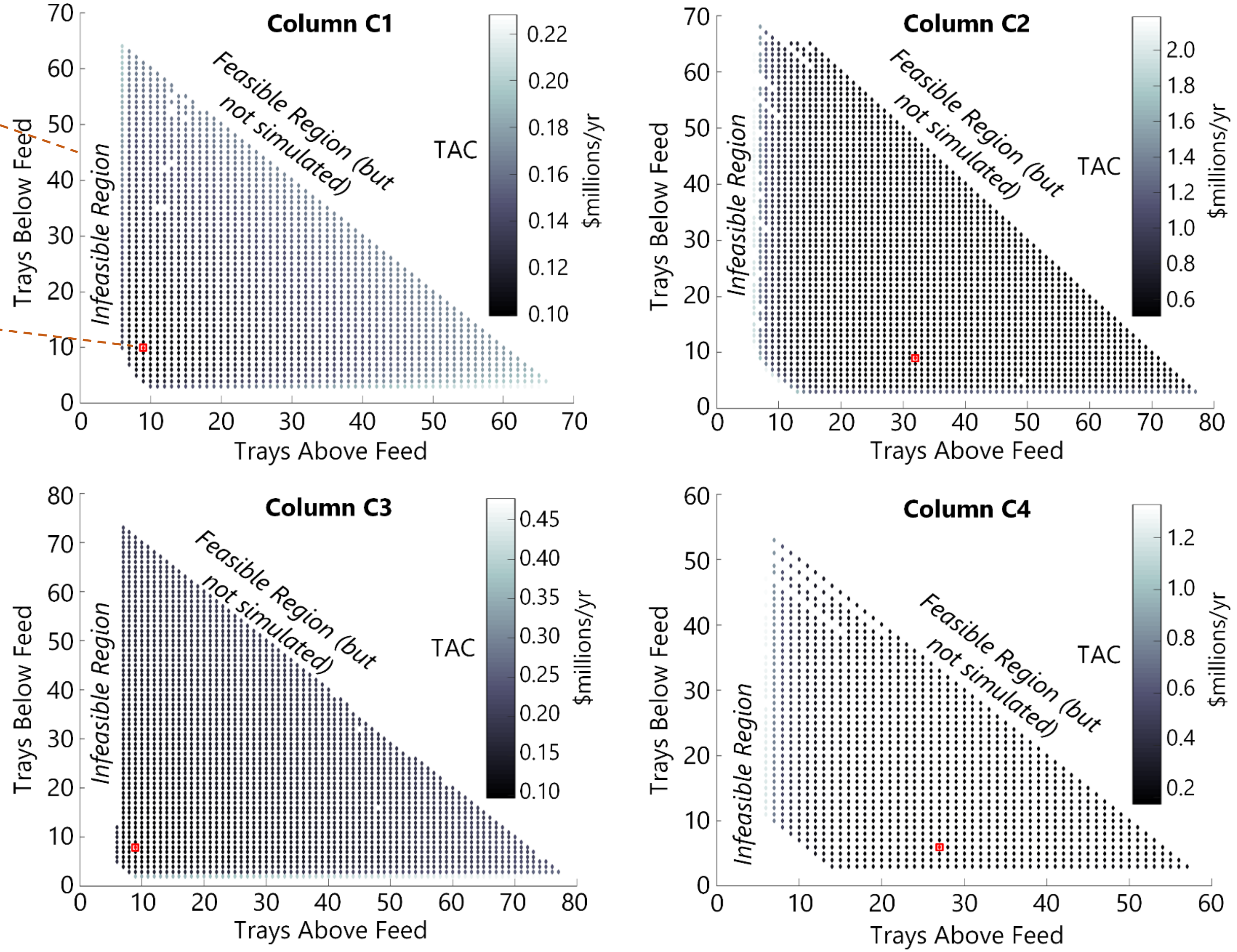
Solve quickly through exhaustive search

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 $\phi_{EXP, D}$



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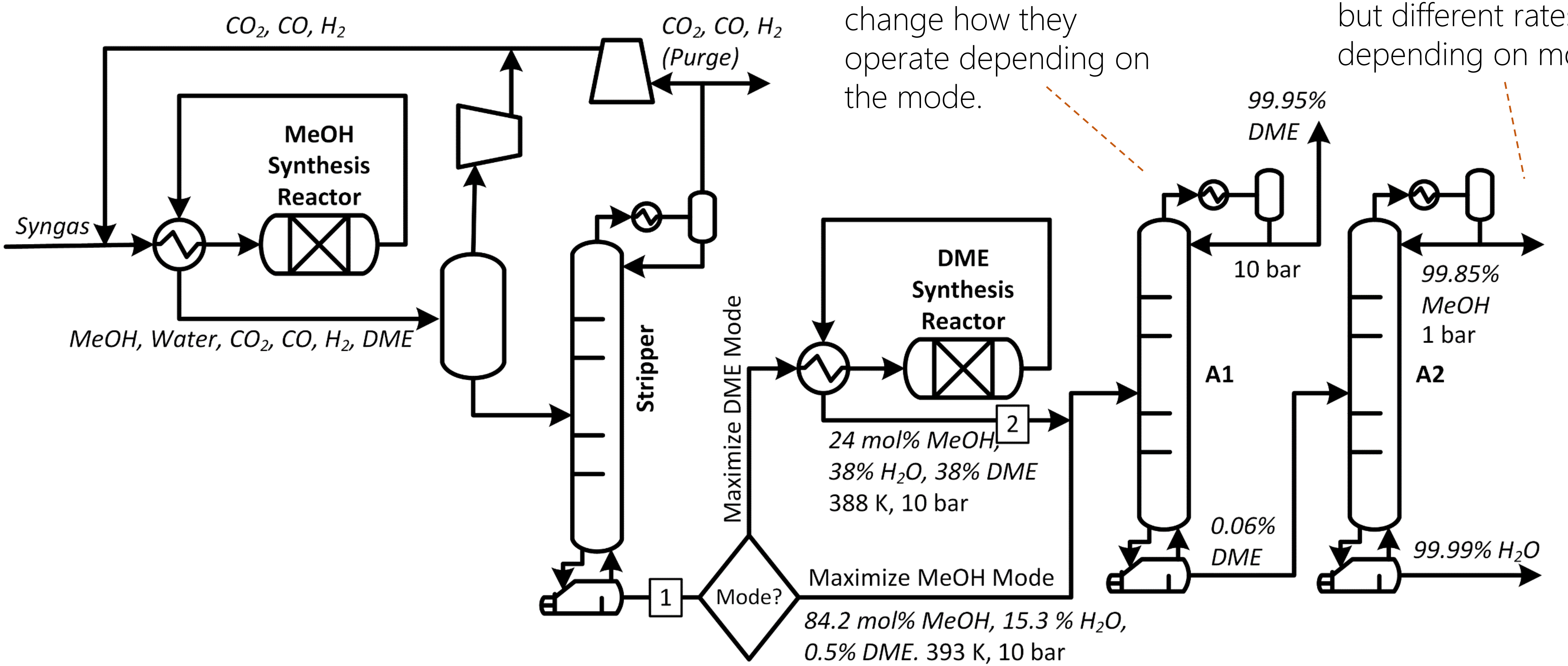
Alternative Design Strategy

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.

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

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

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

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

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

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

Still have the uncertainty factor.

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

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

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

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

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

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

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

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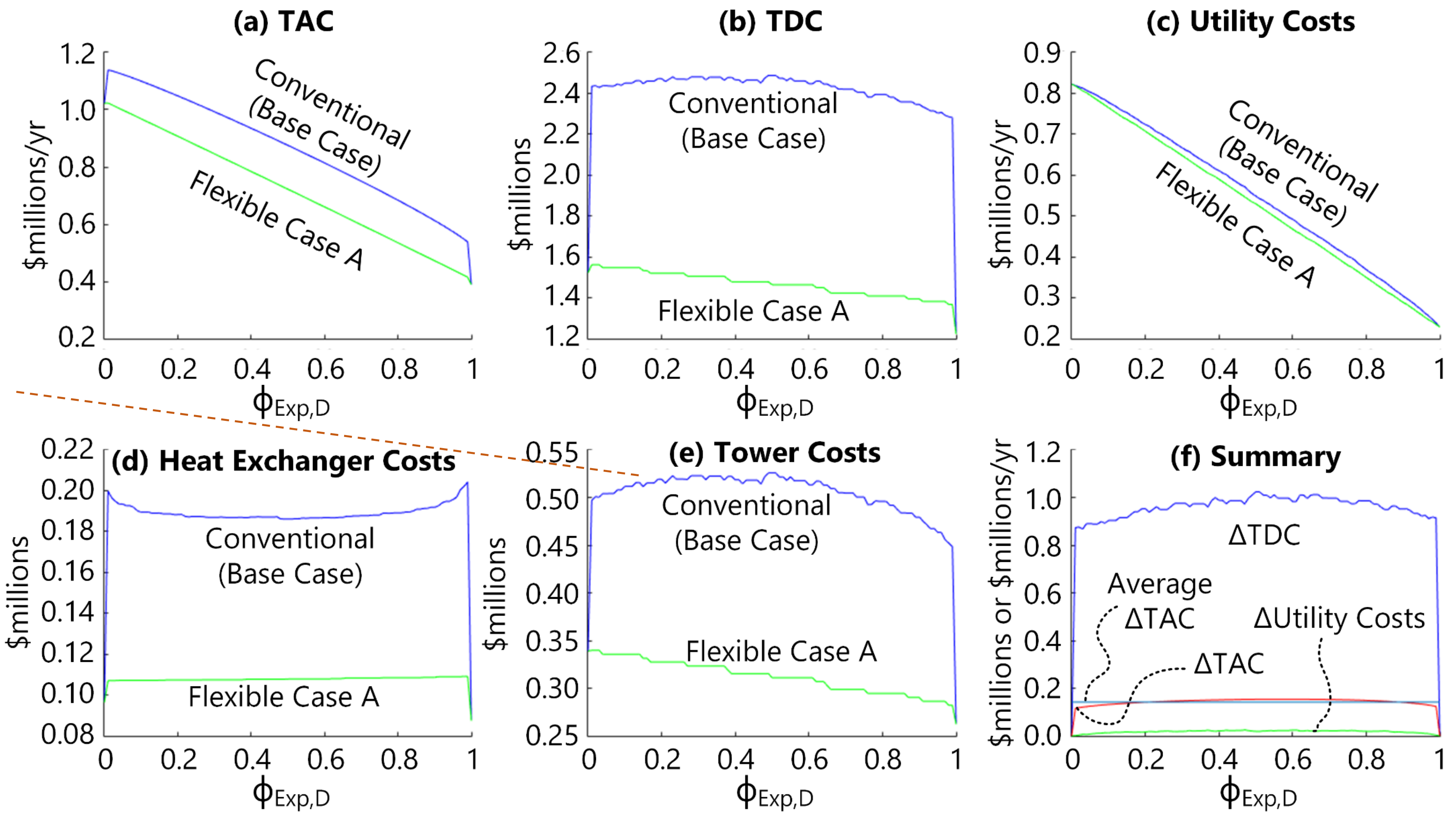
Quantify the Value of Flexibility.

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.



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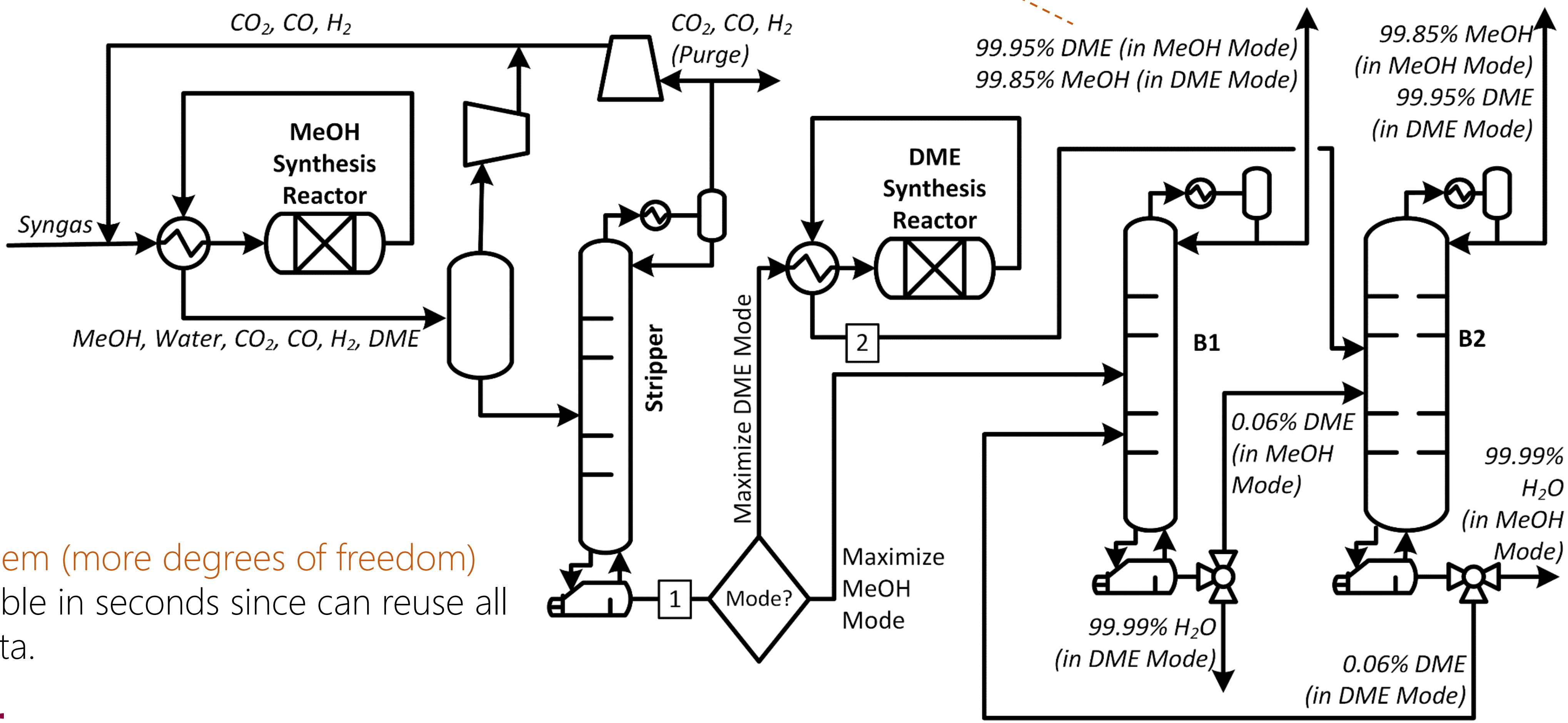
Option B: "Fat / Skinny" columns

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.

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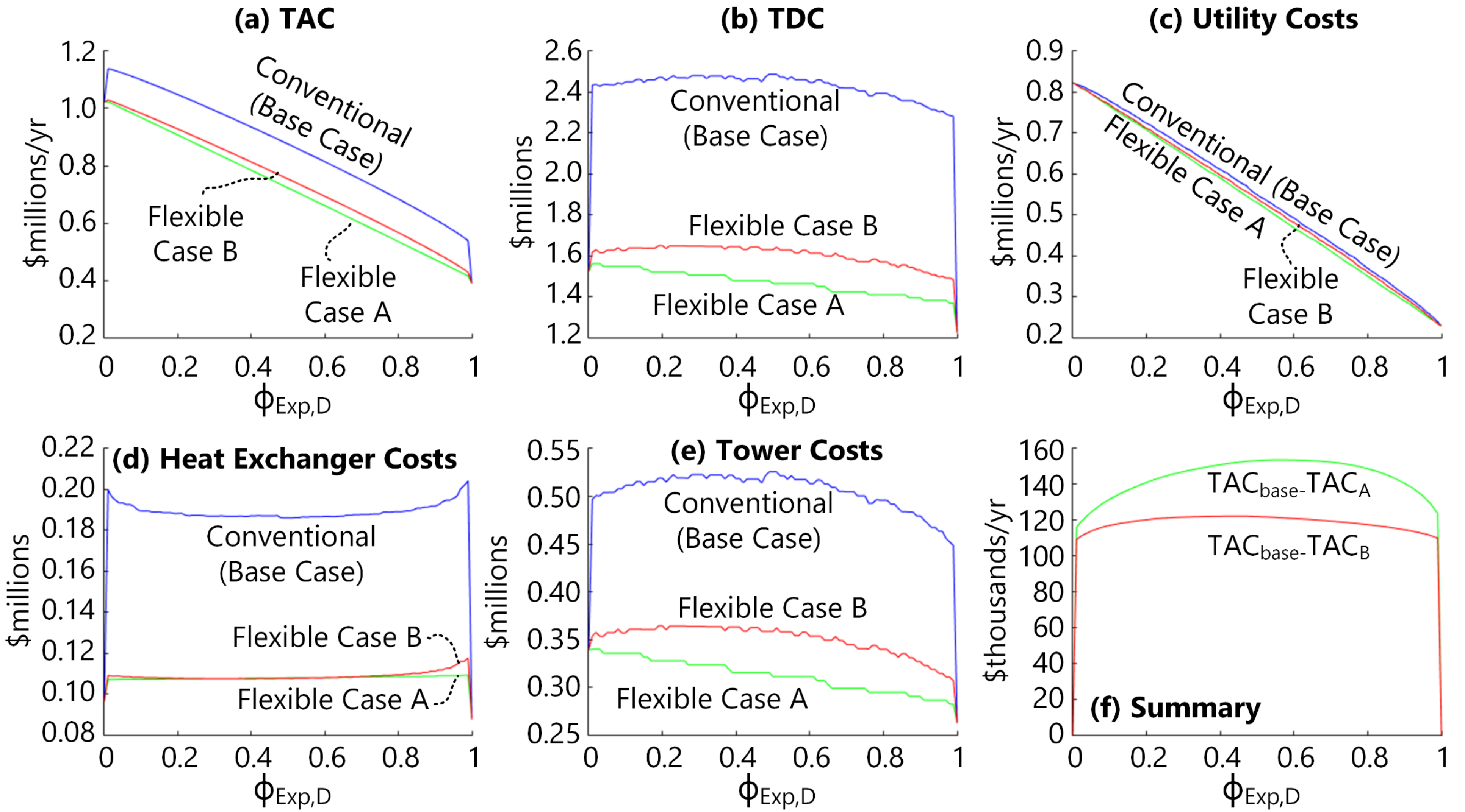
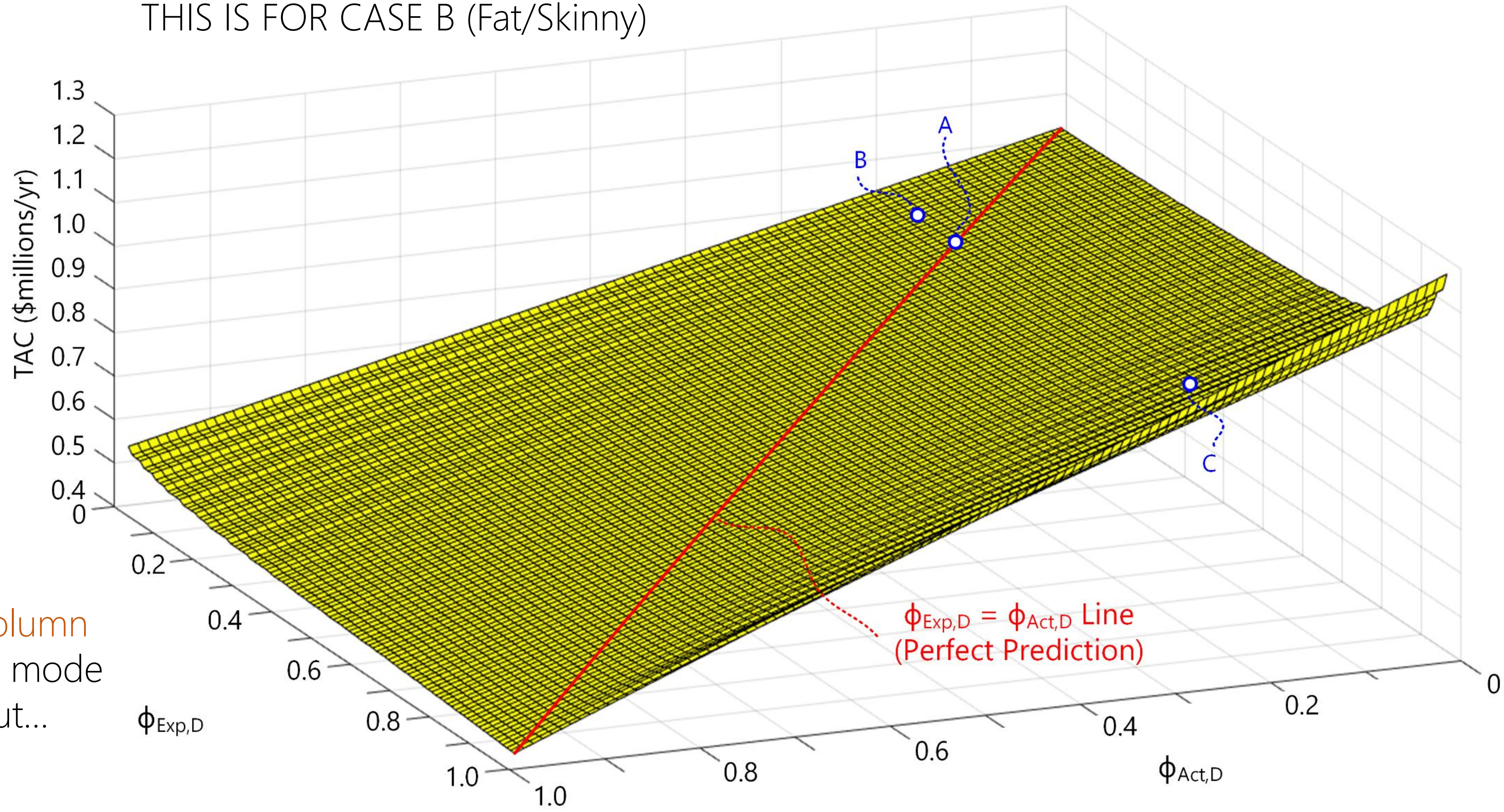
Well, ok, not as good.



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

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

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

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

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

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: 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.

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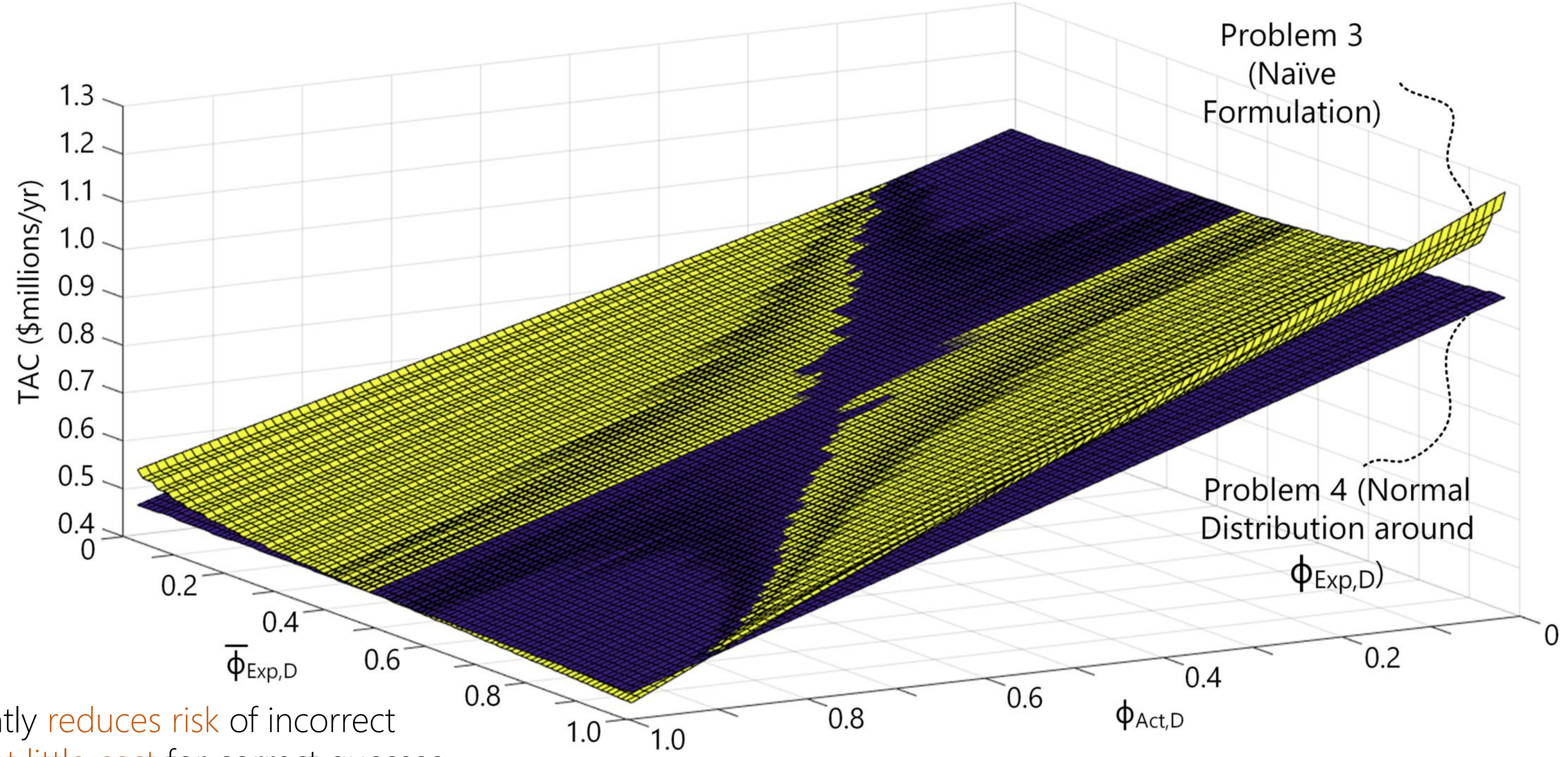
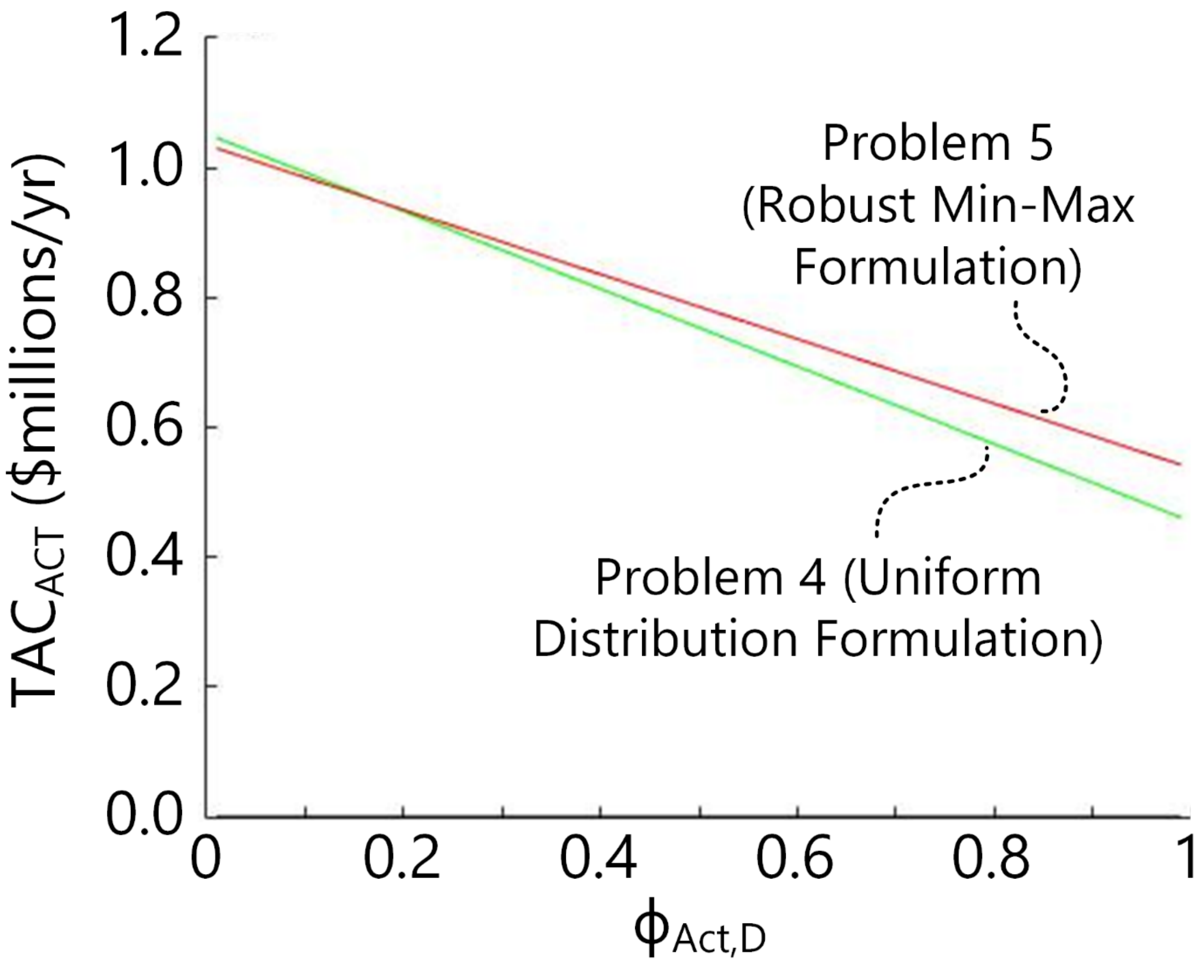
Uncertainty formulation comparison



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