MIXTURE DESIGN OF EXPERIMENTS USING CUSTOM DOE PLATFORM

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WHY USE DOE?

QUICKER ANSWERS,
LOWER COSTS,
SOLVE BIGGER PROBLEMS,
MAKE MORE MONEY!

- More rapidly answer "what if?" questions
- Do sensitivity and trade-space analysis
- Optimize across multiple responses
- By running efficient subsets of all possible combinations, one can – for the same resources and constraints – *solve bigger problems*
- By running sequences of designs one can be as *cost effective as possible* & run *no more trials than are needed* to get a useful answer

SAME HOLDS TRUE FOR MIXTURE DOE

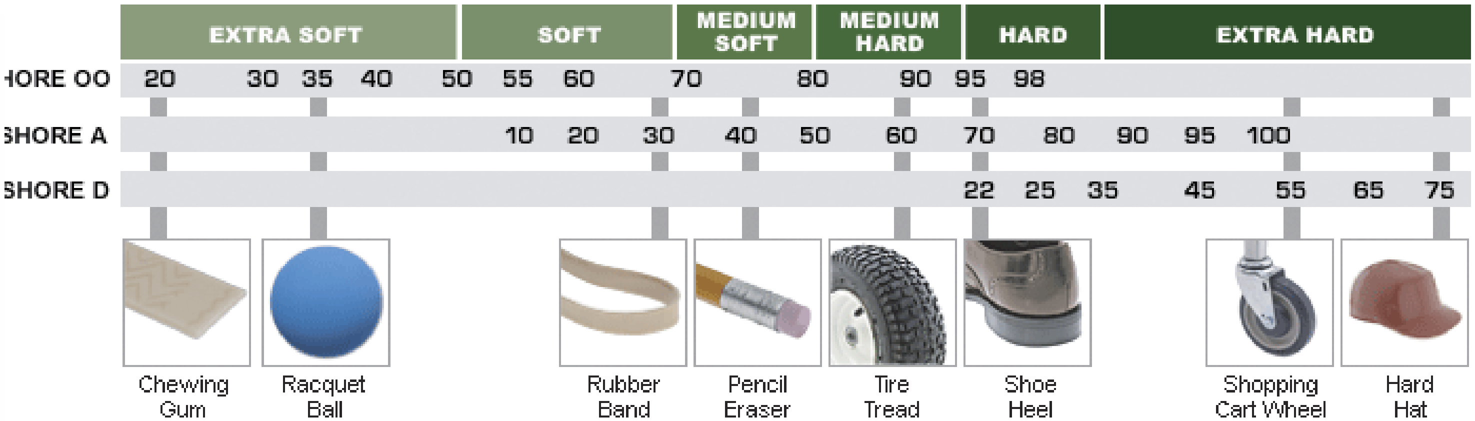
AGENDA

- Do trade-space analysis using models fit to a mixture DOE
- What makes mixture factors (components) and formulation DOE different?
- Several Examples
  - Simple three-component designs using Custom DOE platform

    "Make Designs Fit the Problem – NOT Make Problems Fit the Designs!"
  - Five-component mixture DOE with 3 constraints and response data (revisited)
    - Visualizing process in Fit Model platform
    - Use transformation to prevent physically impossible predictions
  - PDF – Ten-factor = 6 mixture, 2 continuous, 1 categorical and 1 block
    - "Real-world" several type of factors
    - Additional constraints including holding some of mixture constant
  - PDF – Seven-component mixture DOE with 5 and 7 constraints
    - Use constraints to define "mixtures within mixture"
    - Can I find a 3-component blend that's nearly as good as a 7-component blend?
  - *Technically Speaking* – Optimizing Performance of a Multi-Layer Packaging Film
    - Layer thickness expressed as proportions that sum to one = the mixture constraint
    - Can I trade-off thickness and layer resin concentration to target 2 performance metrics & minimize a third?
  - Computational Chemistry - Space-Filling Mixture Design
    - US Army explosive formulation of "Bread."
    - Presented last week at JMP Discovery Summit 2017, St. Louis, MO, USA

NEED TO PREDICT HARDNESS AND COST OF PLASTIC

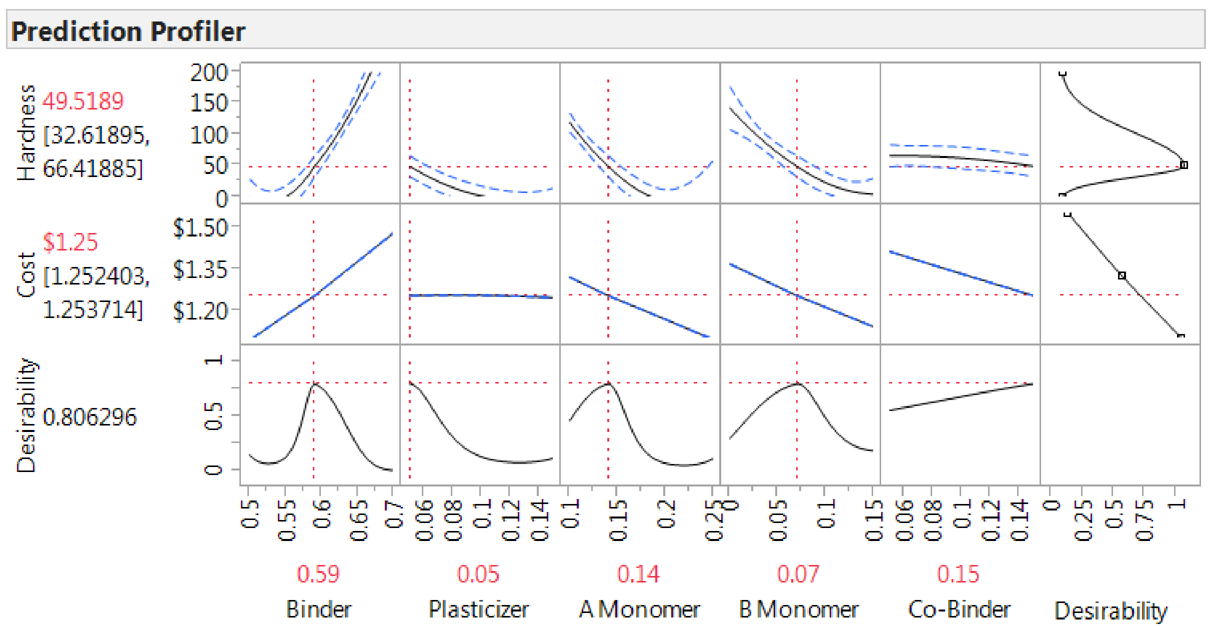
WANT TO MAKE INFORMED BUSINESS DECISIONS TRADING OFF PRODUCT PERFORMANCE AND COST



What formulations yield a Shore A hardness of 50?

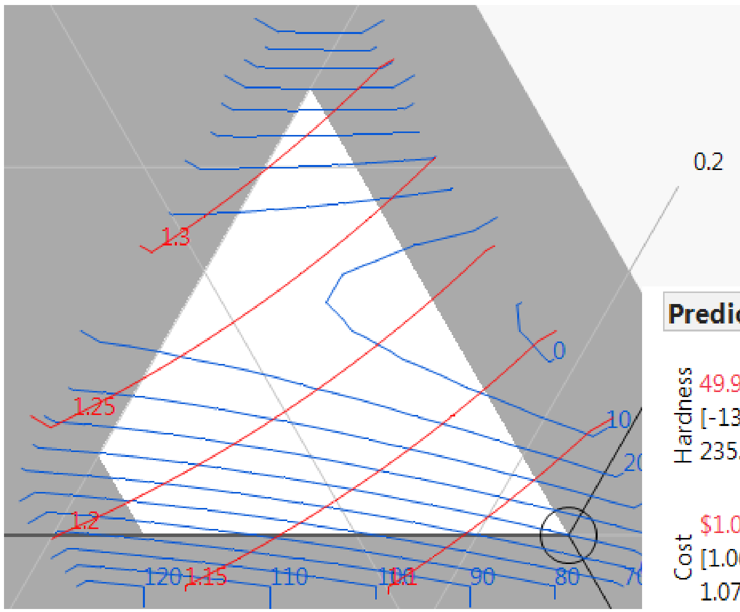
What do these formulations cost?

Can I trade-off hardness and cost?



MODEL OPTIMIZATION SUGGESTS LOWER COST IS POSSIBLE

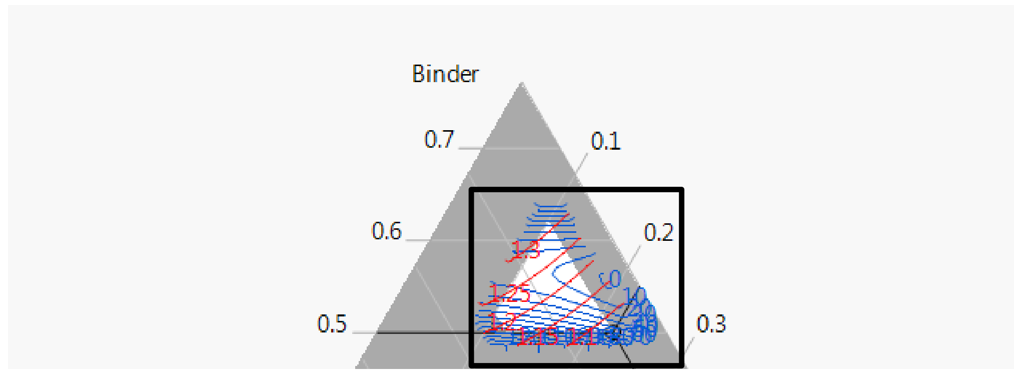
DOES THAT MAKE SENSE?
DOES DATA SUPPORT IT?
RUN CHECKPOINTS THERE.

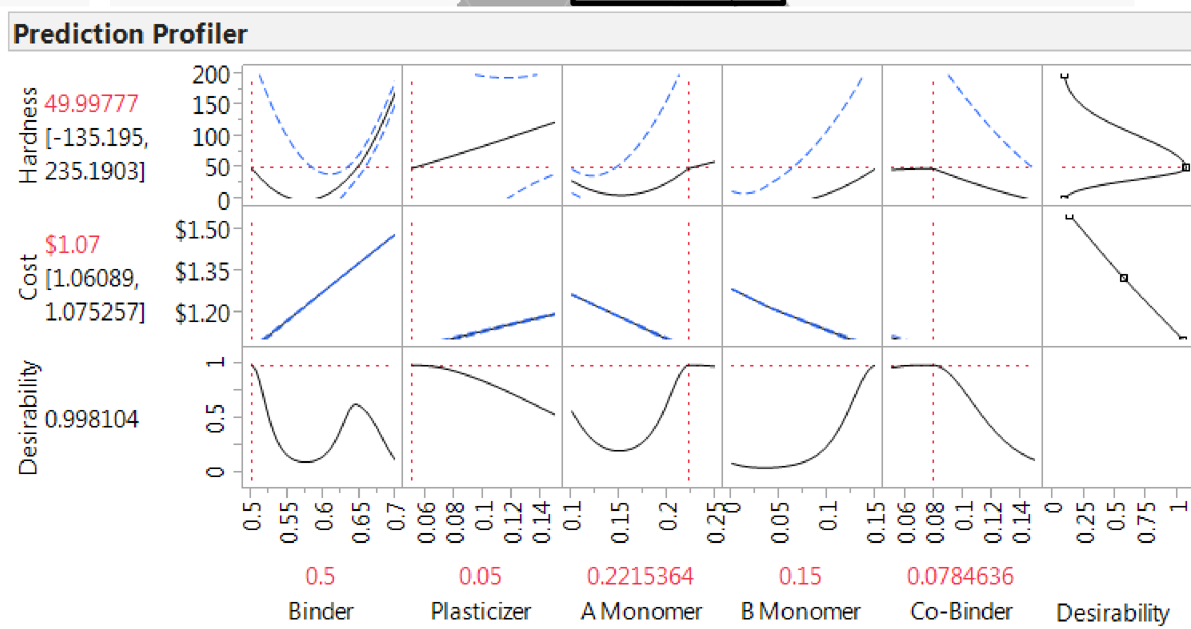


Mixture Profiler

T	L	R	Factor	Current X	Lo Limit	Hi Limit
◉	○	○	Binder	0.5	0.5	0.7
○	◉	○	Plasticizer	0.05	0.05	0.15
○	○	◉	A Monomer	0.2215364	0.1	0.25
○	○	○	B Monomer	0.15	0	0.15
○	○	○	Co-Binder	0.0784636	0.05	0.15

Response	Contour	Current Y	Lo Limit	Hi Limit
Hardness	100	49.997766	.	.
Cost	1.325	1.0680737	.	.





REAL-WORLD DESIGN ISSUES ADDRESSED BY CUSTOM DOE PLATFORM

"Make Designs Fit the Problem – NOT Make Problems Fit the Designs!"

- Work with these different kinds of control variables/factors:
  - **Continuous/quantitative?** (Finely adjustable like *temperature*, *speed*, *force*)
  - **Categorical/qualitative?** (Comes in types, like material = *rubber*, *polycarbonate*, *steel* with mixed # of levels; 3 chemical agents, 4 decontaminants, 8 coupon materials…)
  - **Mixture/formulation? (Blend different amounts of *ingredients* and the process performance is dependent on the *proportions* more than on the amounts)**
  - **Blocking?** (e.g. "lots" of the same raw materials, multiple "same" machines, samples get processed in "groups" – like "eight in a tray," run tests over multiple days – i.e. variables for which there *shouldn't* be a causal effect
- Work with **combinations of these four kinds** of variables?
- Certain **combinations cannot be run**? (too costly, unsafe, breaks the process, subject matter experts say to avoid as "impractical.") **Use constraints.**
- Certain factors are **hard-to-change** (temperature takes a day to stabilize)
- Would like to **add onto existing trials**? (really expensive/time consuming to run)

SIMPLE MIXTURE – MAKING SALAD DRESSING

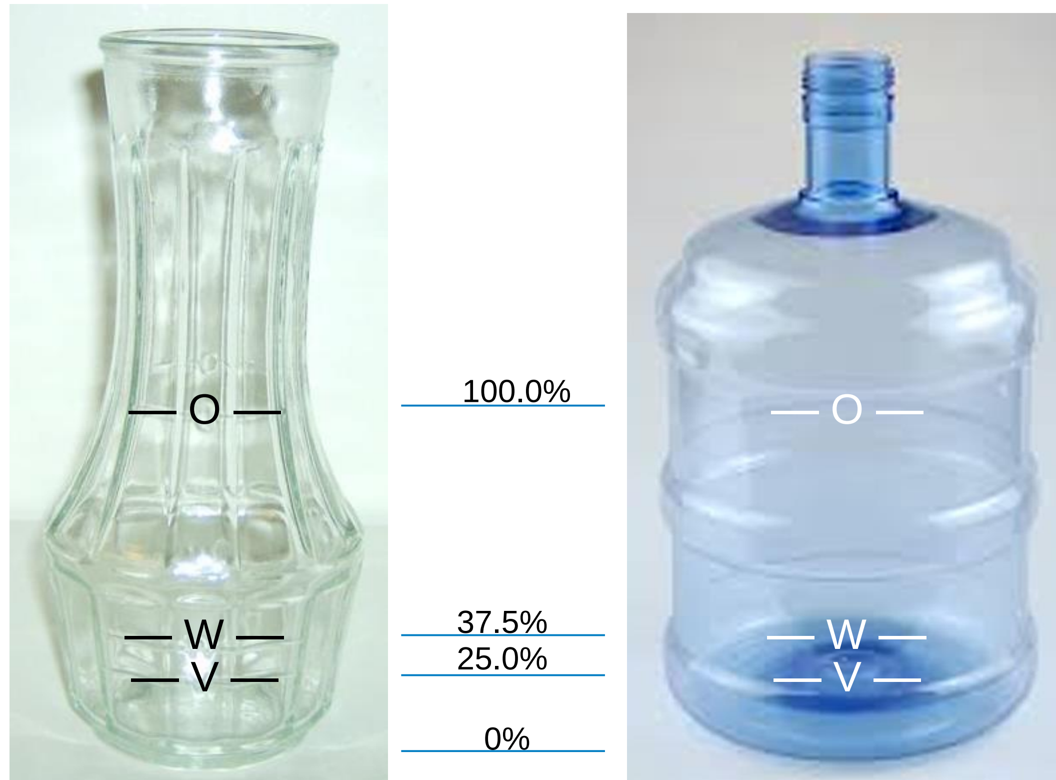
- Relative ***proportions*** of factors or components is more important than actual quantity
- Three liquid components - Oil, Water, and Vinegar
- 8 oz. in Cruet vs. 4 gal. in Jug

5 oz.	"O"	320 oz.	5/8
1 oz.	"W"	64 oz.	1/8
2 oz.	"V"	128 oz.	1/4

- To study these mixture components in a DOE use ranges that are proportions:

O:	0.500 to 0.750	(½ to ¾)
W:	0.000 to 0.250	(0 to ¼)
V:	0.125 to 0.375	(⅛ to ⅜)

- Sum of proportions ***constrained*** to equal 1.



1 = O + W + V so therefore…

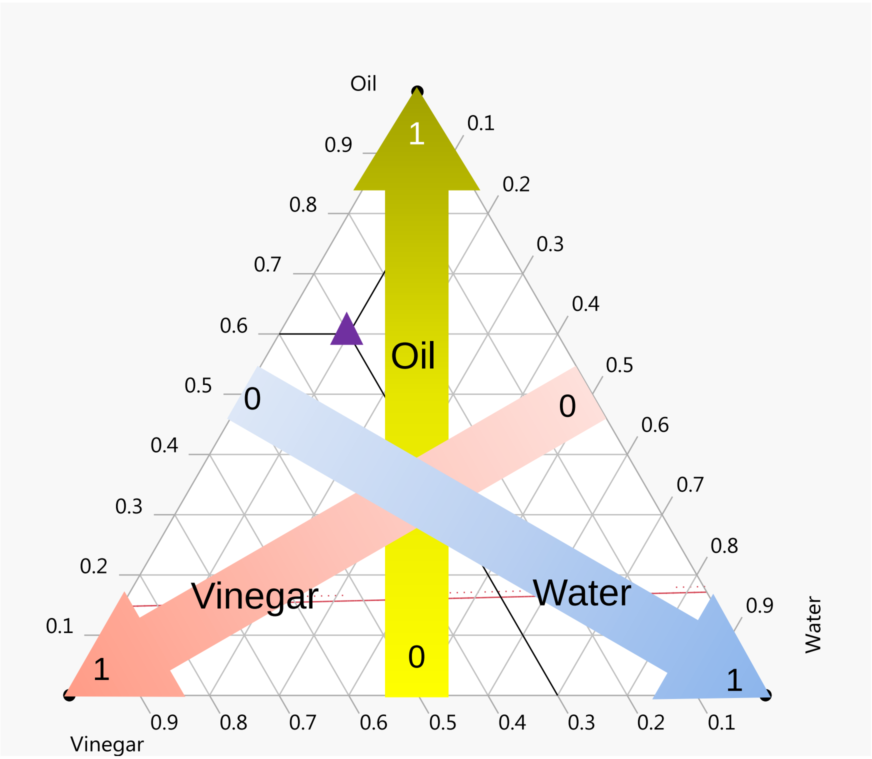
W = 1 – (O + V), O = 1 – (V + W), & V = 1 – (O + W)

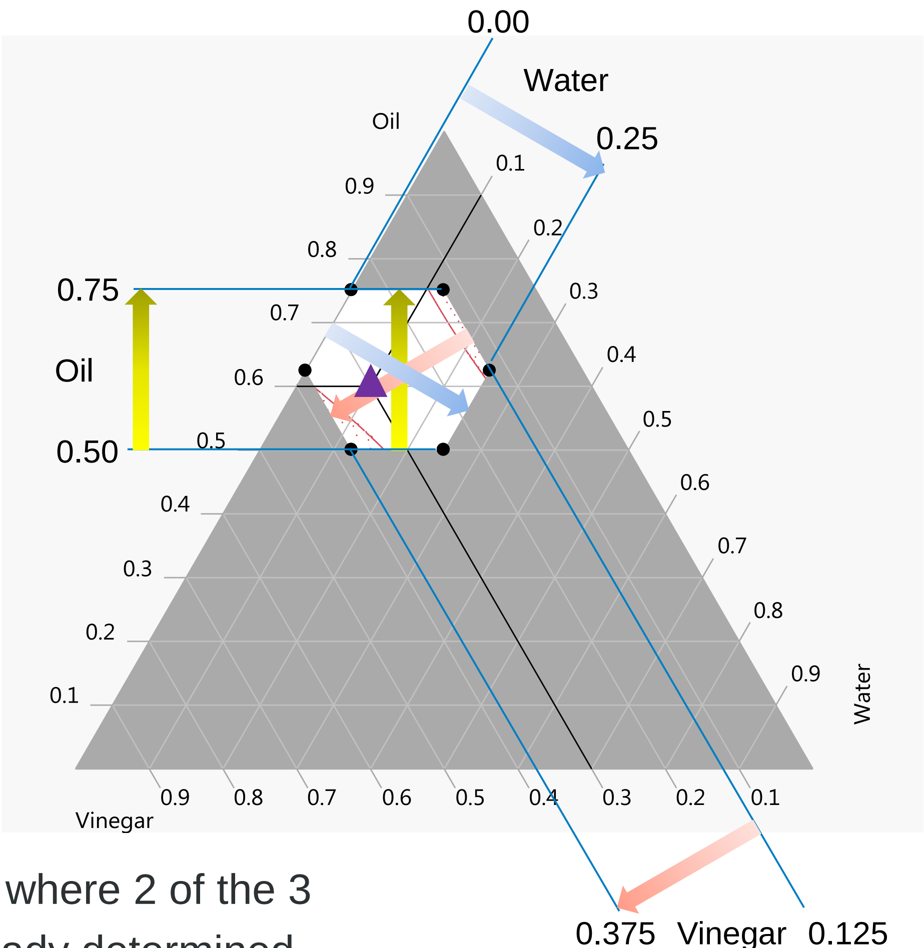
READING TERNARY PLOTS

INCREASE IN PROPORTION IS FROM BASE TO VERTEX

LEFT: FULL RANGE: 0 TO 1

RIGHT: EQUAL WIDTH RANGES: ± 0.125





Ternary plot is constrained so that if one locates where 2 of the 3 coordinates intersect, the third coordinate is already determined.

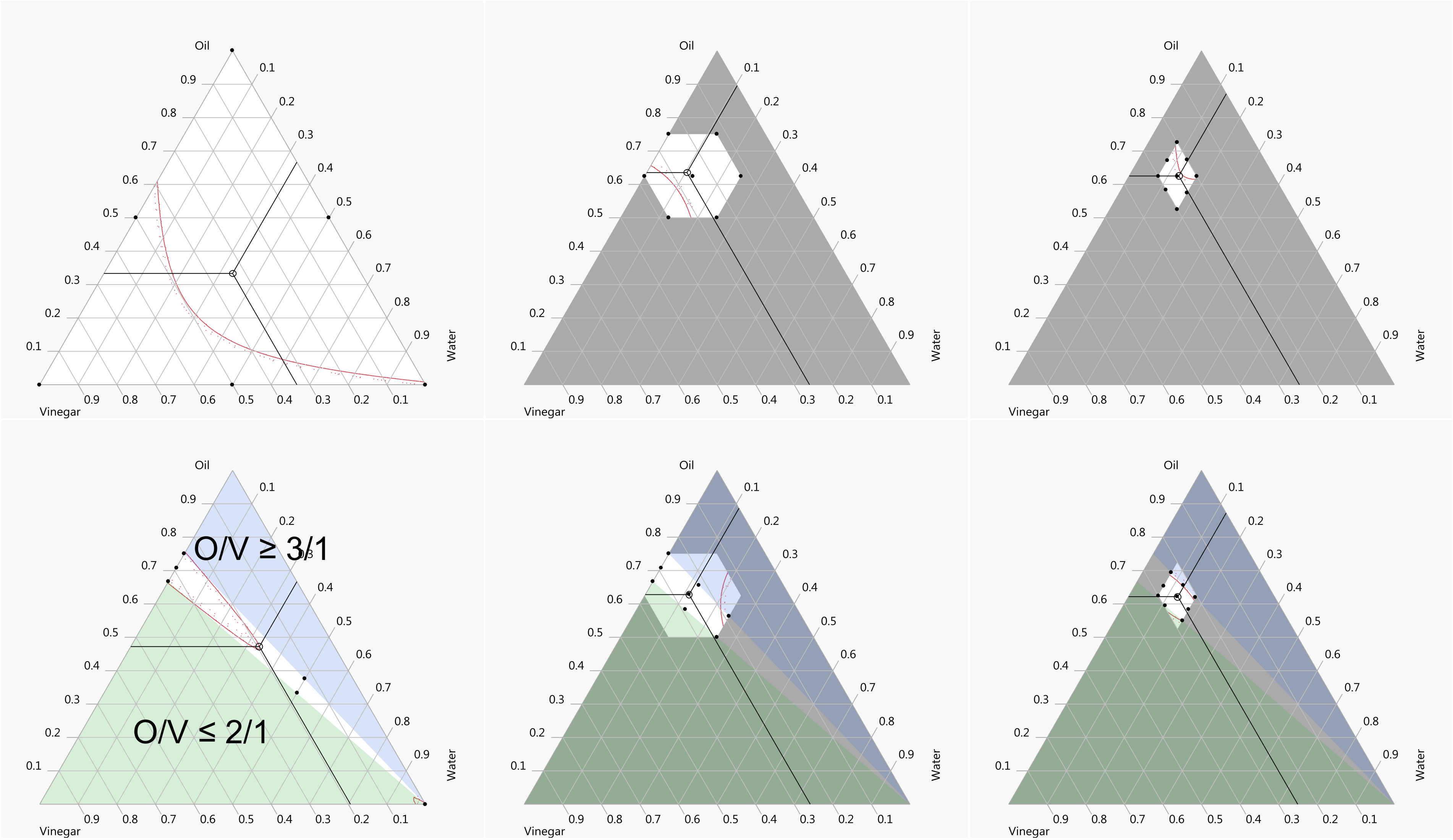
If Oil = 0.6 and Vinegar = 0.3, then Water = 1 – (0.6 + 0.3) = 0.1 (See ▲)

SIX DESIGNS:
TOP: NO CONSTRAINTS
BOTTOM: 2 CONSTRAINTS

Left: Full Range: 0 to 1

Middle: Equal width proportion: ± 0.125 about nominal

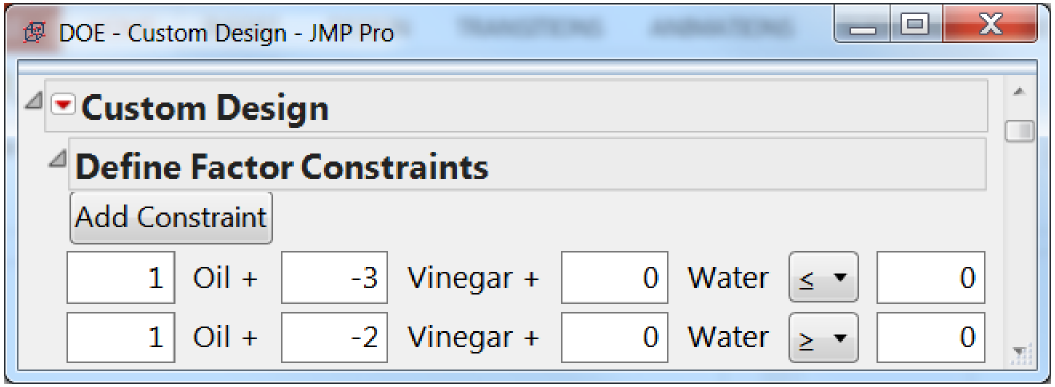
Right: Equal %change: ± 10% of nominal



INEQUALITY CONSTRAINT ALGEBRA

1. Express constraints as proportions
2. Clear fractions (note keeping unit multiplier)
3. Bring all factors to left side of inequality sign
4. Fill in boxes with coefficients and select ≤ or ≥

Oil/Vinegar ≤ 3/1	and	Oil/Vinegar ≥ 2/1
1*Oil ≤ 3*Vinegar	and	1*Oil ≥ 2*Vinegar
1*Oil - 3*Vinegar ≤ 0	and	1*Oil - 2*Vinegar ≥ 0



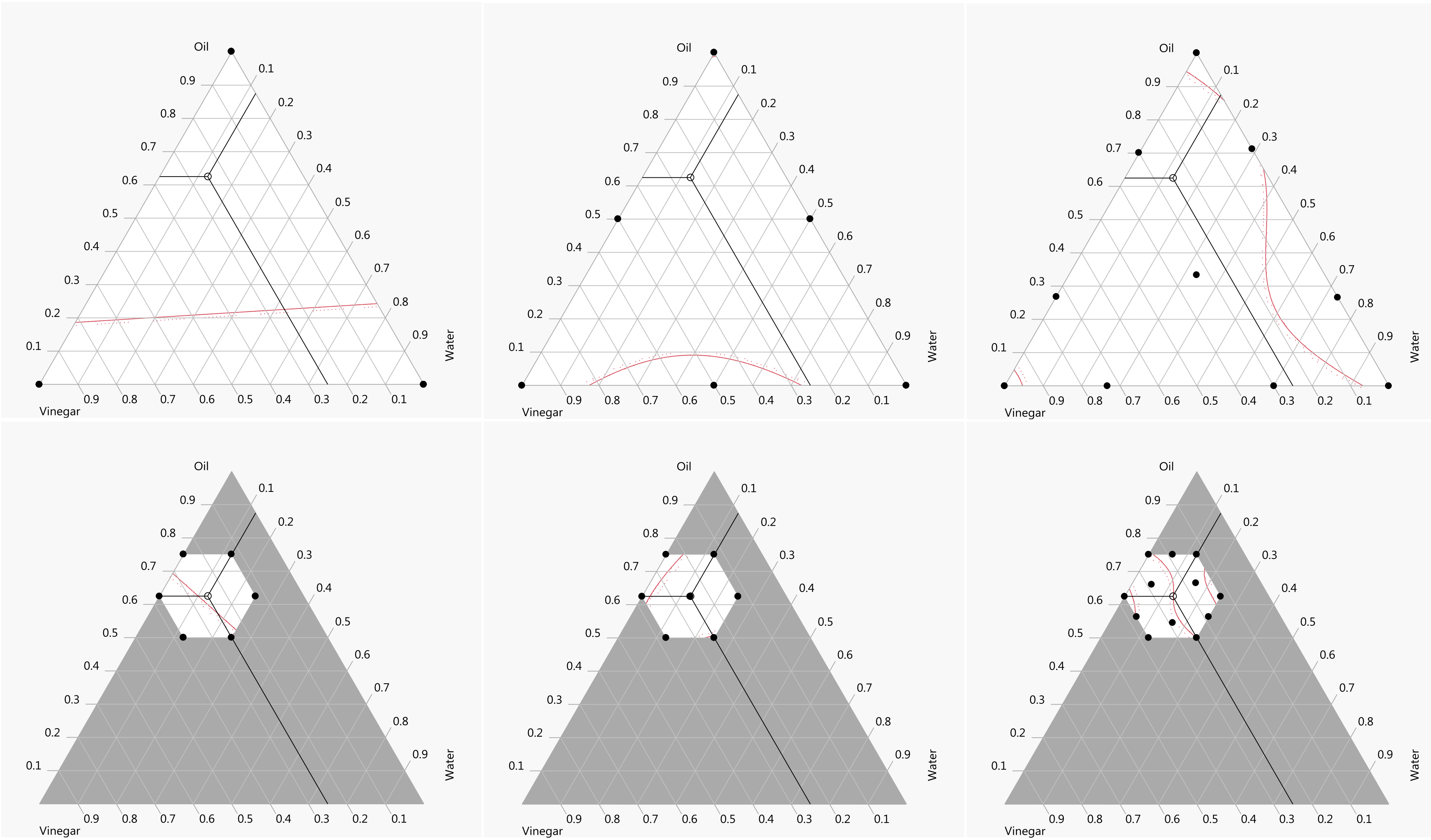
NOTE: Factors not in constraint get multiplied by zero

SIX DESIGNS:
TOP: 0 TO 1 RANGE
BOTTOM: EQUAL WIDTH ± 0.125 ABOUT NOMINAL

Left: Main Effects Model – 1st order

Middle: Interaction = Quadratic model! – 2nd Order

Right: Scheffé Special Cubic model – 3rd Order



MODEL COMPLEXITY

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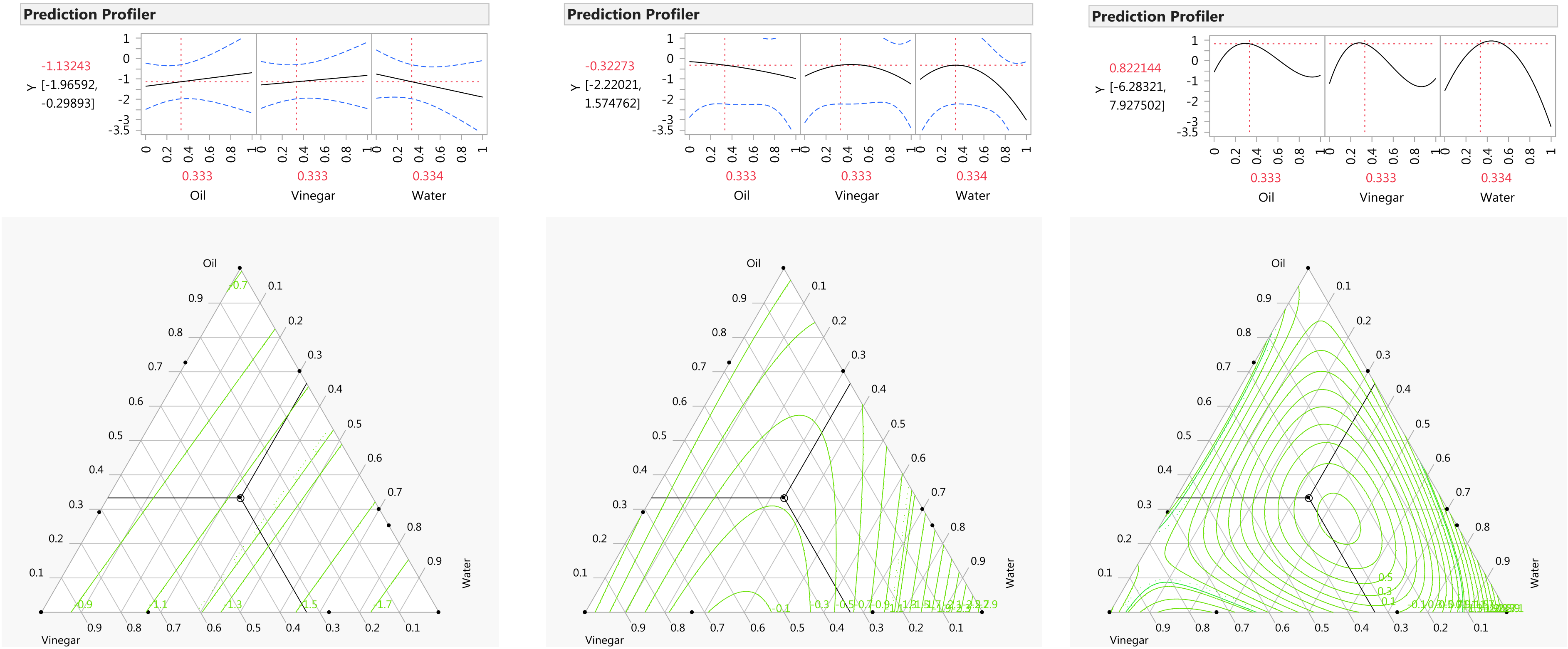


- 1st order for screening – finding the critical few
- 2nd order for prediction and optimization
- 3rd order when 2nd order proves inadequate for prediction (lack-of-fit)

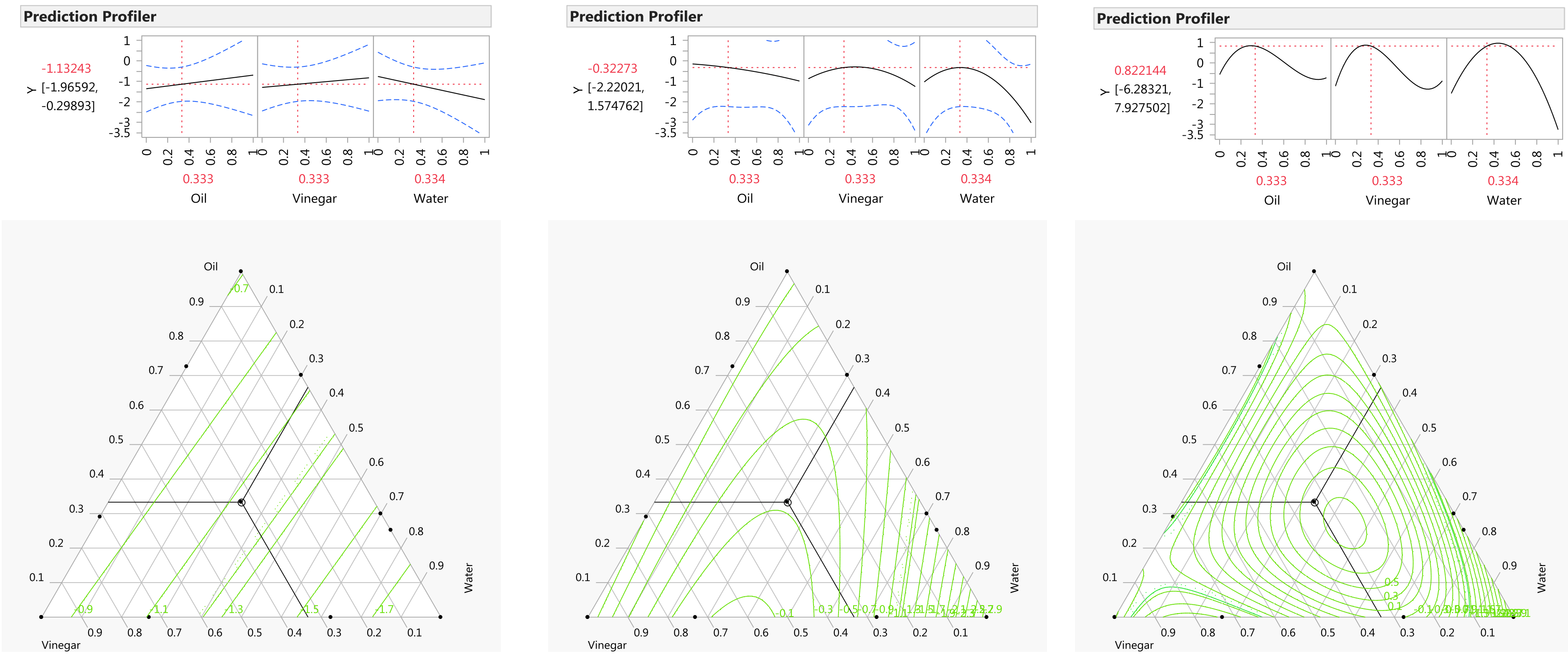
NOTE: For low numbers of components one might consider making a design to support a 3rd order model but analyze first with 2nd order model

MODEL COMPLEXITY

Left: ***Linear Blending**** – 1st order

Middle: ***Nonlinear Blending**** – 2nd Order

Right: Very Nonlinear Blending – 3rd Order



- Linear (additive) blending – need only pure component response values
- Synergistic blending* – improvement in response exceeds additive prediction
- Antagonistic blending* – improvement in response is less than additive prediction

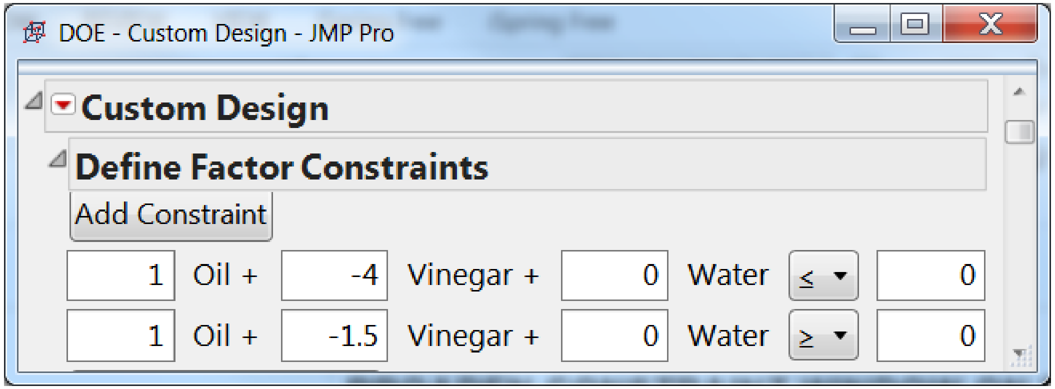
*From Ron Snee's JMP Explorers Event on DOE Strategies for Accelerating Formulation Development

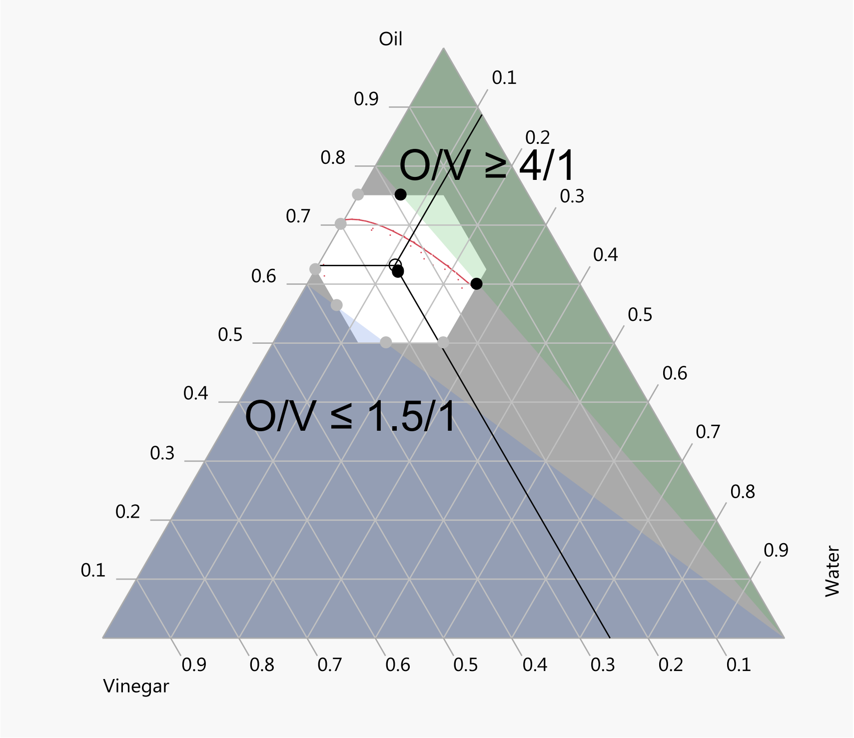
MAKE THIS DESIGN

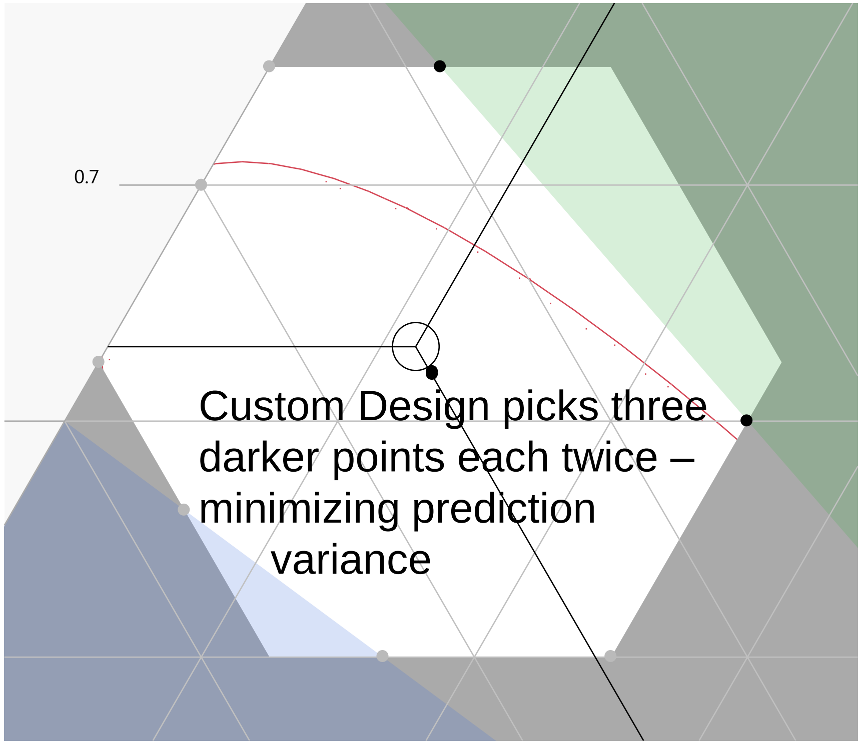
BROADEN CONSTRAINT WINDOW ON RATIO OF OIL/VINEGAR FROM 2 ≤ O/V ≤ 3 TO 1.5 ≤ O/V ≤ 4

O: 0.500 to 0.750 (½ to ¾)
V: 0.125 to 0.375 (⅛ to ⅜)
W: 0.000 to 0.250 (0 to ¼)

Use a 2nd order model







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REVISIT PLASTIC FORMULATION

- 5 components - names & ranges

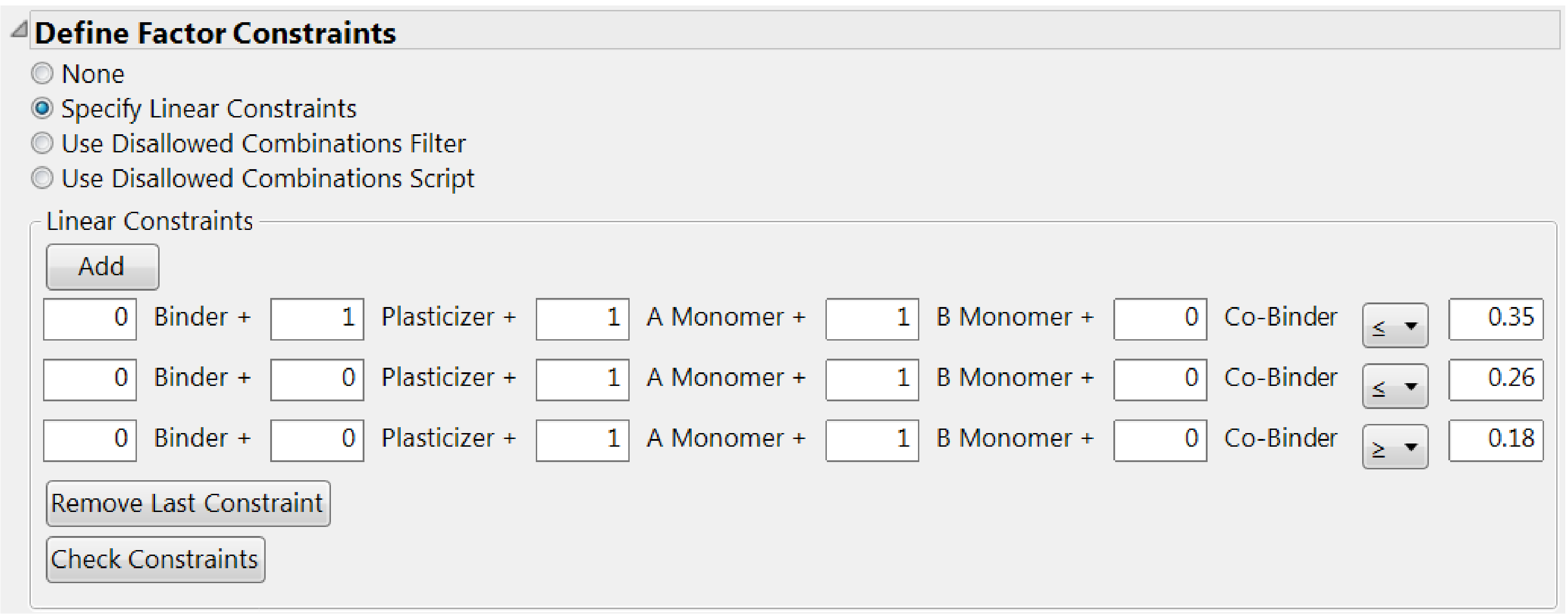
Binder	0.50	-	0.70
Plasticizer	0.05	-	0.15
A Monomer	0.10	-	0.25
B Monomer	0.00	-	0.15
Co-Binder	0.05	-	0.15

- 3 additional constraints

  $0.18 \le$ A_Mon + B_Mon ≤ 0.26

  A_Mon + B_Mon + Plas ≤ 0.35

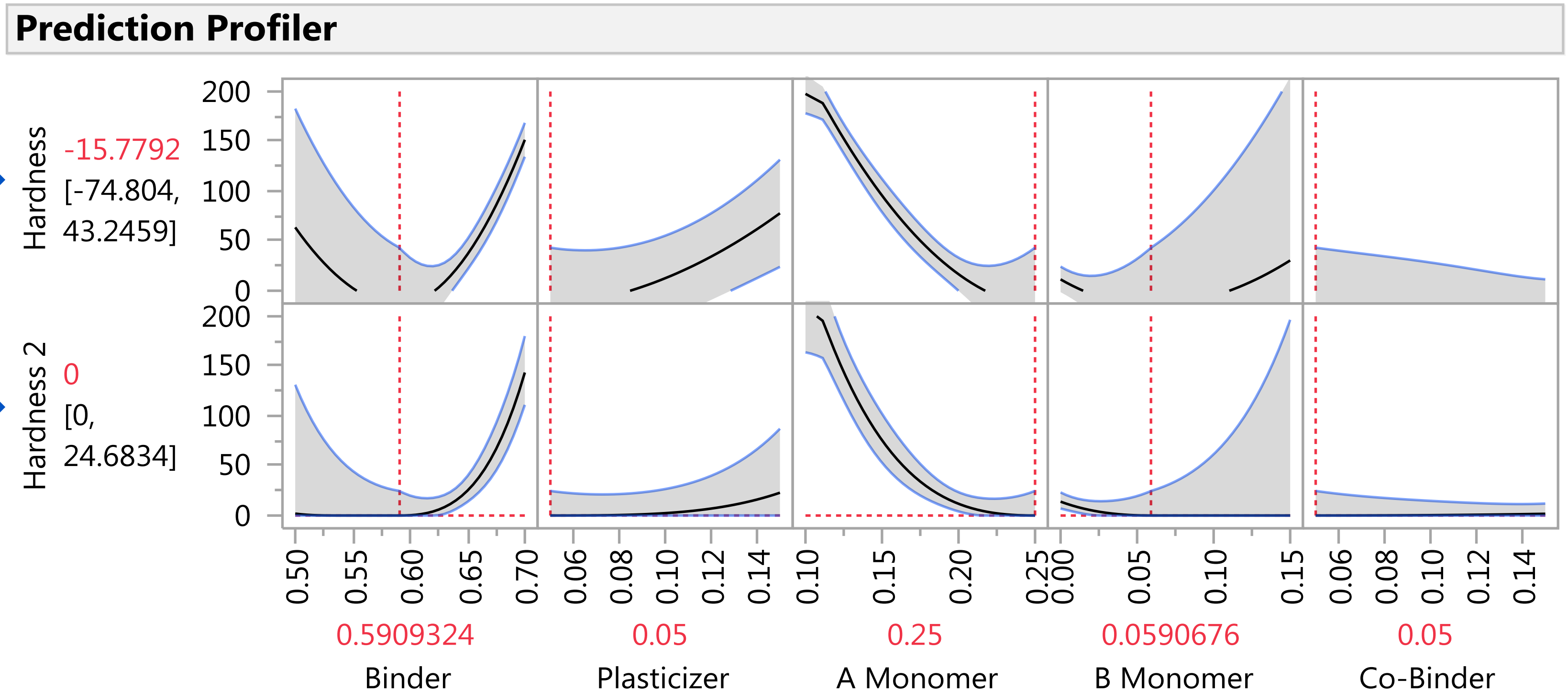
- model is 2^{nd} order = nonlinear blending



POTENTIALLY EMBARRASSING PREDICTIONS

FITTING HARDNESS OF PLASTIC WITHOUT (TOP) AND WITH A SQRT TRANSFORMATION (BOTTOM)

NEGATIVE Value?
NEGATIVE Low Limit?

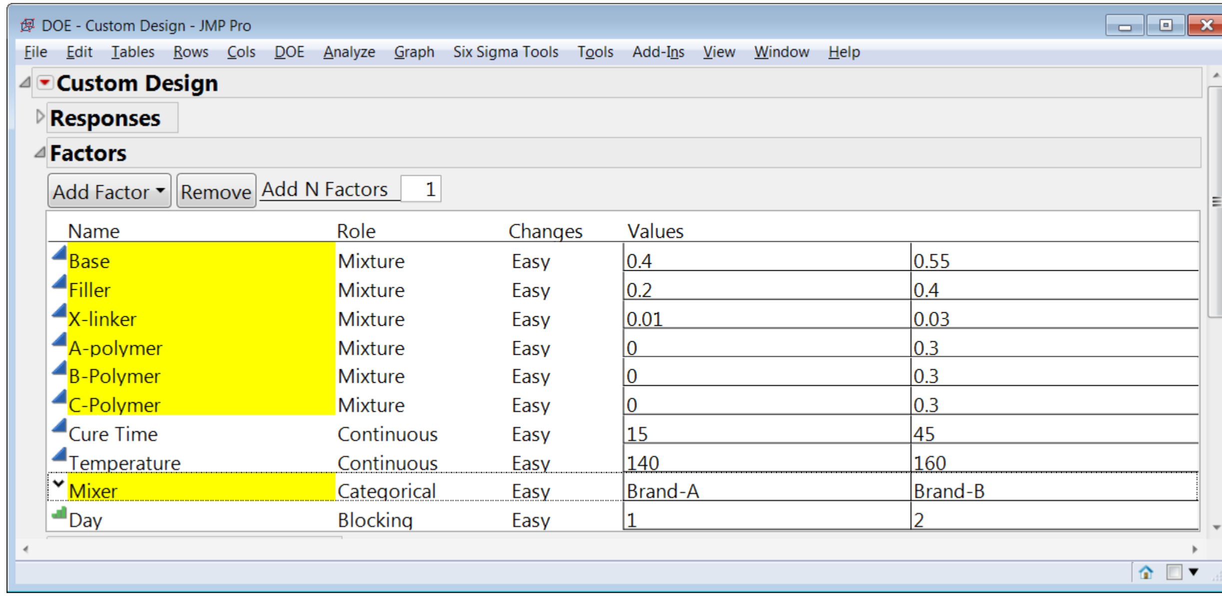


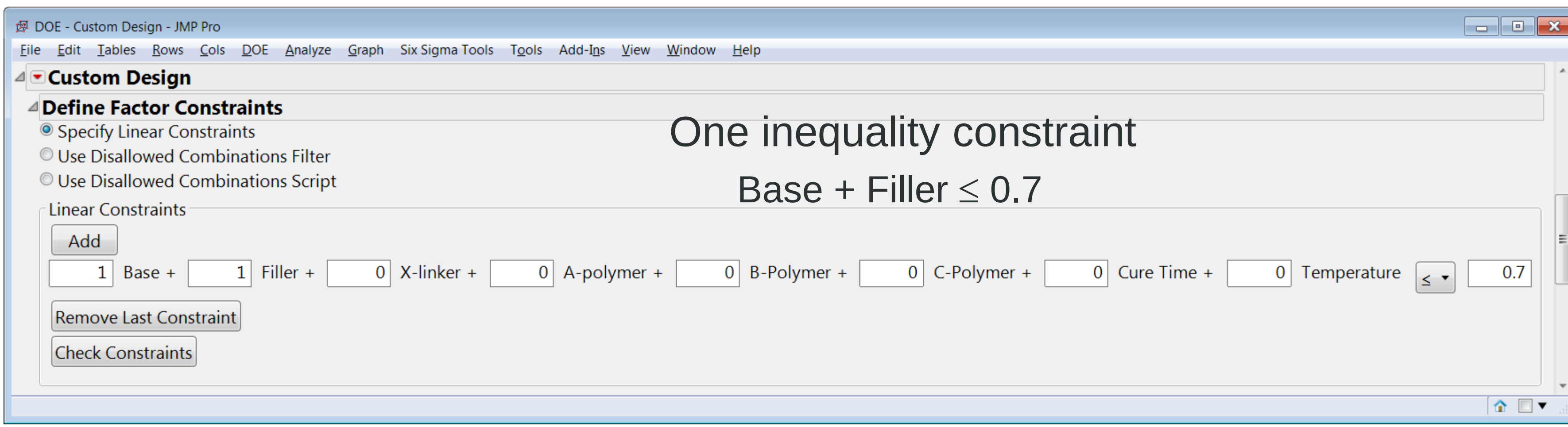
POSITIVE Value!
ZERO Low Limit!

On Transformed Scale (Bottom), Predictions Make Physical Sense

10-FACTOR = 6-MIX, 2-CON, 1-CAT, 1-BLK COMPLEX DOE

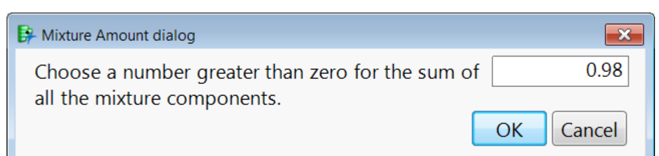
- See step-by-step PDF for details of complex design construction





One inequality constraint

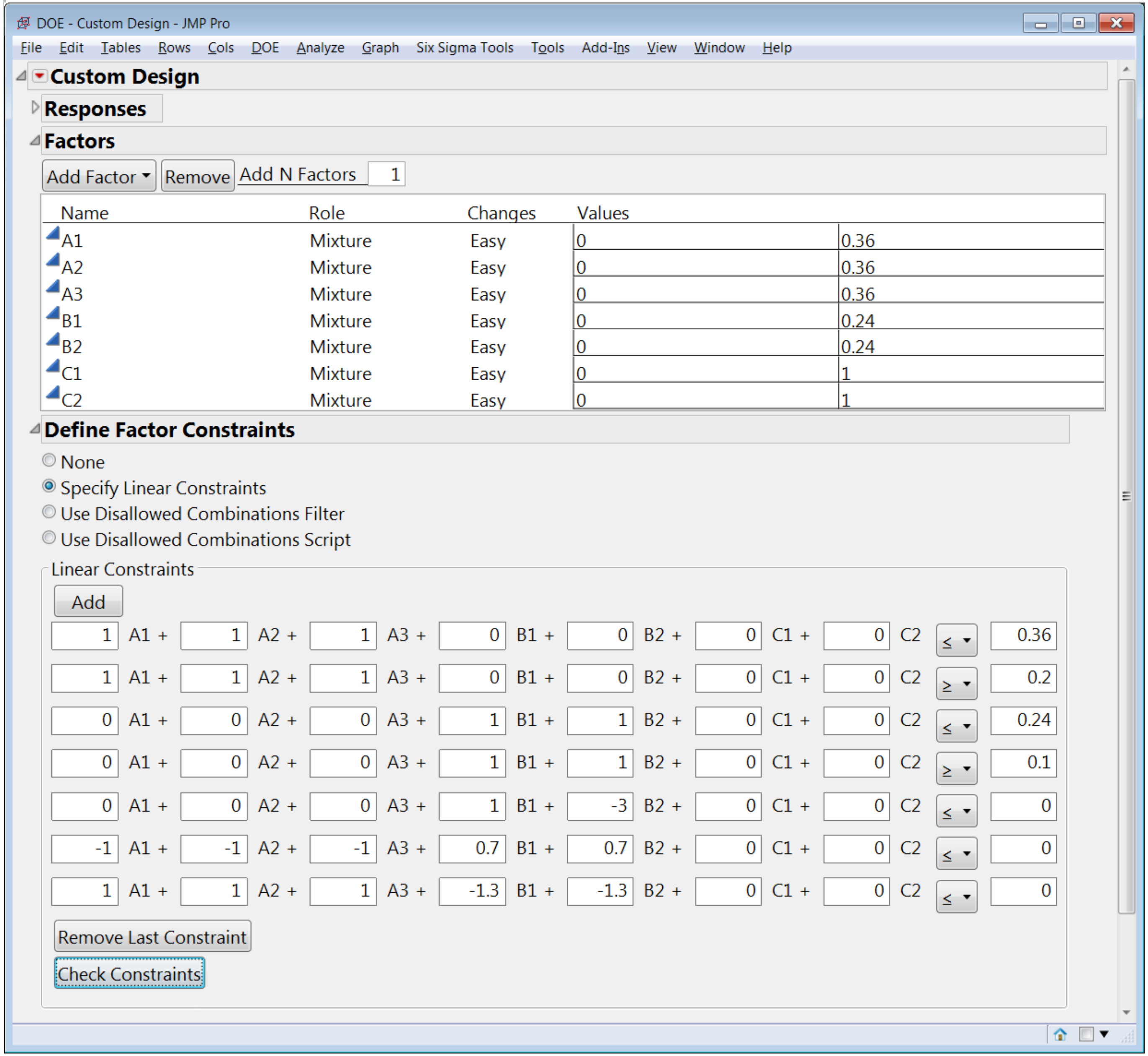
Base + Filler ≤ 0.7



Portion of mixture held constant at 2%

7-COMPONENT AND 7-CONSTRAINTS MIXTURE DOE

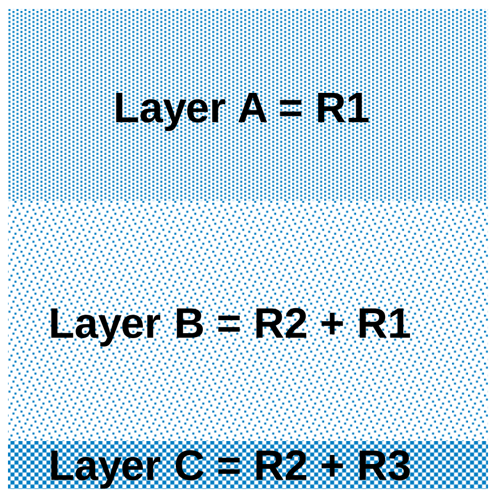
- See step-by-step PDF for details of mixture design construction



THREE-LAYER FILM STRUCTURE, FACTORS AND RANGES

Factor choice and ranges come from you and/or your subject matter experts!

Total *Thickness* of Three-Layer Film is 24 to 48 microns



Layer A is 25% to 55% of Total Thickness

Layer A is 100% Resin 1

Layer B is 30% to 70% of Total Thickness

Layer B is 10% to 90% *Resin 2* and 90% to 10% Resin 1

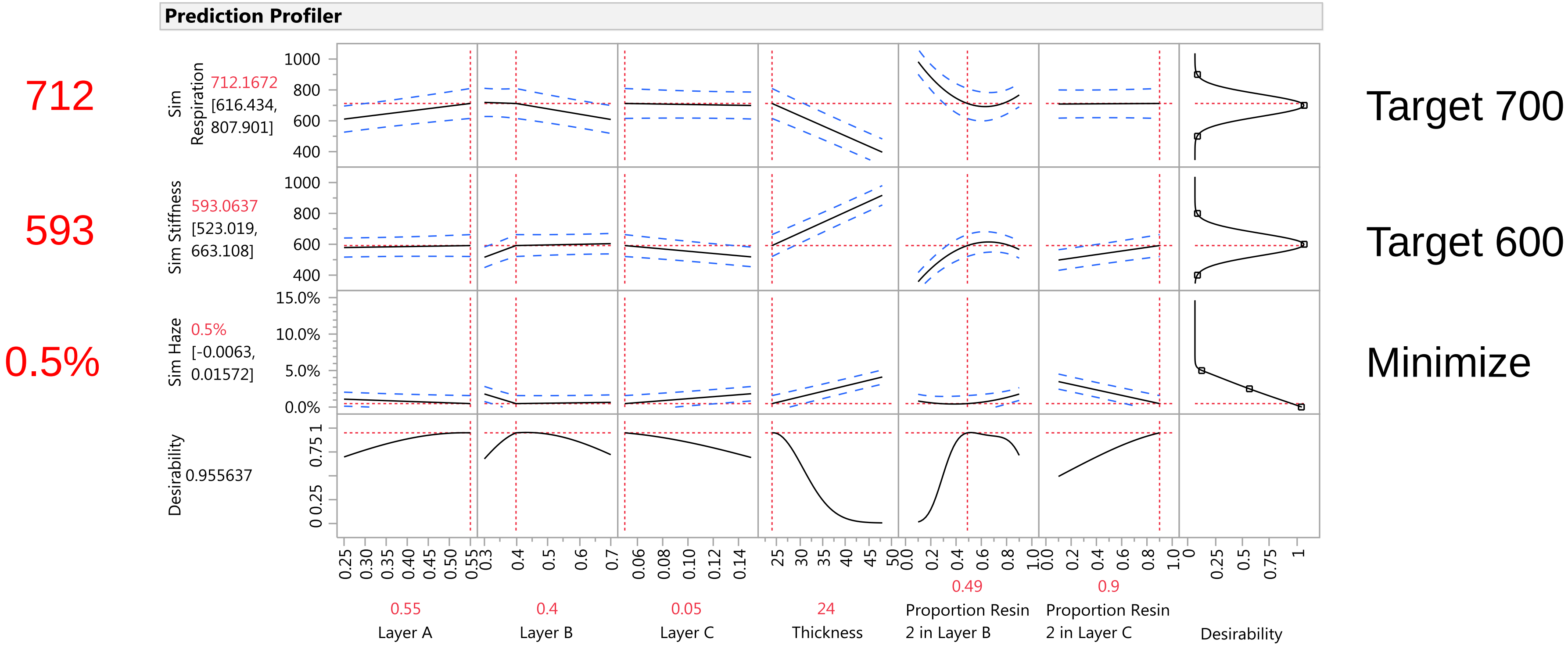
Layer C is 5% to 15% of Total Thickness

Layer C is 10% to 90% *Resin 2* and 90% to 10% Resin 3

GO TO

WWW.JMP.COM/TECHNICALLY-SPEAKING

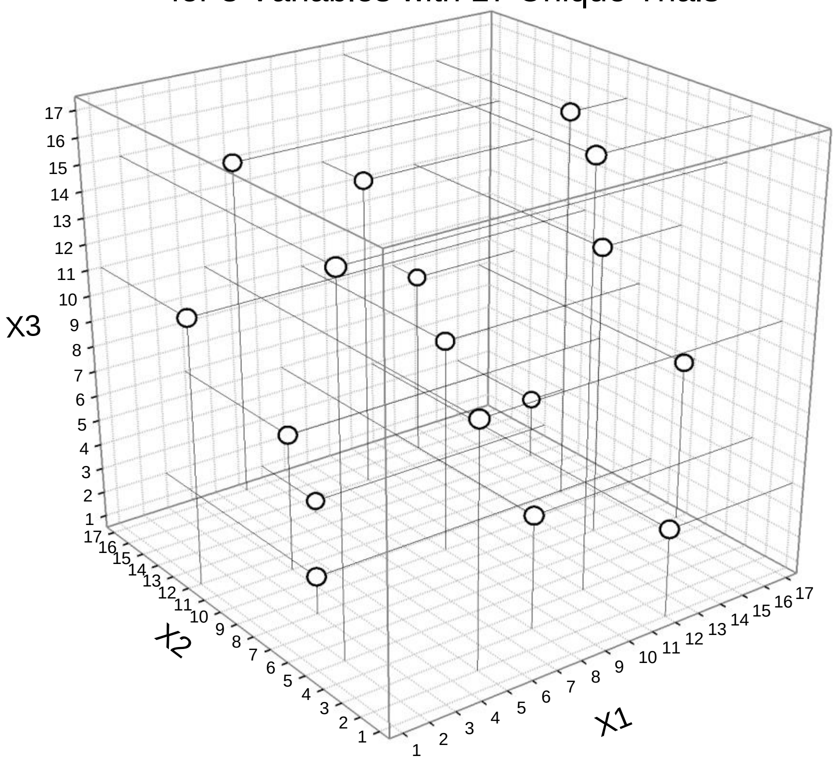
"BOOSTING PERFORMANCE WITH CUSTOM DESIGNED EXPERIMENTS"



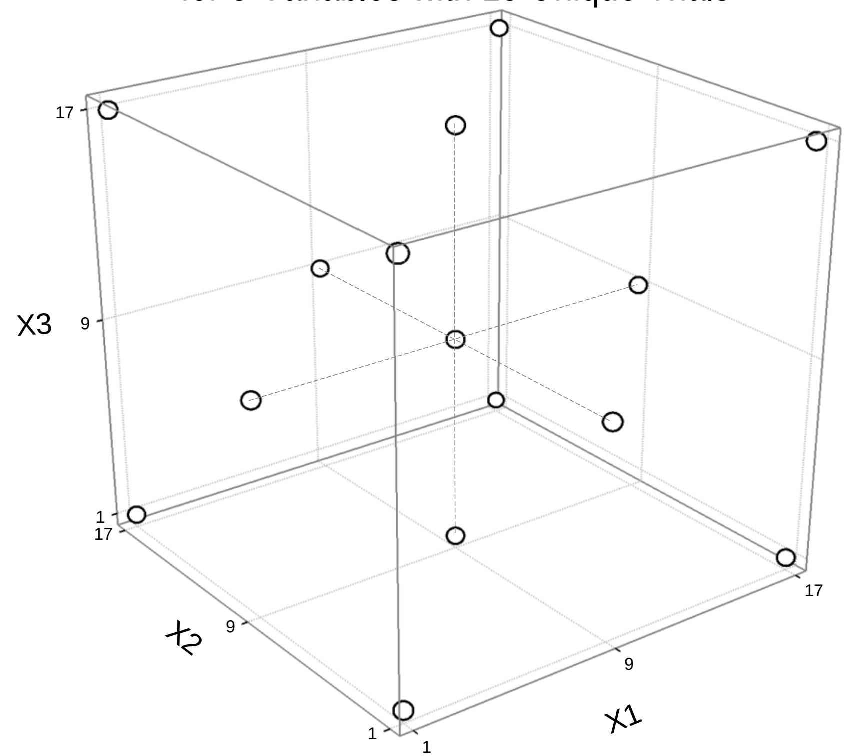
Ask JMP to find the best trade-off in performance among multiple responses for multiple factors

HOW ARE SPACE-FILLING DESIGNS DIFFERENT FROM TRADITIONAL RESPONSE-SURFACE DESIGNS?

Space-Filling Design
for 3 Variables with 17 Unique Trials



Response-Surface Design
for 3-Variables with 15 Unique Trials



Rather than emphasizing high leverage trials (“corners”) for a simple polynomial model, space-filling designs “spread” their trials more uniformly through the space to better capture the local complexities of the simulation model.

SPACE-FILLING MIXTURE DESIGNS

In order to create a space filling design with mixture variables, we have two options-, we can use the mixture design platform with the space filling design option, or we can use the space filling design platform with the appropriate constraints to enforce the sum of the individual ingredient proportions equal to one. As Figure 2 visually demonstrates with an unconstrained three component mixture design, we have nearly equivalent space filling efficiency with either option.

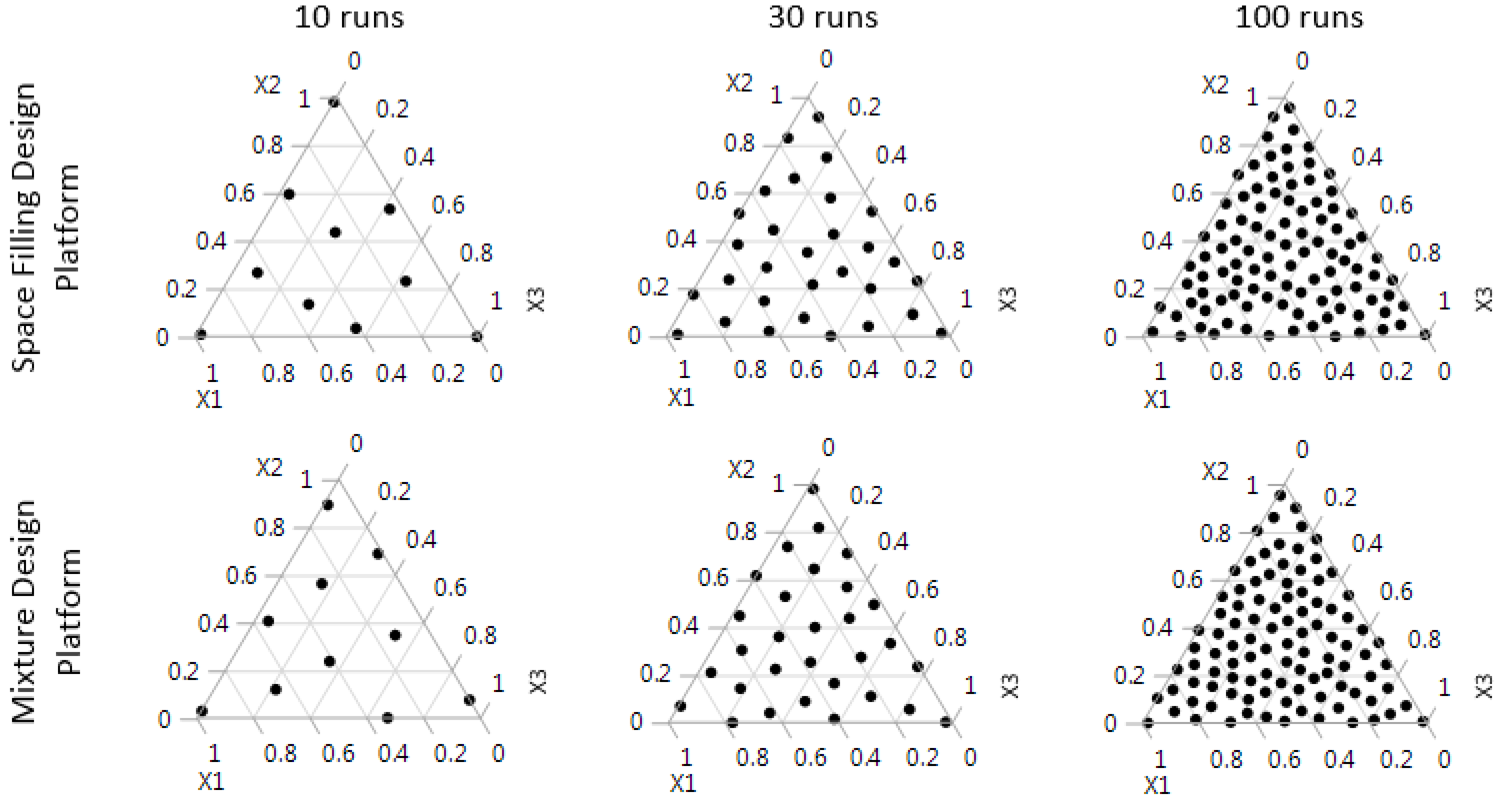
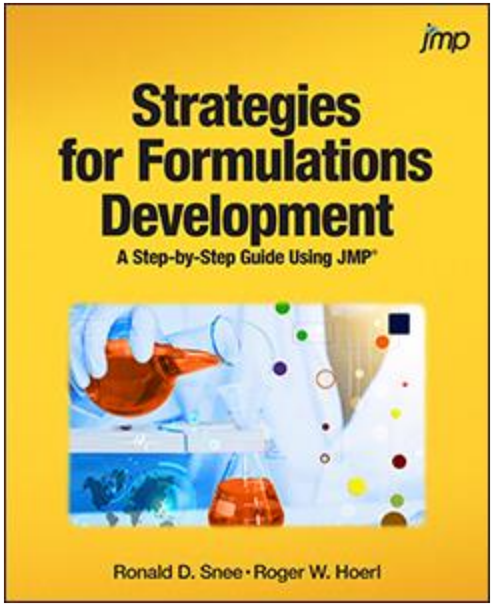


Figure 2: Ternary Plots of 10, 30 and 100-run Space Filling Mixture Designs using the Space Filling Design Platform and the Mixture Design Platform

RESOURCES

LINKS TO WEBCASTS, DOWNLOAD PDFS, AND BOOK

- https://www.jmp.com/en_us/events/ondemand/mastering-jmp/mixture-designs.html
- https://www.jmp.com/en_us/events/ondemand/technically-speaking/boosting-performance-with-custom-designed-experiments.html
- https://www.jmp.com/en_us/events/ondemand/mastering-jmp/transforming-data.html
- https://community.jmp.com/t5/Discovery-Summit-2017/An-Uncertainty-Quantification-Case-Study-Using-Space-Filling/ta-p/44055
- https://community.jmp.com/t5/US-Federal-Government-JMP-Users/Step-by-Step-JMP-DOE-Examples/ta-p/22176



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Thanks.
Questions or comments?

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