Formulation Simplified:
Finding the Sweet Spot via Design and Analysis of Experiments with Mixtures

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P.S. Find slides posted now at www.statease.com/webinar.html and, barring technical issues, a recording put up afterwards.

–Mark

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Reference: Formulation Simplified

Now in 3rd edition.*
1st edition 2018!

* Productivity Press CRC, Taylor & Francis
New York, June 2015.

A Primer on Mixture Design: What’s In It for Formulators?
www.statease.com/pubs/MIXprimer.pdf
The WIIFM for this Webinar

- Introduce tools for multi-component product development and optimization.
- Brief formulators on tailored tools that hone in on optimal recipes.
- Via real-world examples, lay out experiment-designs and models for mixtures that ultimately lead to the “sweet spot” —a formulation meeting all product specifications.

*See how Stat-Ease makes formulation optimization easy for its users!*

*Please press the raise hand now if you are with me.*

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Mixture Design*

*(Pioneered by Henry Scheffé, U Cal., 1957)*

**Considerations:**

- Factors are ingredients of a mixture.
- The response is a function of proportions, not amounts.
- Given these two conditions, fixing the total (an equality constraint) facilitates modeling of the response as a function of component proportions.

*Let’s try forcing a factorial design onto a mixture.*
Forcing (squeezing?) factorial design on a mixture: Lemonade

Mixture Design and Modeling (sweet!)
Two components: Quadratic (synergistic)

\[ \hat{Y} = \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 \quad \beta_{12} > 0 \]

Lemons plus water taste better than either one alone.
Three-Component Mixture

Factorial

Mixture

Ternary Diagram for Mixture Composition
(for example, stainless steel flatware)

\[ x_1 + x_2 + x_3 = 1 \]
Mixture Case Study

Three detergent components are varied:

- 3% ≤ A (water) ≤ 5%
- 2% ≤ B (alcohol) ≤ 4%
- 2% ≤ C (urea) ≤ 4%

The sum of the three active components always equals 9% of the final formulation (all other components held constant at 91%).

A + B + C = 9%

Detergent mix
Using v11 Rebuild,* Run, Analyze
(With Water at 8% high)

Formulation Simplified
In Example 4.5 (p. 140-141), Cornell details an experiment on a tropical beverage formulated from juices of:

A. Watermelon
B. Orange
C. Pineapple
D. Grapefruit

The formulators decided to restrict watermelon to 80% at most, but they wanted mixtures in this region because this juice is so much cheaper than the others.

This complex constraint forms a frustrum of the simplex tetrahedron (top cut off).

*Apple added as 5th component
Slice 3D on pineapple & grapefruit

Figure 4.4. Average flavor scores at the 16 juice blends.
Categorical Factors Combined

In this study a paint chemist working for an automobile manufacturer was tasked to choose:

- Monomer vendor M1 or M2.
- Crosslinker type CL1, CL2 or CL3.
- The optimal mix of
  - A. Monomer, 5 - 20 %
  - B. Crosslinker, 25 - 40 %
  - C. Resin, 55 - 70 %

With these goals for two key response measures:

2. Solids content > 50%.

Categorical Factors Combined: Split Plot

In this study a paint chemist working for an automobile manufacturer was tasked to choose:

- Monomer vendor M1 or M2. <=Hard to Change!
- Crosslinker type CL1, CL2 or CL3.
- The optimal mix of
  - A. Monomer, 5 - 20 %
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*Now you know.*

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[Shari Kraber, Workshop Manager & Master Statistician](mailto:shari@statease.com)  

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“Chemistry is necessarily an experimental science: its conclusions are drawn from data, and its principles supported by evidence from facts.”

- Michael Faraday

Best of luck for your experimenting!
Thanks for listening!

-- Mark

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