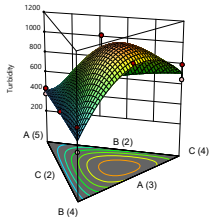
Formulation Simplified: Finding the Sweet Spot via Design and Analysis of Experiments with Mixtures

Making the most of this learning opportunity
Stat-Ease worldwide webinars attract many attendees, so, to prevent audio disruptions, all must be muted by the presenter. Also, to avoid interruptions and keep the presentation to about one hour, please hold all questions until afterwards and address them to stathelp@statease.com.

–Mark

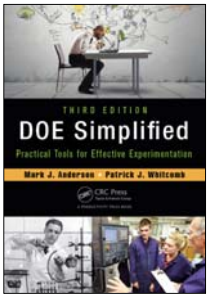
P.S. Find slides posted now at www.statease.com/webinar.html and, barring technical issues, a recording put up afterwards.



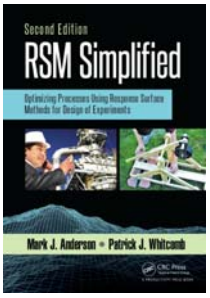
By Mark J. Anderson, PE, CQE
Stat-Ease, Inc., Minneapolis, MN
mark@statease.com

Reference: *Formulation Simplified*

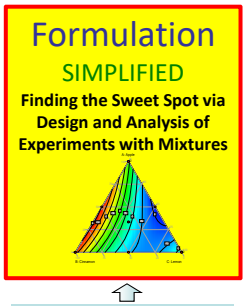
*Now in 3rd edition.**



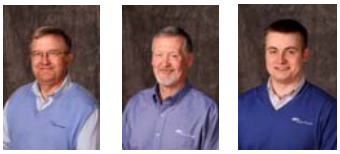
2nd edition 2016.



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.

Mixture Design*

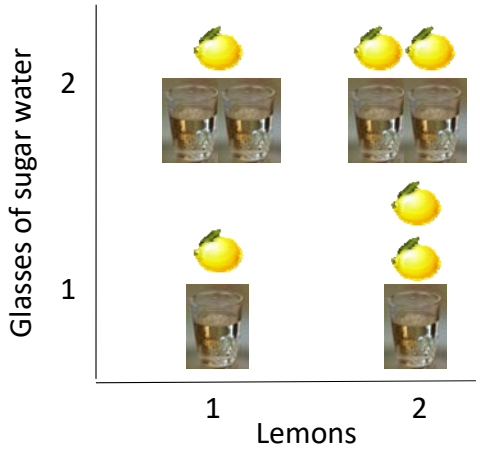
*(Pioneered by Henry Scheffé, U Cal., 1957)

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.

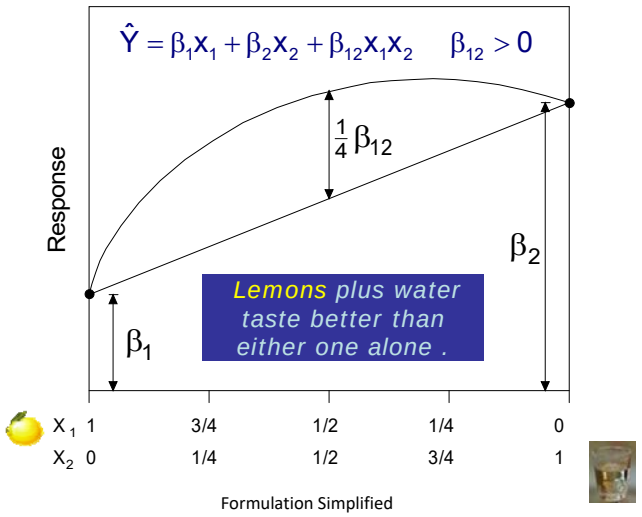
Let's try forcing a factorial design onto a mixture.

Forcing (squeezing?) factorial design on a mixture:
Lemonade

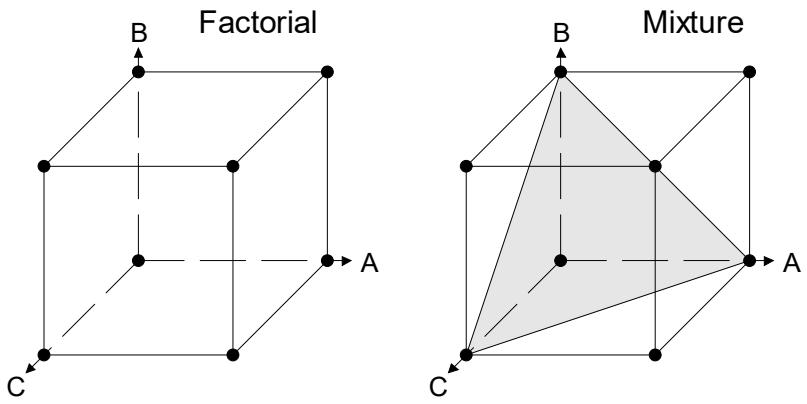


Mixture Design and Modeling (sweet!)

Two components: Quadratic (synergistic)



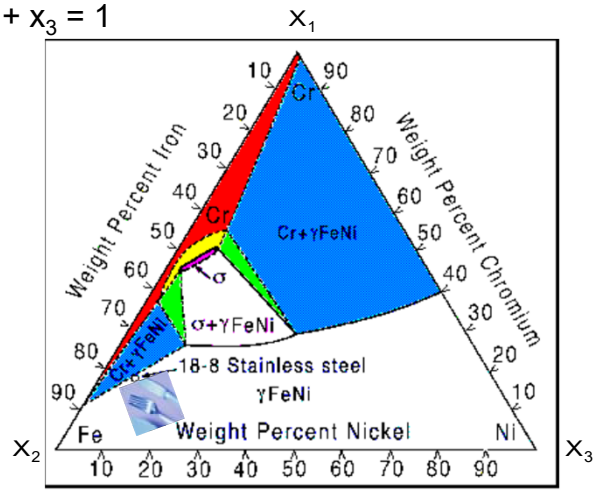
Three-Component Mixture



Formulation Simplified 7

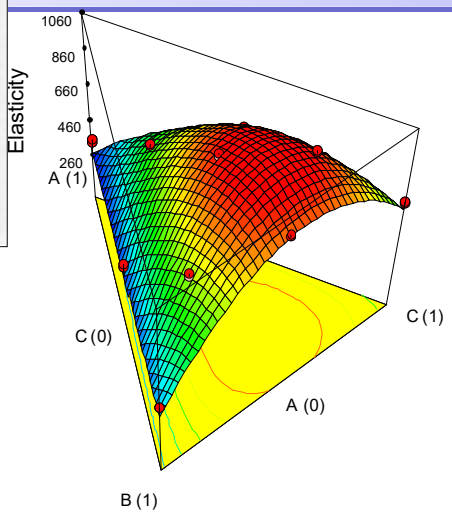
Ternary Diagram for Mixture Composition
(for example, stainless steel flatware)

$x_1 + x_2 + x_3 = 1$



Formulation Simplified 8

M
S



Special cubic model:

Elasticity =
+ 351 * A
+ 446 * B
+ 653 * C
- 6 * AB
+1008 * AC
+1597 * BC
+6141 * ABC

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)*

Complex Constraints (Non-Simplex)
Cornell's Fruit Juice

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.

Complex Constraints
Cornell's Fruit Juice

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

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

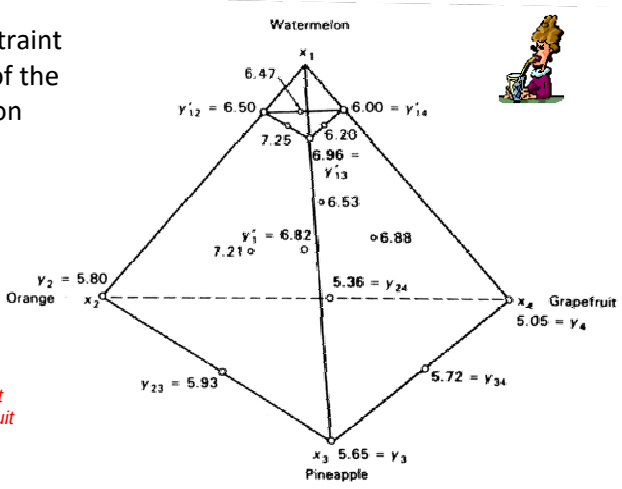


Figure 4.4. Average flavor scores at the 16 juice blends.

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:

1. Knoop hardness > 10.
2. Solids content > 50%.

Autocoat

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 %
  - B. Crosslinker, 25 - 40 %
  - C. Resin, 55 - 70 %

With these goals for two key response measures:

1. Knoop hardness > 10.
2. Solids content > 50%.

Autocoat
Rebuild w vendor HTC
Go with 6 added groups

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!

Now you know.

Stat-Ease Training:
Sharpen Up via Computer-Intensive Workshops

Shari Kraber,
Workshop Manager
& Master Statistician
shari@statease.com

PreDOE
Web-Based (optional)
Stat-Ease Academy

Basic Statistics for Design of Experiments

Designed Experiments for Pharma, Life Sciences, Assay Optimization, Food Science

Experiment Design Made Easy

Modern DOE for Process Optimization

Response Surface Methods for Process Optimization

Factorial
Split-Plot Designs
Stat-Ease Academy

Mixture and Combined Designs for Optimal Formulations

Robust Design and Tolerance Analysis

Plus more classes here!

www.statease.com/training/stat-ease-academy.html

Statistics Made Easy®

Best of luck for your experimenting!

Thanks for listening!

-- Mark

mark@statease.com

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

- Michael Faraday

