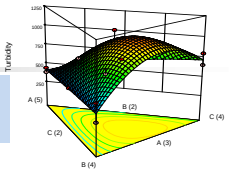
"If your experiment needs statistics, Then you ought to have done a better experiment."
-- Ernest Rutherford (Nobel prize winner for chemistry 1908)
(Chapter 11 *RSM Simplified* "Applying RSM to Mixtures")



An Introduction to Mixture Design for Optimal Formulations*

*Posted at www.statease.com/webinar.html

Presented by Mark J. Anderson
(Email: Mark@StatEase.com)

If you are on a speaker phone, please put your microphone on mute. Thanks. But feel free to speak up with a question. However, I may ask that some of these be put off until the end or emailed to me. Much appreciated -- Mark

Timer by Hank Anderson

It all began with beer:

Pioneering Mixture Experiments

A century ago William Sealy Gossett, a chemist at Guinness Brewery, developed a statistical method called the "t-test" to determine when the yeast content of a particular batch of beer differed significantly from the brewery's standard.

This is a simple comparative experiment that's still widely used to evaluate one material vs another (for example two brews). However, the state of the art for design of experiments (DOE) on mixtures has advanced greatly from here.

Mixture Design*

Considerations:

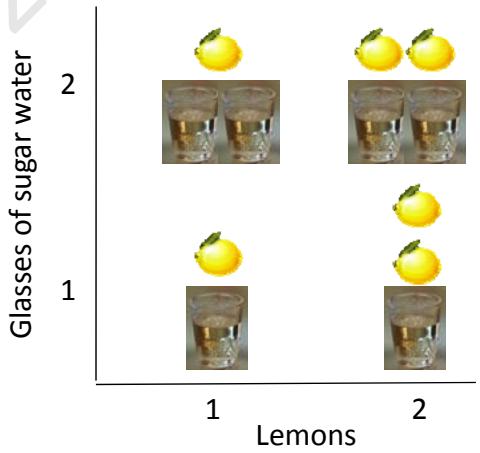
- Factors are ingredients of a mixture.
- The response is a function of proportions, not amounts.
- Given these two conditions, fixing the total (an equality constraint) facilitates modeling of the response as a function of component proportions.

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

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

Forcing (squeezing?) factorial design on a mixture:

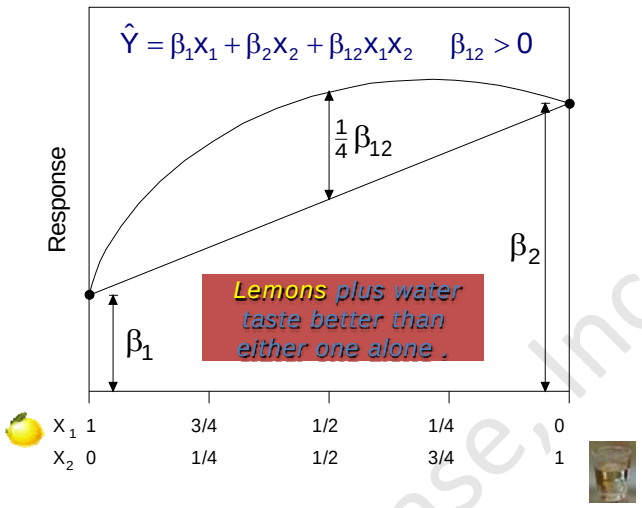
Lemonade



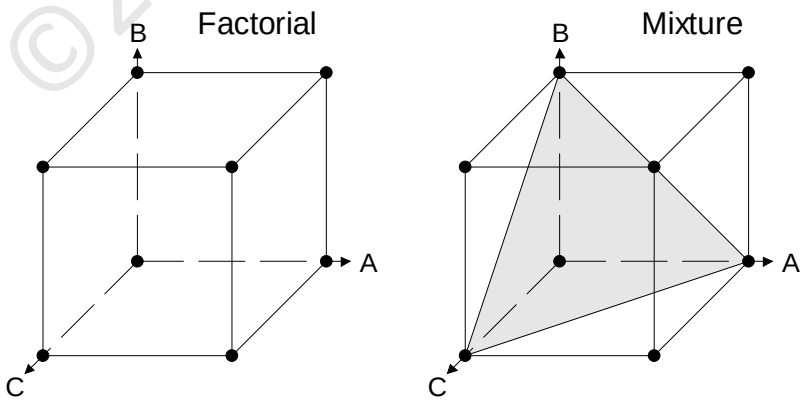
Mixture Design and Modeling (sweet!)

Two components: Quadratic (synergistic)

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

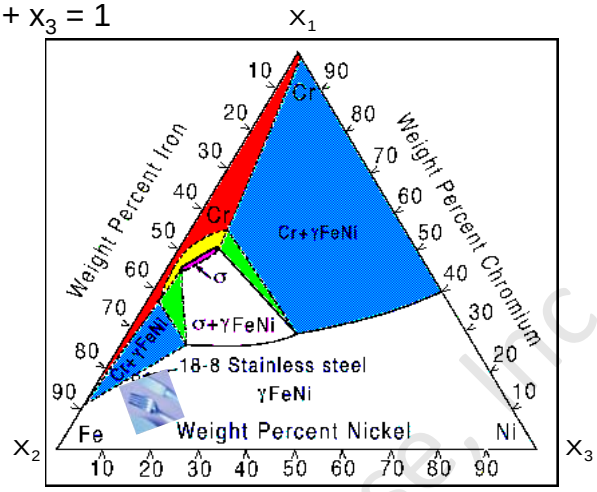


Three-Component Mixture

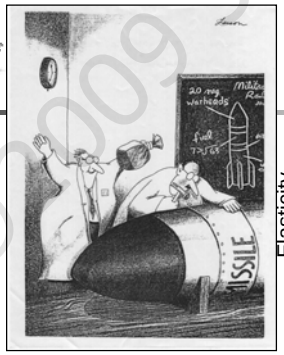


Ternary Diagram for Mixture Composition
(for example, stainless steel flatware)

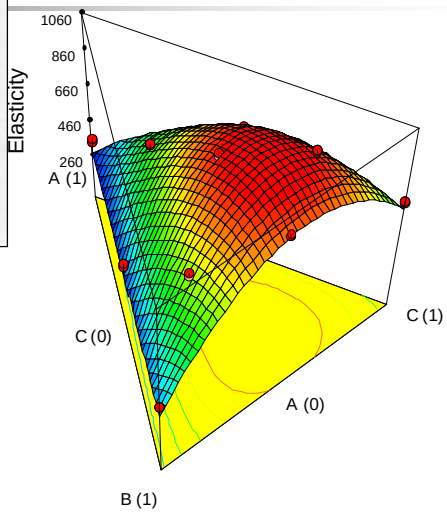
$x_1 + x_2 + x_3 = 1$



Mixture Design:
Solid Rocket Fuel



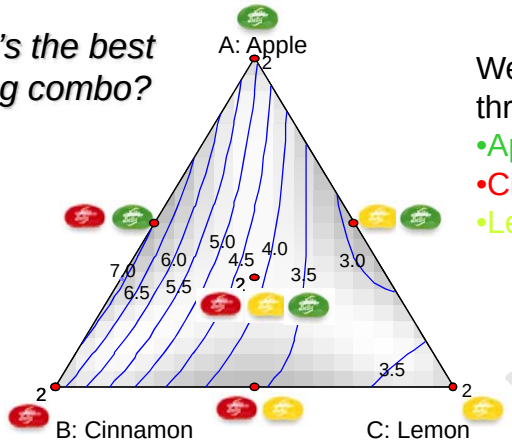
Special cubic model:
Elasticity=
+ 351 * A
+ 446 * B
+ 653 * C
- 6 * AB
+1008 * AC
+1597 * BC
+6141 * ABC



File: Rocket.dxp (V8)

Mixture Design: Homework?
Jelly Beans

What's the best tasting combo?



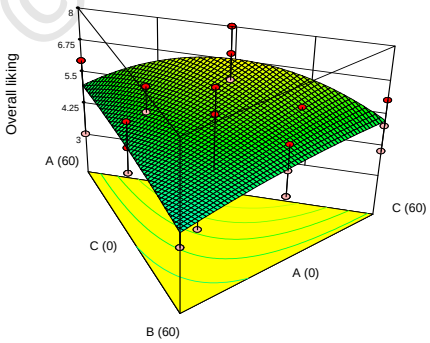
We juggled three beans:
- Apple
- Cinnamon
- Lemon

www.jellybelly.com

File: Teenbean.dxp (V8)

Mixture Design Brews Up New Beer Cocktail – Black & Blue Moon

stateaser



Let's go over this example!

Black & Blue Moon Beer Cocktail

"He was a wise man who invented beer."
-- Plato

Let's analyze results from this blending of beers. Can you detect any component interactions?

Filename: Beer cocktail.dxp (V8)
Rebuild the design.

Text* for Mixture Design

Experiments with Mixtures, 3rd edition

by John A. Cornell, John Wiley, New York, NY (2002).

John is infamous in statistical circles for his Harvey Wallbanger mixture experiment up at 3M Canada, but we will go with another, alcohol -free, example.

*Less academic soft-cover underway by Mark & Pat:
Formulation Simplified: Finding the Sweet Spot via Design and Analysis of Experiments with Mixtures*

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).

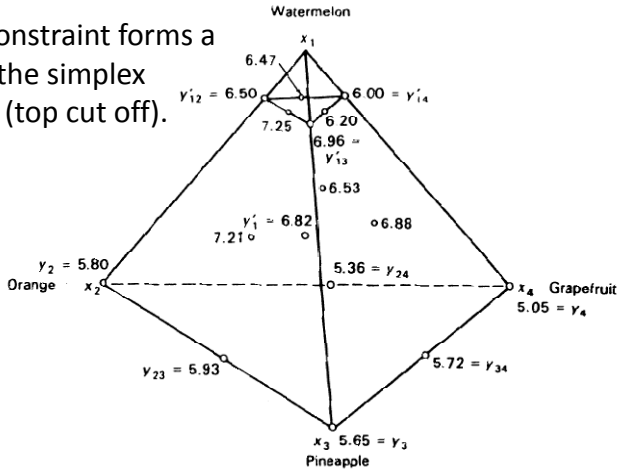


Figure 4.4. Average flavor scores at the 16 juice blends.

Minnesota-Scandinavian Hedonic Taste Scale

9 Yust like lutefisk! ☺
8 Tastes like Mom's
7 Not so bad
6 Could be better
5 Could be worse 😐
4 Helga made something like this once
3 I like it, but ....
2 It's different!
1 Silence ☹

Fruit Juice with Complex Constraints

Let's see how the computer builds an optimal design within this frustrum (non-simplex) experimental region.

Filename: Cornell Ex 4-5 -- fruit juice.dxp (V8)
Rebuild the design. Only analyze if time allows.

The Perils of Parts

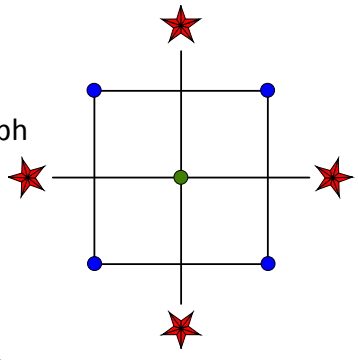
A recent communication:

"I am a Design-Expert user doing a chemical formulation DOE study. I have 2 ingredients to study in relation (by parts) to the base polymer (100 parts). So I don't think it is a mixture design."

Perils of Parts
Polymer RSM Experiment

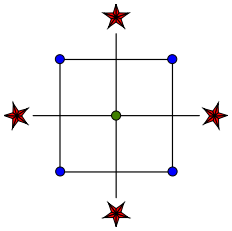
Response surface method (RSM) – a central composite design (CCD) – chosen to optimize filler and plasticizer over a range of parts per hundred (pph) of polymer:

- Polymer is constant at 100.
- Filler varies from 100 to 250 pph of polymer.
- Plasticizer varies from 50 to 100 pph of polymer.
- All other ingredients are held constant at 57 pph of polymer.



Polymer RSM
Perils of Parts

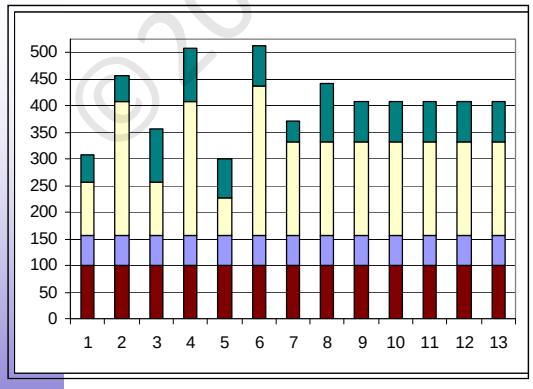
Factor	pph polymer	
Filler	100	250
Plasticizer	50	100
Polymer	100	
Other	57	



Do you see a problem?

- ☑ Factors are ingredients of a mixture.
- ☑ Response is a function of proportions.

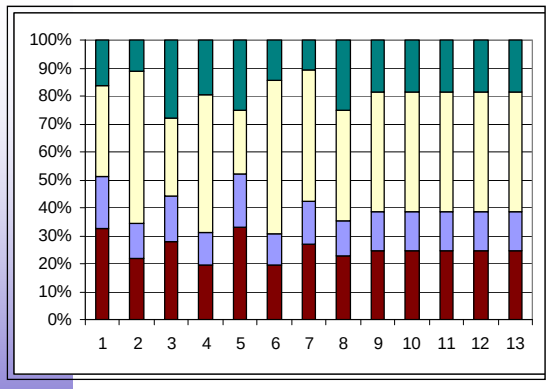
Polymer RSM
Pounds in the Reactor



A		Filler	100	250
B		Plasticizer	50	100
C		Polymer	100	
D		Other	57	

$$\hat{y} = \beta_0 + \beta_1 A + \beta_2 B + \beta_{12} AB + \beta_{11} A^2 + \beta_{22} B^2$$

Polymer RSM
Composition in Cartridge



A		Filler	23%	55%
B		Plasticizer	11%	28%
C		Polymer	19%	33%
D		Other	11%	19%

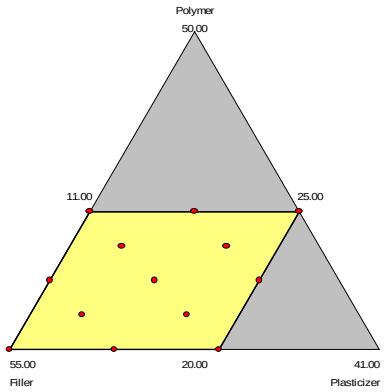
$$\hat{y} = \beta_0 + \beta_1 A + \beta_2 B + \beta_{12} AB + \beta_{11} A^2 + \beta_{22} B^2$$

This equation excludes C and D, which are both varying!

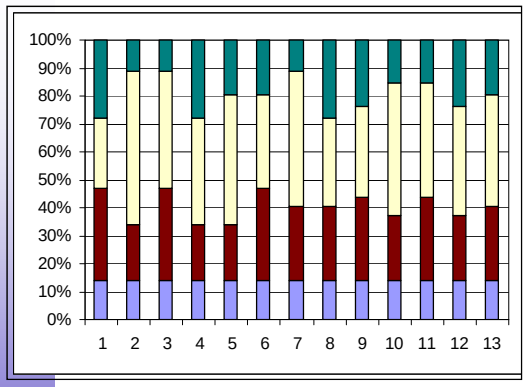
Polymer Experiment
As a Mixture Design

The factors studied are ingredients and performance is a function of proportions - - this is a mixture!

- Vary polymer from 20 to 33%.
- Vary filler from 25 to 55%.
- Vary plasticizer from 11 to 28%.
- All other ingredients are held constant 14%.



Polymer Mixture Design
Composition in Cartridge



A		Filler	25%	55%
B		Plasticizer	11%	28%
C		Polymer	20%	33%
D		Other	14%	

$$\hat{y} = \beta_1 A + \beta_2 B + \beta_3 C + \beta_{12} AB + \beta_{13} AC + \beta_{23} BC$$

D is held constant at 14%.

Take home message!

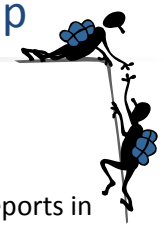
When you are:

- studying ingredients (components), and
- the response is a function of the proportions.

Use Mixture DOE

Pat suggests that formulators ask themselves an easy question:
"If I double everything, will I get a different result?"
If the answer is "No," such as it would for a food or beverage recipe, then mixture design will be the best approach to experimentation.

How to get help



- Search publications posted at www.statease.com.
- In Stat-Ease software press for Screen Tips, view reports in annotated mode, look for context-sensitive Help (right-click) or search the main Help system.
- Explore Experiment Design Forum http://forum.statease.com and post your question (if not previously answered).
- E-mail stathelp@statease.com for answers from Stat-Ease's staff of statistical consultants.
- Call 612.378.9449 and ask for "statistical help."

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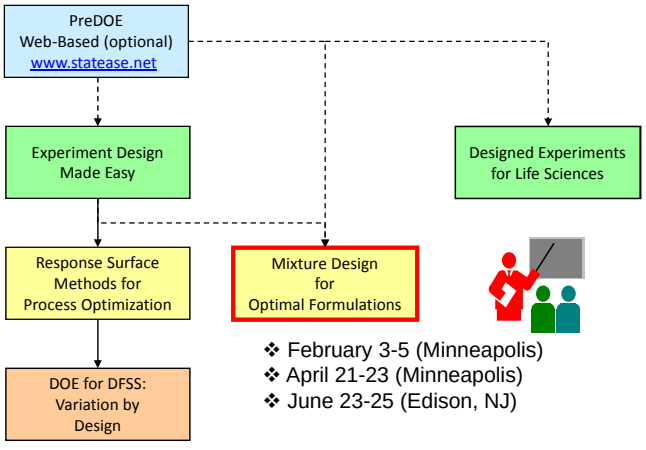

- February 3-5 (Minneapolis)
- April 21-23 (Minneapolis)
- June 23-25 (Edison, NJ)

Statistics Made Easy®

"Each pint is like a child.
You have to mind it through the entire process."
-- Fergal Murray, Guinness brew master

Best of luck for your experimenting!

Thanks for listening!

-- Mark

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