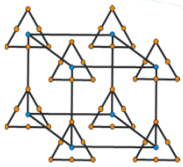

How to Unveil Breakthrough Synergisms Between Mixture and Process Variables

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mark@statease.com

- **Layout of combined mixture-process designs *(fish patties)***
- Streamlined option to 'brute force' crossed models: "KCV"
- KCV combining mixture with categorical variables *(composite)*
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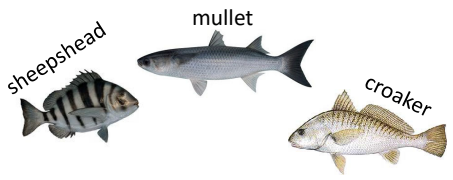
Cornell's* Fish Patty Experiments

Three mixture components:

- x_1 mullet
- x_2 sheepshead
- x_3 croaker



Three process factors:

- z_1 oven temperature: 375 or 425 °F
- z_2 time in oven: 25 or 40 minutes
- z_3 time of deep frying: 25 or 40 seconds

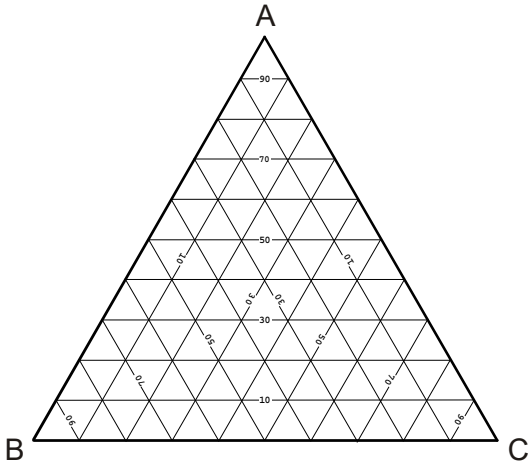
One Response:

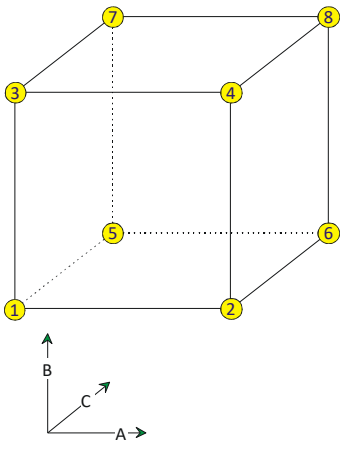
- R_1 Texture

*(*Experiments with Mixtures, 3rd edition*, John Wiley, Chapter 7)

Mixture-Process Experiments

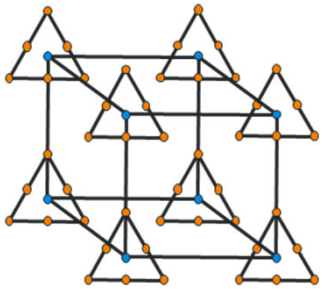
Elements of Combined Design: Mixture Components & Process Factors





Mixture-Process Experiments

Three Mixture Components and Three Process Factors Combined



If all 7 blends laid out in the mixture design (triangles) are done at all 8 (2^3) process conditions (cube), then <u>all</u> terms can be fitted to a crossed 3FI (three-factor interaction) x SC (special cubic) model, all the way up to $X_1X_2X_3Z_1Z_2Z_3$ (6^{th} order!).

Mixture: $Y(x) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{123} x_1 x_2 x_3$

Process: $Y(z) = \alpha_0 + \alpha_1 z_1 + \alpha_2 z_2 + \alpha_{12} z_1 z_2 + \alpha_3 z_3 + \alpha_{13} z_1 z_3 + \alpha_{23} z_2 z_3 + \alpha_{123} z_1 z_2 z_3$

$$\eta(x,z) = \quad Y(x) \times Y(z) \quad = \quad 56 \text{ terms}$$

Mixture-Process Experiments

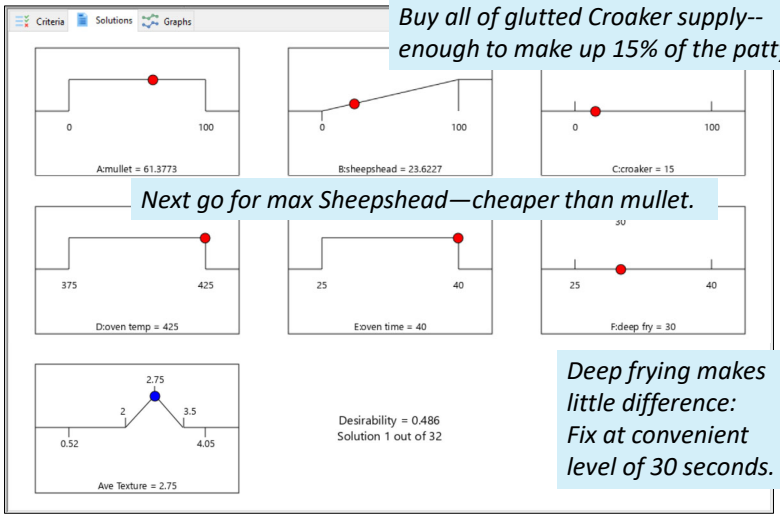
Resulting Textures from Completely Crossed Mixture-Process Design

Process Factors			Mixture Composition (x_1,x_2,x_3)						
z_1	z_2	z_3	(1,0,0)	(0,1,0)	(0,0,1)	(½,½,0)	(½,0,½)	(0,½,½)	(⅓, ⅓,⅓)
-1	-1	-1	1.84	0.67	1.51	1.29	1.42	1.16	1.59
1	-1	-1	2.86	1.10	1.60	1.53	1.81	1.50	1.68
-1	1	-1	3.01	1.21	2.32	1.93	2.57	1.83	1.94
1	1	-1	4.13	1.67	2.57	2.26	3.15	2.22	2.60
-1	-1	1	1.65	0.58	1.21	1.18	1.45	1.07	1.41
1	-1	1	2.32	0.97	2.12	1.45	1.93	1.28	1.54
-1	1	1	3.04	1.16	2.00	1.85	2.39	1.60	2.05
1	1	1	4.13	1.30	2.75	2.06	2.82	2.10	2.32

Confirmed by the statistical modeling, many combos of mullet, sheepshead and croakers met the 2 to 3.5 goal when processed at the right settings for oven temp & time and frying. ☺

Mixture-Process Experiments

Applying the Predictive Model to Unveil Desirable Results in 'What-If' Scenario



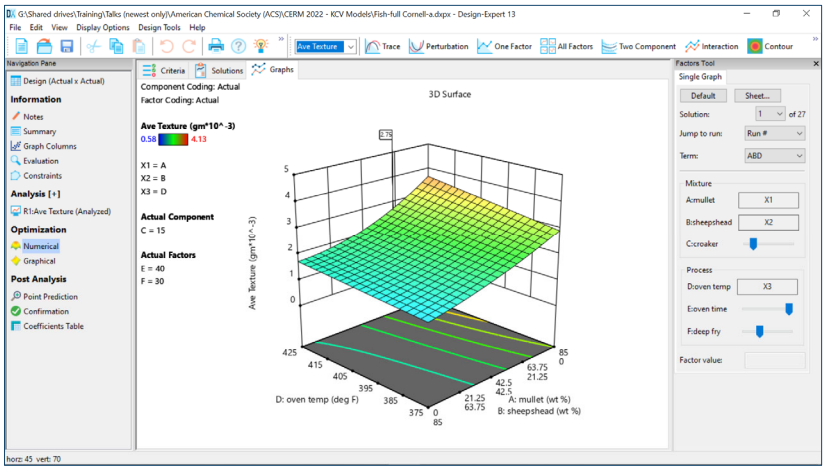
Buy all of glutted Croaker supply-- enough to make up 15% of the patty.

Next go for max Sheepshead—cheaper than mullet.

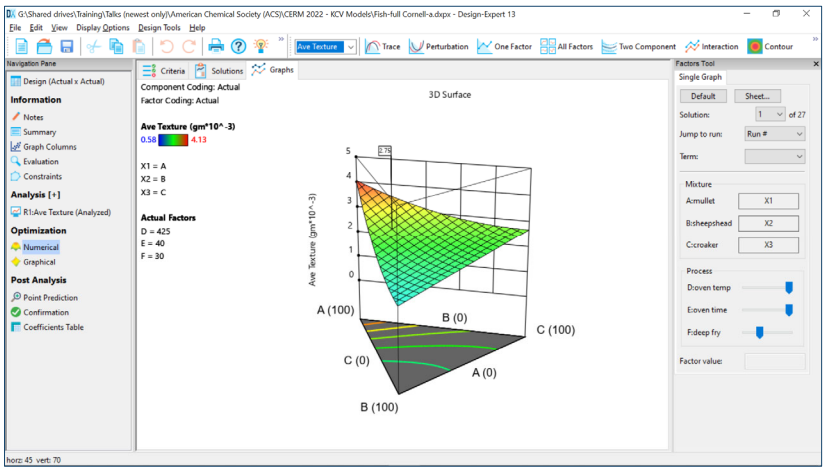
Deep frying makes little difference: Fix at convenient level of 30 seconds.

Mixture-Process Experiments

Model Graphs: Process View Optimal Settings for Factors and Components



Model Graphs: Mixture View
Optimal Settings for Factors and Components



- Layout of combined mixture-process designs *(fish patties)*
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KCV* Model for Combined Designs

Problem:

Standard crossed models generate far more terms than needed to detect likely interactions between mixture and process variables.

Elegant Solution:

Kowalski, Cornell and Vining (KCV) simplified the equation by only crossing the linear models; adding mixture and process terms beyond that. This streamlined model when used for an optimal (custom) design, saves many runs, yet it detects probable combination effects between components and factors (*and/or categorical variables*).

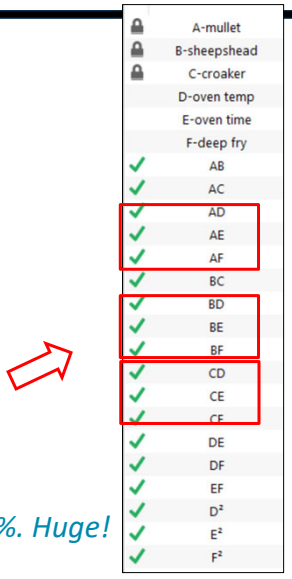
KCV makes mixture-process combined designs far more practical!

*Scott Kowalski , John A. Cornell & G. Geoffrey Vining, "A new model and class of designs for mixture experiments with process variables, *Communications in Statistics - Theory and Methods*, 29:9-10, 2255-2280, 2000.

Applying the KCV Model to Fish Patties

Three Process Factors & Three Mixture Components

- The crossed 2FI-by-SC (special cubic) model generates 56 coefficients.
  - It includes many high-order terms that will almost certainly be insignificant, e.g., AD^2, ABCDE, $ABCD^2$, etc. All these terms must be fitted by a unique run. Wasteful!
- The KCV model only needs 21 coefficients.
  - The linkage between mixture components (A, B, C) and process factors (D, E, F) is restricted to simple component-by-factor interactions. Other terms are either purely mixture or purely process. Elegant!



KCV's generally cut design sizes by over 50%. Huge!

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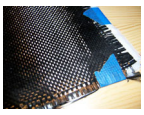
KCV Design Applied to a Combined Mixture & Categorial Experiment on a Composite Material

Aerospace engineers aimed to maximize the impact and tensile strength of an epoxy-fiber composite by varying the materials as follows (a 4-component mixture combined with two categoric factors):

A. Elastomer, 5 – 20% (two types—Factor E)
B. Fiber, 54 – 62% (three types—Factor F)
C. Hardener, 0 – 100%
D. Epoxy resin, 0 – 100%



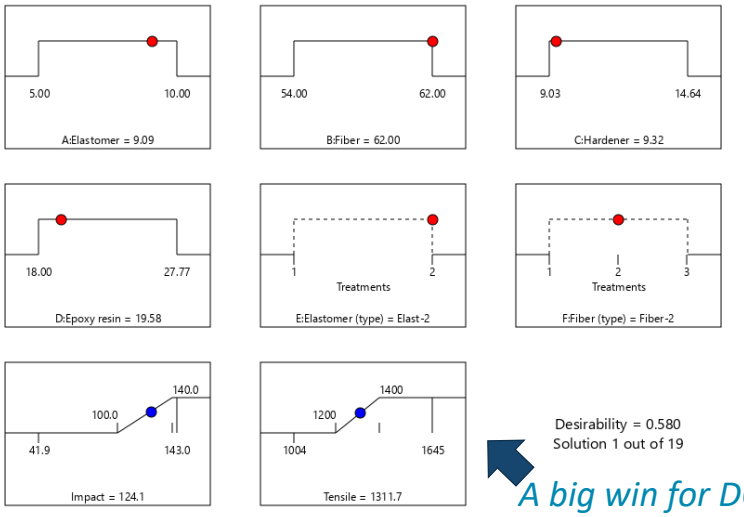
Subject to this multicomponent ratio constraint to achieve proper stoichiometry for the reaction:

C/D. Epoxy/hardener, 1.8 – 2.1

Applying an optimal design customized for KCV modeling reduced the number of terms (& runs) from 60 for crossed 2FI-Q (quadratic) to 24. ☺

*Source: "Mixture Design for Optimal Formulation" workshop, Stat-Ease, Inc.

Settings for Most Desirable Composite



A big win for DOE!

Mixture-Process Experiments

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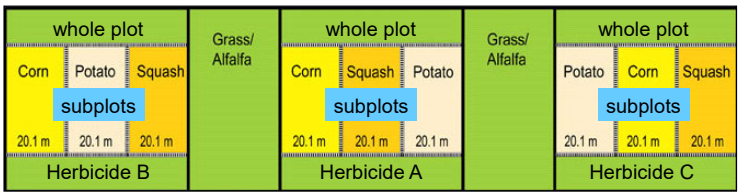
Split-Plot Designs

The "split-plot" design originated in the field of agriculture. For convenience, agronomists applied one "hard-to-change" (HTC) treatment (*e.g., herbicide*) to "whole plots" (3 in this case) and "easy-to-change" (ETC) inputs (*e.g., crop*) to smaller "subplots" (3 per whole plot in this experiment). Both whole and sub plots are randomized for statistical validity. The convenience of HTC grouping (versus complete randomization) comes at a price: Far trickier stats than a completely randomized design (but software can handle it) and reduced power.

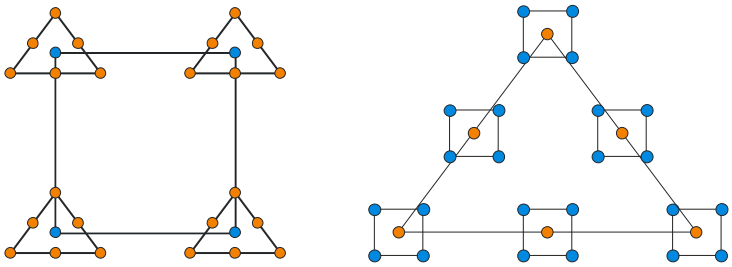


Mixture-Process Experiments

Split-Plot Combined Designs

In combined designs it's common that either the process factors or the mixture components are hard to change (HTC), e.g., mixing and baking chocolate-chip cookies,* which could go either way.

Process Factors HTC	Mixture Components HTC
Mix each cookie at random (ETC)	Mix up a batch.
Bake a bunch on a tray.	Bake one cookie at a time (ETC).



*Pictured: "Perfect Chocolate Chip Cookies," Kimberly Vardeman, Wikipedia Commons

Mixture-Process Experiments

Reference Publications

- "Background on the KCV Designs," Geoff Vining, Stat-Ease blog, Feb. 21, 2020, www.statease.com.

  "*KCV significantly reduces the overall design size while still preserving the ability to estimate highly informative models*."

- "Design of Experiments (DOE):How To Handle Hard-to-change Factors Using A Split Plot," Mark J. Anderson, *Chemical Engineering*, Sept. 1, 2016.

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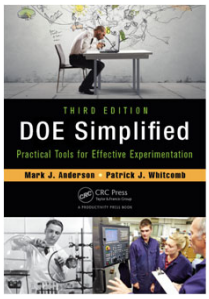
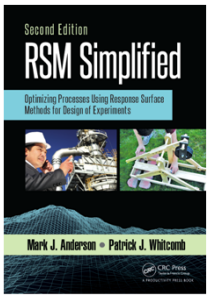
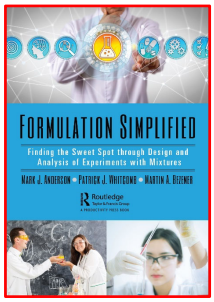
Reference Books
*DOE/RSM/Formulation Simplified Series**

**Anderson, et al, Taylor & Francis, Productivity Press, New York, NY.*







For details on mixture-process designs, including KCV and split plot, see:
Formulation Simplified
"Working Amounts, Categorical and Process Factors Into the Mix",
Chapter 9.

Mixture-Process Experiments

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