Mixture Design for Optimal Food and Beverage Formulation

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Abstract

Mixture design is a specialized branch of design of experiments (DOE) uniquely suited to food and beverage formulation, where responses depend on the *proportions* of ingredients rather than their absolute amounts. Three case studies of increasing complexity — a two-component lemonade, a three-component jellybean mixture, and a five-component constrained fruit juice blend—illustrate how mixture designs and specialized models efficiently characterize nonlinear blending behavior, identify synergistic and antagonistic ingredient interactions, and drive multi-response optimization of flavor and cost. All designs and analyses were conducted using Design-Expert® software (Stat-Ease, Inc.).

1. The Right Tool for the Job

Food and beverage R&D presents a formulation challenge that is fundamentally different from process optimization. In a process experiment, factors such as temperature, pressure, and time can be varied independently. In a formulation experiment, they cannot increase the proportion of one ingredient, and at least one other must decrease. The components are linked by an equality constraint — they must sum to a fixed total, such as 100% by weight or volume. This collinearity makes standard factorial and response surface method (RSM) designs structurally inappropriate for mixture problems.

A common error among practitioners who have embraced multifactor DOE is to apply these familiar designs to formulation work — what might be called the "new hammer syndrome," where a powerful new tool gets applied indiscriminately. The consequences are redundant experimental runs, obscured blending effects, and missed opportunities to find the true optimum.

Mixture design addresses this by restricting the experimental space to a *simplex* space— a line segment for two components, a triangle for three, a tetrahedron for four — and fitting responses using specialized "Scheffé" polynomials, which are geared to mixtures. The following three case studies demonstrate the application of this methodology to food and beverage formulation, progressing from a straightforward two-component simplex to a five-component constrained design.

2. Lemonade: The Mixture Constraint and Scheffé Modeling

2.1 The Problem with a Factorial Approach

Consider optimizing the ratio of lemon juice to sugar water in a lemonade formulation. A two-factor, two-level factorial design would assign independent low and high levels to each ingredient, generating four treatment combinations: (1 lemon, 1 glass sugar water), (2 lemons, 1 glass), (1 lemon, 2 glasses), and (2 lemons, 2 glasses). The critical flaw is immediately apparent: the (1,1) and (2,2) combinations represent identical *proportions* — 50% lemon, 50% sugar water — and will therefore produce identical taste responses. The factorial design wastes experimental effort and cannot distinguish proportion effects from amount effects.
The correct approach collapses both ingredients onto a single mixture axis, with pure lemon juice ($X_1 = 1$, $X_2 = 0$) at one extreme and pure sugar water ($X_1 = 0$, $X_2 = 1$) at the other, with intermediate blends tested at evenly spaced proportions.

2.2 Nonlinear Blending and the Scheffé Quadratic Mixture Model

If ingredients do not react, the taste response would track along a straight line between the two pure-component endpoints. This is referred to as "linear blending." However, in many cases synergistic or antagonistic interactions between components cause the response to deviate from linearity — a phenomenon captured by the binary blending term β_{12} in the Scheffé quadratic model:

$$\hat{y} = \beta_1 X_1 + \beta_2 X_2 + \beta_{12} X_1 X_2$$

For lemonade, pure lemon juice scores approximately 3 on a 9-point hedonic scale (too sour), while pure sugar water scores approximately 7 (very tasty!). The 75% sugar water / 25% lemon blend, however, scores approximately 8 — well above the linear interpolation of ~6.5 — demonstrating strong positive (synergistic) blending. The β_{12} coefficient captures this uplift. At the 50/50 blend point, the blending term X_1X_2 reaches its maximum value of 0.25, contributing $\frac{1}{4}\beta_{12}$ to the predicted response. Design-Expert fits this model from experimental data and generates predictions across the entire mixture space.

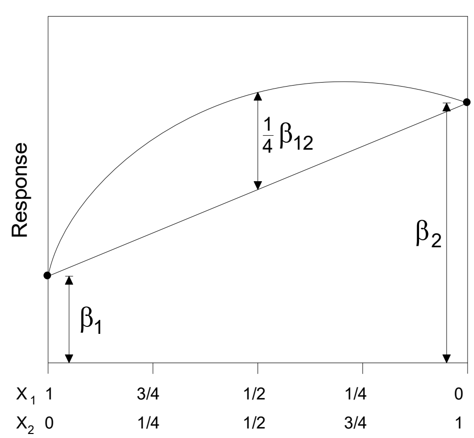

FIGURE 1: Scheffé quadratic blending curve for lemonade, showing nonlinear response vs. proportion of lemon juice (X_1) and sugar water (X_2)

3. Jellybeans: Three-Component Simplex Design

3.1 Experimental Design

To demonstrate a three-component simplex, our Stat-Ease staff served as a tasting panel to evaluate blends of three jellybean flavors: Apple (A), Cinnamon (B), and Lemon (C). The 11-run design covered the pure-component vertices, binary edge midpoints (centroid edges), and the overall centroid — sufficient to fit a Scheffé quadratic model. Responses were initially blocked by individual taster to account for person-to-person variation, then averaged across the panel to simplify the final analysis — a "keep it simple statistically" (KISS) approach.

Table 1. Jellybean Simplex Design and Taste Response Data (9-point hedonic scale)

Run	Space Type	Apple (%)	Cinnamon (%)	Lemon (%)	Taste Score
1	Center	33.3	33.3	33.3	4.3
2	Vertex	100	0	0	5.2
3	Vertex	100	0	0	5.1
4	Vertex	0	0	100	4.0
5	CentEdge	50	0	50	2.8
6	CentEdge	0	50	50	3.5
7	Center	33.3	33.3	33.3	4.2
8	Vertex	0	0	100	4.5
9	CentEdge	50	50	0	6.9
10	Vertex	0	100	0	7.0
11	Vertex	0	100	0	6.5

3.2 Results and Interpretation

The pure-component vertex scores establish the baseline preferences of the adult panel: Cinnamon scores highest (6.5, 7.0), apple scores moderately (5.1, 5.2), and lemon scores lowest (4.0, 4.5). The binary blend results reveal the nonlinear blending behavior that motivates mixture design. The apple-cinnamon edge midpoint (50% each) scores 6.9 — higher than either pure component — a clear demonstration of synergistic blending between components A and B. Conversely, the apple-lemon midpoint scores only 2.8, well below both pure components, indicating a pronounced antagonistic interaction. The overall centroid (equal thirds) scores 4.2–4.3, pulled down by lemon's drag on the blend.

The fitted Scheffé quadratic model captures these effects through the binary blending coefficients β_AB, β_AC, and β_BC. Multi-response optimization via Design-Expert software's desirability function identified the optimal formulation at approximately **70% cinnamon / 30% apple** — consistent with the strong synergy observed on the A-B edge of the simplex.

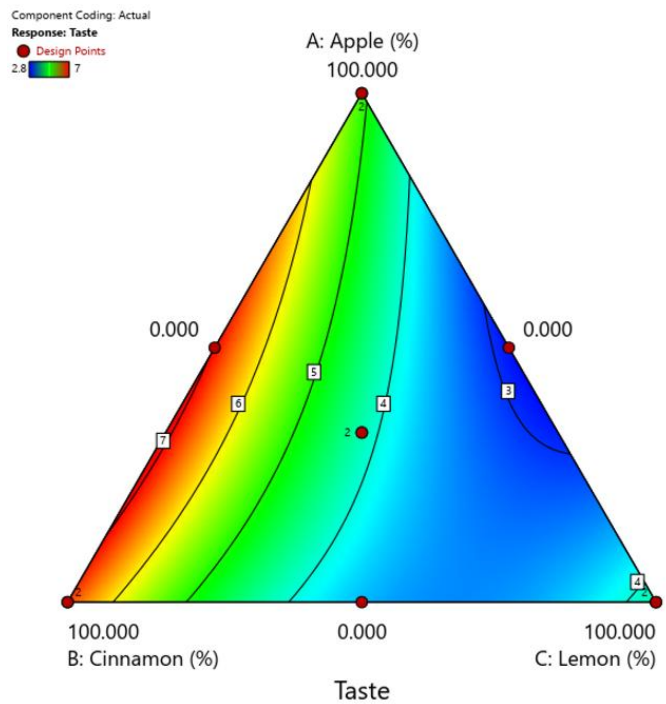

FIGURE 2: Ternary contour plot of jellybean taste scores across the apple/cinnamon/lemon simplex space, showing peak response in the cinnamon-rich region

4. Fruit Juice: Non-Simplex Design with Optimal Custom Design

4.1 Background

This case study, based on work originally documented in Cornell's *Experiments with Mixtures* — the standard reference text for mixture-design methodology — addresses the optimization of a tropical fruit juice blend comprising five components: watermelon (A), orange (B), apple (C), pineapple (D), and grapefruit (E). A fifth component (apple) was added to the original four-component Cornell formulation in the case presented here. The experiment design is complicated by an upper-bound constraint on watermelon: formulators restricted it to a maximum of 80% (proportion ≤ 0.80). Although watermelon is by far the least expensive ingredient, food science knowledge established that consumers reject juices exceeding this threshold due to dilution of flavor. This upper-bound constraint truncates the simplex tetrahedron, forming a *frustrum* — a non-simplex feasible region that standard simplex-lattice designs cannot accommodate.

4.2 I-Optimal Custom Design

When component constraints create a non-simplex feasible region, computer-generated optimal designs are required. Design-Expert employs an **I-optimal** criterion for mixture optimization problems, which minimizes average prediction variance across the design space. This criterion is preferable to D-optimality in this context: D-optimal designs concentrate points at the boundary and leave the interior poorly estimated, whereas I-optimal designs distribute estimation precision more uniformly throughout the feasible region.

The 35-run design incorporated model points, lack-of-fit check points, and replicate runs — for example, runs 11 and 16 at identical proportions — to enable pure error estimation independent of model lack of fit.

Table 2. Selected Fruit-Juice Runs Illustrating the Flavor-Cost Trade-off

Run	Watermelon	Orange	Apple	Pineapple	Grapefruit	Flavor	Cost (¢/L)
1	0.425	0.175	0.300	0.050	0.050	8.63	60.75
8	0.300	0.300	0.300	0.050	0.050	7.98	63.25
34	0.420	0.170	0.170	0.120	0.120	6.90	62.50
30	0.300	0.550	0.050	0.050	0.050	6.48	65.75
6	0.800	0.050	0.050	0.050	0.050	5.72	55.75

The data reveal a clear flavor-cost trade-off driven by Watermelon content. Run 6, at the maximum Watermelon constraint (80%), delivers the lowest cost at 55.75 ¢/L but also the lowest flavor score in the dataset at 5.72. Run 1, with a more balanced blend of watermelon, orange, and apple, achieves the highest flavor score of 8.63 at a modest cost premium. Higher watermelon proportion consistently reduces both cost (range: 55.75–66.50 ¢/ L) and flavor (range: 5.63–8.63) — the central tension this optimization must resolve.

A special cubic Scheffé model was fitted to the flavor response, capturing linear blending effects, pairwise synergies and antagonisms, and three-component interaction terms. Cost was modeled as a deterministic linear function of ingredient proportions, requiring no statistical fitting and yielding an exact cost prediction for any blend within the feasible region.

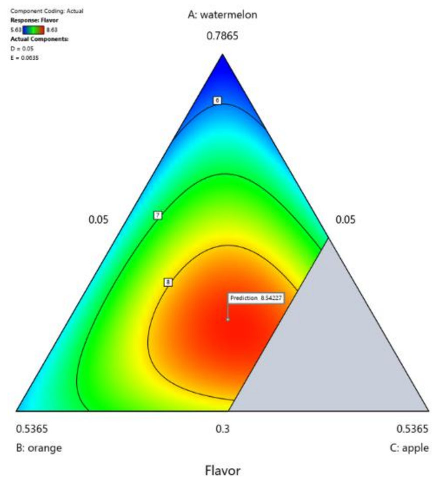

FIGURE 3: Contour plot of flavor score across the constrained fruit juice mixture space (low levels of D and E)

4.3 Multi-Response Optimization

With models established for both flavor and cost, Design-Expert's numerical optimization simultaneously maximized flavor and minimized cost using a composite desirability function. The relative weighting of these objectives can be adjusted to reflect business priorities, providing a practical decision-support tool for formulation trade-off analysis.

With equal weighting, the optimal blend was identified at approximately **48% watermelon**, with the balance distributed primarily among orange and apple and smaller contributions from pineapple and grapefruit. This formulation achieved a predicted flavor score near the upper range of the dataset while maintaining cost well below orange- or apple-dominated blends. Shifting priority toward cost minimization drives the solution toward higher watermelon content — a useful capability when ingredient prices fluctuate.

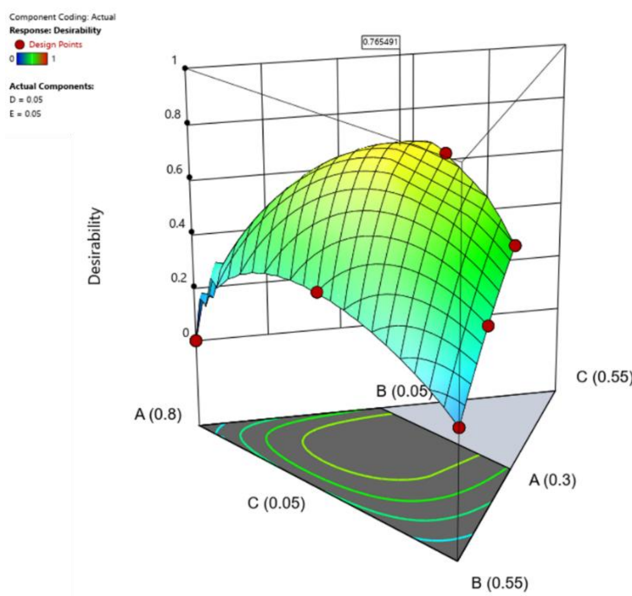

FIGURE 4: Desirability plot showing the feasible region satisfying both flavor and cost targets simultaneously

5. Selecting the Appropriate Mixture Design

The three case studies illustrate a progression in mixture design complexity. A **simplex-lattice design** is appropriate when all components can range freely from 0 to 100% without additional constraints, as in the jellybean case. A **computer-generated optimal design** is required when upper or lower bound constraints on one or more components create a non-simplex feasible region, as in the fruit juice case. Attempting a standard simplex design in the latter situation places experimental runs outside the feasible region, generating physically unrealizable blends and wasting resources.

In both situations, the **Scheffé polynomial** is the appropriate model. Unlike standard regression polynomials, Scheffé models are parameterized in terms of component proportions and implicitly respect the mixture constraint. Model degree — linear, quadratic, or special cubic — should be selected based on the complexity of blending behavior observed, with stepwise reduction used to eliminate non-significant terms subject to model hierarchy, arriving at a well-fitted result.

6. Conclusions

Mixture design is an indispensable tool for food and beverage formulation R&D. It remains underutilized by practitioners more familiar with factorial and RSM methods. The case studies presented here demonstrate several consistent findings across systems of varying complexity:

Standard factorial and RSM designs are structurally inappropriate for mixture problems. The lemonade example illustrates the reasons: redundant treatment combinations, wasted experimental effort, and no ability to distinguish proportion effects from amount effects.

When component constraints create a non-simplex feasible region, optimal computer-generated designs provide well-distributed coverage of the irregular experimental space and enable fitting of higher-order mixture models with confidence.

Multi-response optimization via composite desirability functions enables simultaneous balancing of competing objectives — such as flavor versus cost — and provides a practical simulation capability for formulation trade-off decisions once models are in hand.

Design-Expert and Stat-Ease 360 software (Stat-Ease, Inc.) provide an integrated platform for mixture design construction, Scheffé model fitting and reduction, diagnostic evaluation, and multi-response optimization, making these methods accessible to food scientists and formulation chemists without requiring deep statistical programming expertise.

References

1. Anderson, M.J., Whitcomb, P.J., *DOE Simplified: Practical Tools for Effective Experimentation*, 3rd ed., Taylor & Francis / Productivity Press, New York, NY.
2. Anderson, M.J., Whitcomb, P.J., *RSM Simplified: Optimizing Processes Using Response Surface Methods for Design of Experiments*, 2nd ed., Taylor & Francis / Productivity Press, New York, NY.
3. Anderson, M.J., Whitcomb, P.J., Bezener, M.A., *Formulation Simplified: Finding the Sweet Spot through Design and Analysis of Experiments with Mixtures*, Taylor & Francis / Productivity Press, New York, NY.
4. Cornell, J.A., *Experiments with Mixtures: Designs, Models, and the Analysis of Mixture Data*, 3rd ed., Wiley, New York, NY.
5. Kidane, S.W., "Application of RSM in Food Process Modeling and Optimization," *Response Surface Methodology in Engineering Science*, Oct 2021, IntechOpen. www.intechopen.com/chapters/78667
6. Stat-Ease, Inc., *Design-Expert Software*, Minneapolis, MN. www.statease.com