

# A Primer on Experiments with Mixtures

JOHN A. CORNELL

University of Florida  
Department of Statistics  
Gainesville, FL

 **WILEY**

A JOHN WILEY & SONS, INC., PUBLICATION

# Contents

<b>Preface</b>	<b>ix</b>
<b>1. Introduction</b>	<b>1</b>
1.1 The Original Mixture Problem, 2	
1.2 A Pesticide Example Involving Two Chemicals, 2	
1.3 General Remarks About Response Surface Methods, 9	
1.4 An Historical Perspective, 13	
References and Recommended Reading, 17	
Questions, 17	
Appendix 1A: Testing for Nonlinear Blending of the Two Chemicals Vendex and Kelthane While Measuring the Average Percent Mortality (APM) of Mites, 20	
<b>2. The Original Mixture Problem: Designs and Models for Exploring the Entire Simplex Factor Space</b>	<b>23</b>
2.1 The Simplex-Lattice Designs, 23	
2.2 The Canonical Polynomials, 26	
2.3 The Polynomial Coefficients As Functions of the Responses at the Points of the Lattices, 31	
2.4 Estimating The Parameters in the $\{q, m\}$ Polynomials, 34	
2.5 Properties of the Estimate of the Response, $\hat{y}(\mathbf{x})$ , 37	
2.6 A Three-Component Yarn Example Using A $\{3, 2\}$ Simplex-Lattice Design, 38	
2.7 The Analysis of Variance Table, 42	
2.8 Analysis of Variance Calculations of the Yarn Elongation Data, 45	
2.9 The Plotting of Individual Residuals, 48	
2.10 Testing the Degree of the Fitted Model: A Quadratic Model or Planar Model?, 49	

- 2.11 Testing Model Lack of Fit Using Extra Points and Replicated Observations, 55
- 2.12 The Simplex-Centroid Design and Associated Polynomial Model, 58
- 2.13 An Application of a Four-Component Simplex-Centroid Design: Blending Chemical Pesticides for Control of Mites, 60
- 2.14 Axial Designs, 62
- 2.15 Comments on a Comparison Made Between An Augmented Simplex-Centroid Design and a Full Cubic Lattice for Three Components Where Each Design Contains Ten Points, 66
- 2.16 Reparameterizing Scheffé's Mixture Models to Contain A Constant ( $\beta_0$ ) Term: A Numerical Example, 69
- 2.17 Questions to Consider at the Planning Stages of a Mixture Experiment, 77
- 2.18 Summary, 78

References and Recommended Reading, 78

Questions, 80

Appendix 2A: Least-Squares Estimation Formula for the Polynomial Coefficients and Their Variances: Matrix Notation, 85

Appendix 2B: Cubic and Quartic Polynomials and Formulas for the Estimates of the Coefficients, 90

Appendix 2C: The Partitioning of the Sources in the Analysis of Variance Table When Fitting the Scheffé Mixture Models, 91

- 3. Multiple Constraints on the Component Proportions 95**
  - 3.1 Lower-Bound Restrictions on Some or All of the Component Proportions, 95
  - 3.2 Introducing *L*-Pseudocomponents, 97
  - 3.3 A Numerical Example of Fitting An *L*-Pseudocomponent Model, 99
  - 3.4 Upper-Bound Restrictions on Some or All Component Proportions, 101
  - 3.5 An Example of the Placing of an Upper Bound on a Single Component: The Formulation of a Tropical Beverage, 103
  - 3.6 Introducing *U*-Pseudocomponents, 107
  - 3.7 The Placing of Both Upper and Lower Bounds on the Component Proportions, 112
  - 3.8 Formulas For Enumerating the Number of Extreme Vertices, Edges, and Two-Dimensional Faces of the Constrained Region, 119
  - 3.9 McLean and Anderson's Algorithm For Calculating the Coordinates of the Extreme Vertices of a Constrained Region, 123
  - 3.10 Multicomponent Constraints, 128

3.11	Some Examples of Designs for Constrained Mixture Regions: CONVRT and CONAEV Programs, 131	
3.12	Multiple Lattices for Major and Minor Component Classifications, 138	
	Summary, 154	
	References and Recommended Reading, 155	
	Questions, 157	
<b>4.</b>	<b>The Analysis of Mixture Data</b>	<b>159</b>
4.1	Techniques Used in the Analysis of Mixture Data, 160	
4.2	Test Statistics for Testing the Usefulness of the Terms in the Scheffé Polynomials, 163	
4.3	Model Reduction, 170	
4.4	An Example of Reducing the System from Three to Two Components, 173	
4.5	Screening Components, 175	
4.6	Other Techniques Used to Measure Component Effects, 179	
4.7	Leverage and the Hat Matrix, 190	
4.8	A Three-Component Propellant Example, 192	
4.9	Summary, 195	
	References and Recommended Reading, 196	
	Questions, 197	
<b>5.</b>	<b>Other Mixture Model Forms</b>	<b>201</b>
5.1	The Inclusion of Inverse Terms in the Scheffé Polynomials, 201	
5.2	Fitting Gasoline Octane Numbers Using Inverse Terms in the Model, 204	
5.3	An Alternative Model Form for Modeling the Additive Blending Effect of One Component In a Multicomponent System, 205	
5.4	A Biological Example on the Linear Effect of a Powder Pesticide In Combination With Two Liquid Pesticides Used for Suppressing Mite Population Numbers, 212	
5.5	The Use of Ratios of Components, 215	
5.6	Cox's Mixture Polynomials: Measuring Component Effects, 219	
5.7	An Example Illustrating the Fits of Cox's Model and Scheffé's Polynomial, 224	
5.8	Fitting A Slack-Variable Model, 229	
5.9	A Numerical Example Illustrating The Fits of Different Reduced Slack-Variable Models: Tint Strength of a House Paint, 233	
5.10	Summary, 239	

References and Recommended Reading,	240
Questions,	242
<b>6. The Inclusion of Process Variables in Mixture Experiments</b>	<b>247</b>
6.1 Designs Consisting of Simplex-Lattices and Factorial Arrangements,	249
6.2 Measuring the Effects of Cooking Temperature and Cooking Time on the Texture of Patties Made from Two Types of Fish,	251
6.3 Mixture-Amount Experiments,	256
6.4 Determining the Optimal Fertilizer Blend and Rate for Young Citrus Trees,	262
6.5 A Numerical Example of the Fit of a Combined Model to Data Collected on Fractions of the Fish Patty Experimental Design,	269
6.6 Questions Raised and Recommendations Made When Fitting a Combined Model Containing Mixture Components and Other Variables,	272
6.7 Summary,	277
References and Recommended Reading,	278
Questions,	280
Appendix 6A: Calculating the Estimated Combined Mixture Component–Process Variable Model of Eq. (6.10) Without the Computer,	282
<b>7. A Review of Least Squares and the Analysis of Variance</b>	<b>285</b>
7.1 A Review of Least Squares,	285
7.2 The Analysis of Variance,	288
7.3 A Numerical Example: Modeling the Texture of Fish Patties,	289
7.4 The Adjusted Multiple Correlation Coefficient,	293
7.5 The Press Statistic and Studentized Residuals,	293
7.6 Testing Hypotheses About the Form of the Model: Tests of Significance,	295
References and Recommended Reading,	298
<b>Bibliography</b>	<b>299</b>
<b>Answers to Selected Questions</b>	<b>317</b>
<b>Appendix</b>	<b>337</b>
<b>Index</b>	<b>347</b>