Case Study : An efficient product re-formulation using The Unscrambler®

Purpose of the study:

- Re-formulate the existing product (Shampoo) and optimize its properties after a major ingredient has been substituted.

Data Description:

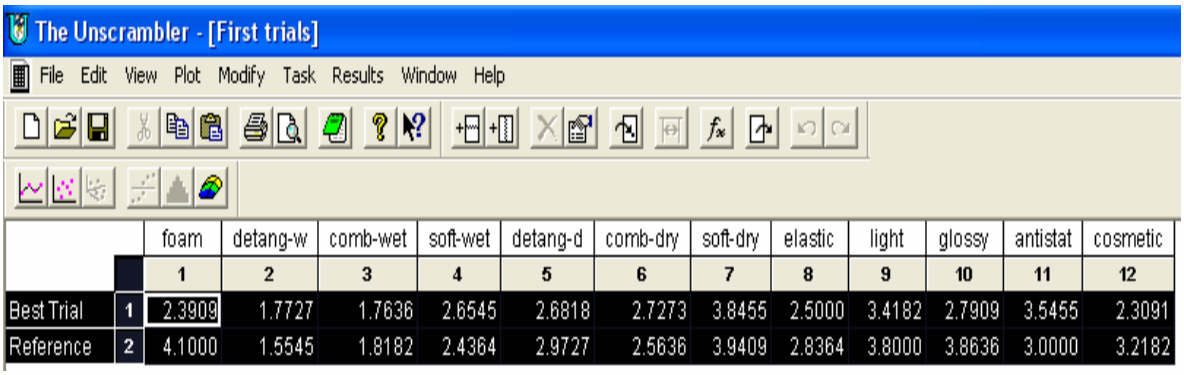
- A cosmetics manufacturer wants to substitute a detergent in the formula of its most popular shampoo, in order to make it milder.
- It is of utmost importance to achieve the same cosmetic properties as the currently marketed product, so that the consumer should not be disappointed.

Experimental Strategy:

- We will start with a screening design, to understand which ingredients and their combinations are responsible for the largest variations in the product properties.
- If necessary, an optimization design will then let us model the response surface as a function of the most important ingredients.

After substituting a milder detergent for the old one, the product development team has tried to adjust the other ingredients so as to achieve the same cosmetic properties as today's product's (reference)

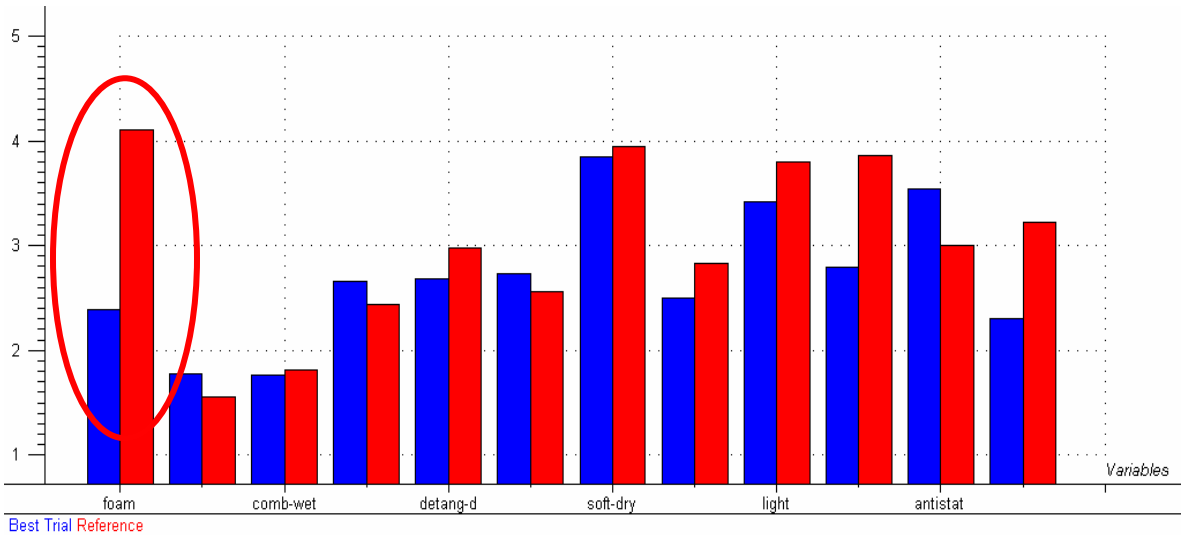
This data table contains the cosmetic profile of their best trial, as well as of today's shampoo: 12 sensory properties, measured on a scale from 0 to 5 by trained judge



		foam	detang-w	comb-wet	soft-wet	detang-d	comb-dry	soft-dry	elastic	light	glossy	antistat	cosmetic
		1	2	3	4	5	6	7	8	9	10	11	12
Best Trial	1	2.3909	1.7727	1.7636	2.6545	2.6818	2.7273	3.8455	2.5000	3.4182	2.7909	3.5455	2.3091
Reference	2	4.1000	1.5545	1.8182	2.4364	2.9727	2.5636	3.9409	2.8364	3.8000	3.8636	3.0000	3.2182

picture1: The cosmetic profile of their best trial, as well as of today's (reference) shampoo

Visual comparison of two shampoos by using Line plot



Picture 2 : Line plot of sensory properties over Best trail and reference products.

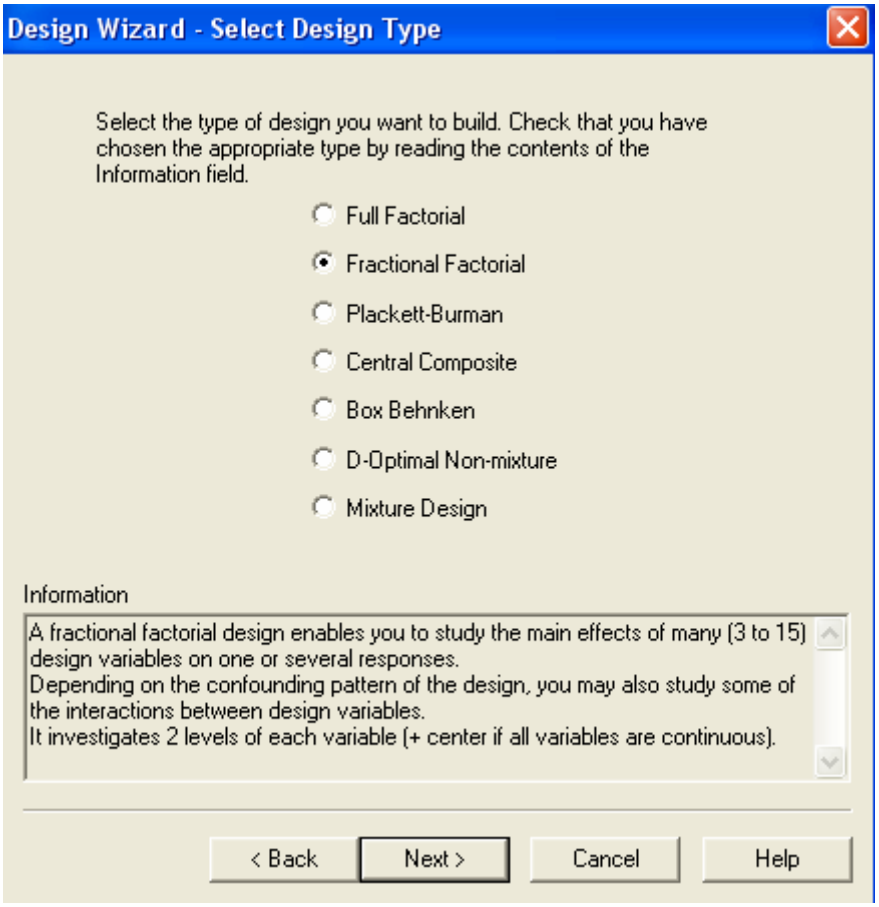
Our best trial so far is close to the reference product for most properties, but lacks Foam, Glossiness and overall Cosmetic effect. Foam in particular should be improved dramatically: from 2.39 to 4.10.

Obviously, trial and error is not efficient enough to solve our complex problem. We need experimental design.

A brainstorming session has identified 8 formulation parameters which might influence the cosmetic performances.

First Experimental Design: Screening Design

Let us create a fractional factorial design to investigate the effects of these 8 variables.



Picture 3: Fractional Factorial design template

Fractional factorial design with resolution IV gives 16 experiments and 2 center samples along with two reference samples in total we have 20 experiments to conduct.

We have prepared the 20 shampoos and evaluated their performances as per experimental design.

Now we are ready to study the effects of the 8 design variables on product performance. Let us run an Analysis of Effects (ANNOVA).

File Edit View Plot Task Results Window Help

Effects Overview
Significance Testing Method: Center

Variable	foam	detang-w	comb-wet	soft-wet	detang-d	comb-dry	soft-dry	elastic	light	glossy	antistat
Detergent	+	NS	-	NS	NS	NS	-	+	NS	+	+
Cationic	NS	NS	NS	NS	NS	NS	NS	NS	NS	+	NS
Anionic	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS
Silicon	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS
Vitamin	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS
Pearlizer	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS
Emulsl	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS
Emuls2	-	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS
Dete*Cati	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS
Dete*Anio	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS
Dete*Sili	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS	NS

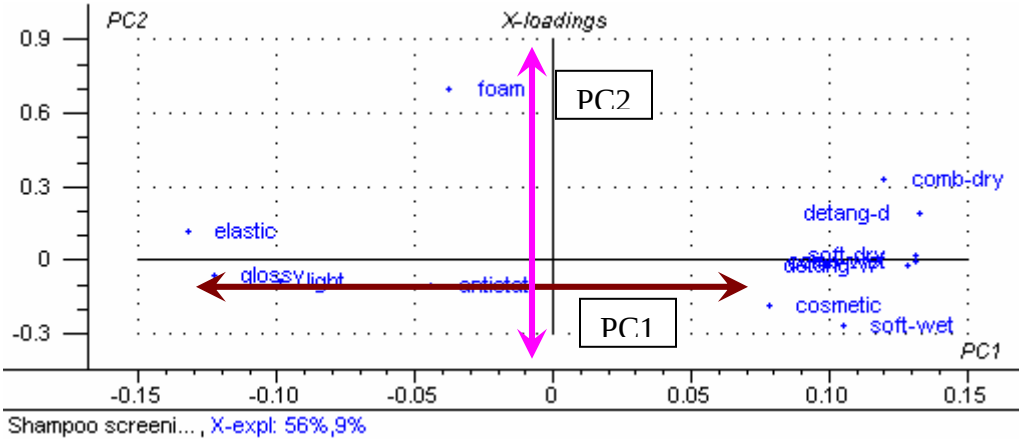
Picture4: Effects Overview

Detergent (A) and Cationic agent (B) have significant positive effects on Glossiness. Detergent (A) has significant effects on several responses, including Foam. Emulsifier 2 (H) also has a significant effect on Foam.

The overall Cosmetic performance is influenced by A, B, G, H and an interaction (AB=CG=DH=EF). Since both A and B have significant main effects, the most likely interpretation for this confounded interaction is AB.

Multivariate Analysis of sensory attributes by Principle Component Analysis (PCA).

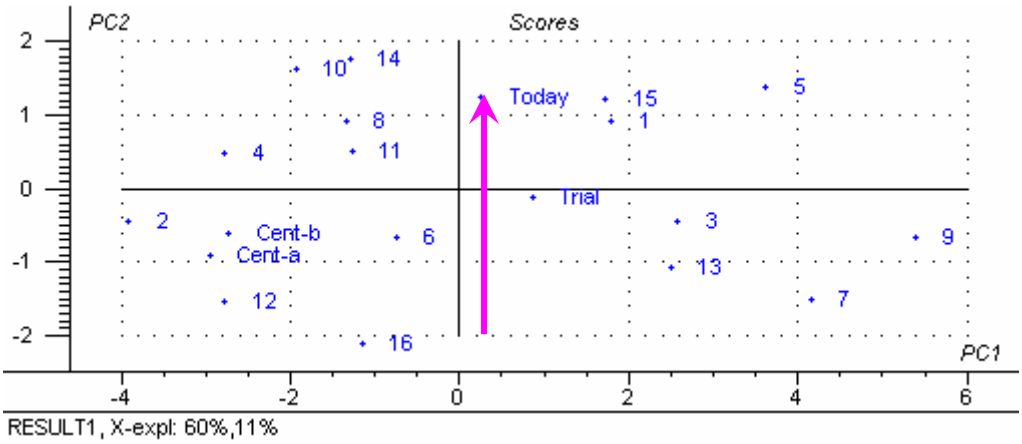
Let us run a PCA to understand how the 12 cosmetic properties are linked to each other, and which design samples could be close enough to today's product regarding all properties together.



Picture5: Loading plots explains variables relationships.

Along PC1, properties Elastic, Glossy and light (to the left) are linked. They are negatively correlated with most other cosmetic properties (to the right).

Along PC2, Foam varies independently from the other properties.



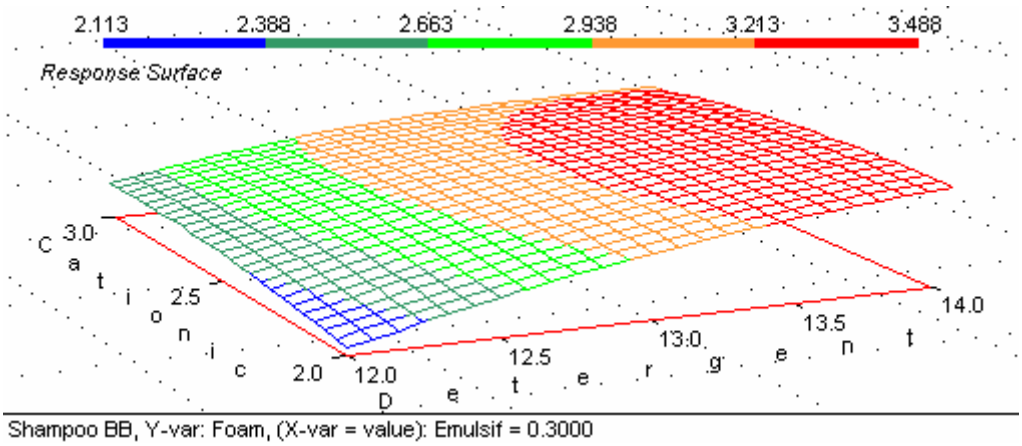
Picture 6: Scores plot explains sample relationships.

Today's (Reference) shampoo is projected to the top, far away from our previous trial. This visualizes the difference in Foam between these two products. The good news is that several design samples have about as much Foam as today's product: Samples 10 and 14, for example.

Screening to Optimization:

The amounts of Detergent, Cationic agent and Emulsifier2, have significant effects and interactions on the most important cosmetic responses.
We need an optimization to find out how we can combine the levels of these 3 variables to achieve the desired properties.

The design is a Box-Behnken with 3 center samples. We have prepared the 15 new shampoos, and measured their cosmetic performances.
Now we are going to interpret the results from our Response Surface Analysis.



Picture 7: Response surface

The model for Foam looks excellent: the R-square is close to 1. We have found a solution which almost matches today's product's performances. Detergent: 14%, Cationic agent: 3%, Emulsifier: 0.1%.

Conclusion:

The Unscrambler has helped solve our product development problem in two steps.

Step 1: Build Screening design and Multivariate Analysis (PCA)

We started by building a suitable screening design where we varied the concentrations of 8 ingredients. We prepared 18 new shampoos.

Analysis of Effects told us about the significance of the main effects and interactions. PCA gave us an overview of the 18 new shampoos compared to today's product.

Step 2: Screening to Optimization

We prepared 15 more shampoos, and run a Response Surface Analysis. After diagnosing and interpreting our models, we found a satisfactory compromise between the major responses.

By combining experimental design with multivariate analysis, The Unscrambler provides you with the tools you need for efficient product development.