An Application of Computers to the Flavor Development Process

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The development of flavors can be enhanced through the use of computer software because a large part of the performance of a flavor system depends on the ratio of specific ingredients to each other. For example, ingredient ratios can determine flavor characteristics for strawberry ranging from a jammy, seedy type to a fresh sweet, fruity type.

Knowing how to combine the ingredients into just the right mixture to yield the best possible flavor profile requires expertise, time, and energy. The level of flavor expertise depends on the developer's knowledge and understanding of flavor chemistry. The computer addresses time and energy issues by providing a systematic approach to optimizing the ratio of ingredients.

In the development of flavors, the independent variables are the flavoring ingredients which produce a response or flavor profile. The flavorist developes a concept of how a particular flavor should perform, and then based on flavor skills and expertise, creates several prototypes and evaluates them. In this process much time and energy may be spent on these prototypes in order to combine all of the different ingredients into just the right mixture to yield the best and most acceptable flavor profile.

Details of the Process

When the goal is to enhance the fresh, fruity charactertistics of a strawberry flavor base, the first step is to select those ingredients that will deliver the desired flavor characteristics. This step requires some understanding and knowledge of flavor chemistry. For this application, I selected natural bitter almond oil, γ-undecalactone (aldehyde C-14), and γ-nonalactone (aldehyde C-18). The bitter almond oil contributes a fresh, sweet, cherry-like taste. Aldehyde C-14 yields a sweet, oily-fruity, peach-like character and the aldehyde C-18 delivers a creamy, delicately fruity and coconut-type profile.

The working ranges established for each ingredient were:

Aldehyde C-14:	0.05-0.15%
Bitter almond oil:	0.15-0.30%
Aldehyde C-18:	0.005-0.015%
Ethanol (solvent):	0.50-1.00%

When the ingredients and their ranges are entered into the computer program,[1] it constructs an experimental mixture design to produce the flavor prototypes. The amounts of each ingredient to be blended are shown in the left window named DESIGN.ECH in Table I. Each prototype

Table I. A (left) is DESIGN.ECH, and B (right) is RESPONSE.ECH

A B

Experiment Design					Response Data	
Trial #	Aldehyde C-14	Bitter Almond	Aldehyde C-18	Ethanol	Trial #	Quality
1	0.15	0.30	0.015	0.5350	1	3
2	0.05	0.15	0.005	0.7950	2	3
3	0.15	0.15	0.015	0.6850	3	1
4	0.05	0.30	0.015	0.6350	4	2
5	0.15	0.23	0.005	0.6200	5	3
6	0.10	0.30	0.005	0.5950	6	2
7	0.10	0.15	0.005	0.7450	7	3
8	0.05	0.15	0.015	0.7850	8	2
9	0.10	0.23	0.010	0.6650	9	2
10	0.15	0.15	0.010	0.6900	10	3
11	0.05	0.30	0.005	0.6450	11	2
12	0.15	0.30	0.010	0.5400	12	2
13	0.15	0.15	0.005	0.6950	13	2

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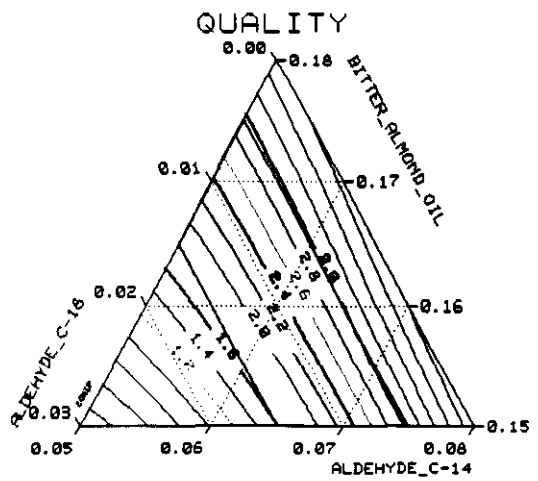

Figure 1A. 2-D contour plot with off-axis variable Ethanol = 0.77

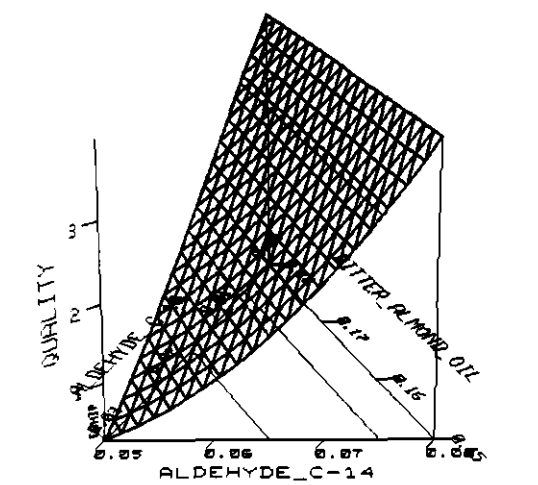

Figure 1B. Corresponding 3-D response surface, Ethanol = 0.77

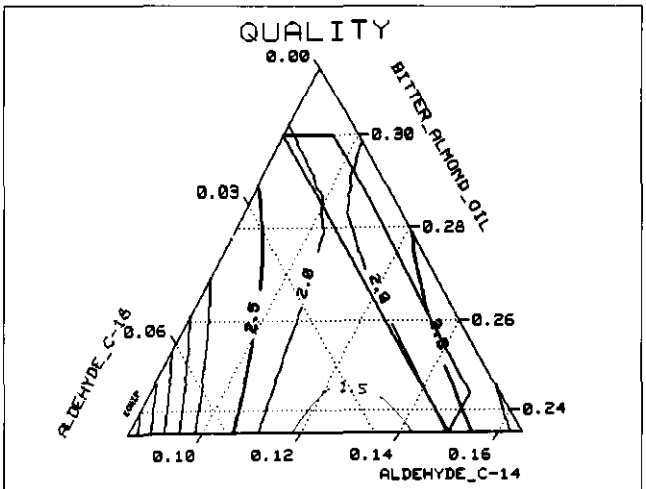

Figure 2A. 2-D contour plot with off-axis variable Ethanol = 0.60

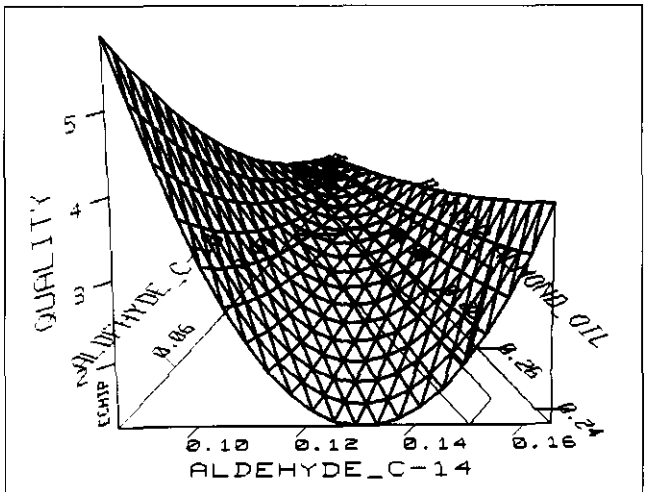

Figure 2B. Corresponding 3-D response surface, Ethanol= 0.60

is tasted without referring back to the design sheet. My own response data is generated by rating each sample against a quality scale. The responses are non-linear because, for example, an excellent overall quality rating is not three times better than a poor one. Quality values corresponding to each trial in the design are shown in the right window named RESPONSE.ECH in Table I.

The computer program creates a 2-D contour map (Figure 1A) which points toward those ingredient combinations that yield the best flavor profile based on taste evaluations. The contour map is the projection of the 3-D response surface (Figure 1B). Quality is plotted versus three of the four ingredients while the fourth ingredient, in this case ethanol, is held constant at 77% of the mixture. By quickly examining these plots, valuable research time and effort is saved by identifying and eliminating those ingredient combinations that produce below average prototypes (lower left portion of the triangle). I can focus my creative flavor skills in experimental regions of the map (upper right side of the triangle) that are likely to deliver the most promising flavor options. The 2-D contour map and the 3-D response surface shown in Figures 2A and 2B, respectively, are obtained by changing the off-axis ingredient, ethanol, to 60% of the mixture. This allows the exploration of potential response values for more new prototypes and it gives me direction for planning the next series of experiments. I validate all of my selected flavor prototypes with taste evaluations.

More than three ingredients can be handled very easily by the software. Any three ingredients may be selected for the contour plot. The remaining ingredients are held off-axis at their optimum value. The contour plot is still interactive because by scrolling the off-axis variables, new plots can be explored which may reveal even better flavor

combinations.

I have found that ten ingredients at a time are manageable. If more than ten ingredients are required, I divide the flavor into separate flavor keys. For example, the strawberry flavor may contain a "berry" key with ten ingredients, a "jammy" key with seven ingredients and a "creamy" key with five ingredients. Once I have identified the desired flavor profile for each key, the software helps me determine how much of each key (ppm, percent, grams, etc) is needed to achieve the right flavor balance or impact. Each key may be perfectly blended by itself, but if one key is used at the wrong level, the overall performance of the final flavor is affected. I am able to determine not only the best ingredient combinations, but also their optimal usage rates.

Additional Applications

In most cases, flavor systems are developed using a combination of many different types of ingredients. However, the same approach can be applied to complex flavor formulations. The effects table can be used to identify important ingredient interactions. Formulations can be optimized by eliminating those ingredients with very small contributions to the desired finished flavor. This approach can also be applied to flavor duplication work. The target sample serves as the reference point. Prototypes can be judged as to how close they approximate the flavor of the Control. The same experimental process can be used to "zero in" on the characteristics of the reference sample and accomplish the objective.

Summary

Because the responses are non-linear, the emphasis of this approach is not necessarily on locating the most simultaneously optimal data observation. The idea is to save time and energy by identifying the most promising prototypes in areas of greatest interest to the developer so that his or her own flavor skills can be maximized. Once an area has been defined, the developer can select prototypes from that region for further refinements and fine-tuning.

Our decision-making skills have improved because we can achieve and integrate the greatest amount of flavor information from the fewest number of prototype mixtures. By involving the computer in our development efforts, we are able to successfully deliver new flavor systems against challenging timetables.

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Reference

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1. ECHIP Version 5.0 by E Chip, Inc, Hockessin, Delaware