The experimental mixture design: an efficient tool to model the odor quality of complex mixtures

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1 Introduction

The experimental mixture design (EMD) constitutes a reliable approach to studying and optimizing mixtures. From pharmaceuticals and alcoholic beverages to ceramics and chemical solvents, the EMD allows understanding the contribution of each component of a mixture to the manifestation of a certain phenomenon, in addition to the interactions among the various constituents; with lesser required experiments and time consumption [1].

Even though the applications of the EMD are diversified, the approach has never been used to address olfactory-related questions, especially since understanding odor mixtures and their effects on the odor quality is still an open question [2]. Previous efforts to model the odor quality in terms of chemical composition are scarce and limited to binary mixtures. Nevertheless, the need for more complex models is growing notably for perfumes blending, food and beverages industries, ambiance and indoor aromas, environmental nuisance, etc.

For these reasons, we opted to combine the experimental mixture design and sensory analysis in hopes to obtain reliable models to predict the odor quality of a complex mixture and understand the interactions among the odorants.

2 Theory

To develop such a model, we combined the experimental mixture design method with a sensory approach, the Langage des Nez® (LdN) [3]. The experimental mixture design used was Scheffe's simplex lattice design. The LdN is an odor quality description approach that uses a collection of 26 pure odorants as odor nature referents, distributed around 7 poles.

3 Material and methods

A mixture of 3 odorants was studied: propane-1-thiol, furfuryl mercaptan, and α-pinene. Since they were going to be used at a gaseous state, the stability of the odorants was verified in canisters and Nalophan® bags using gas chromatography before the analysis.

Odorants were mixed at different odor activity values (OAV) (equation 1) in Nalophan® bags.

$$OAV = \frac{\text{Chemical concentration}}{\text{Odor perception threshold}} \qquad (1)$$

The sum of OAVs was fixed at 30.

The ON of each mixture was described by a panel of 9 experts, using the poles of the LdN as odor descriptors.

4 Results and discussion

From all the LdN odor attributes, only four were used: pyrogenic, sulfurous, and terpenic. The variation of the odor nature (ON) was modeled with the composition of the mixture using a reduced third-order polynomial model. Thus, for each attribute, a model was created. Based on the resulting models, different interactions may be interpreted, e.g., masking or synergism, along with the individual contribution of each odorant to the global ON of the mixture.

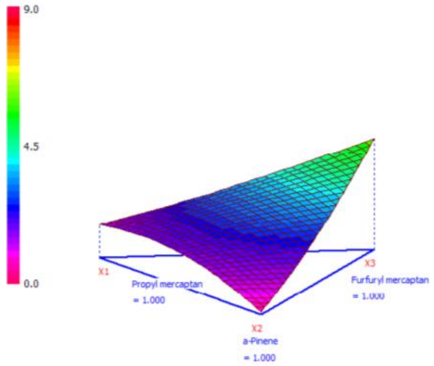

Figure 1 – 3D projection of the pyrogenic attribute model for an example mixture of propylmercaptan, α-pinene and furfuryl mercaptan.

The models were constructed with a minimum number of required experiments, less time consumption and proved to be valid and of good descriptive quality.

5 Conclusion

The models, constructed via the combination of the EMD and LdN, allowed unraveling the interactions among the various constituents of the odor mixture and the prediction of the ON. Indeed, the transposition of the models on other odorants with similar qualities and the addition of the other attributes may strengthen the models. However, the first results showed to be promising.

6 References

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