Improving Fragrance Performance Using Intensity Plots (iPlots[a])

by Michael Incorvia, Tim Young, Cynthia Mussinan and Nicolas Godinot, International Flavors & Fragrances Inc, Union Beach, NJ

One of the challenges faced by functional perfumery is balancing olfactive intensity and character of a fragrance through each product utilization stage. For a laundry detergent, such stages include directly out of the package (also called "point-of-purchase"), damp cloth im–mediately after washing, and dry cloth (typically 24 h) after washing. Differences in the intensity or character of a fragrance between stages play an important role in con–sumer acceptance and likeability.

Researchers at IFF have developed a perfumery tool called iPlots that seeks to measure such intensity and character changes. The tool visually represents intensity and character attributes by simultaneously plotting psy–chophysical sensory and analytical headspace data. The sensory dose response data provide fragrance character attributes, and the analytically measured headspace concentration data provide fragrance intensity attributes. These attributes can be determined for each product utilization stage.

Discussion

Sensory dose response curves: The sensory dose re–sponse curve of an aroma chemical is a plot of the olfactive intensity as a function of concentration. The curves are typically "S" shaped, as illustrated in Figure 1. The main elements of a dose response curve are:

- Threshold value: The lowest concentration at which an aroma chemical is perceived.[1]
- Saturation point: The point above which increasing the concentration does not result in a significant increase in perceived intensity.
- Effective usage range and rate of return: The effective usage range is the region between the threshold value and saturation point. Also associated with this range is the "rate of return" value (or slope) that indicates how much of an intensity change is brought about by a dosage change.

While the threshold value is important in identifying aroma chemicals that could have significant odor impact at low usage levels, it certainly does not provide all the information of value to perfumery, including the psycho-physical properties of an aroma chemical. For example, Figure 2 shows three aroma chemicals with equivalent threshold values, but significantly different dose response curves. Looking beyond the threshold value to the quantity necessary to achieve a moderate intensity, it is clear that other factors are very important. For example, to achieve a moderate intensity for Compound A, a dosage level of 172 ppm — six times its threshold concentration — is needed. To achieve the same intensity, 1,014 ppm and 16,000 ppm

Figure 1. Sensory dose response curve (note S-shape)

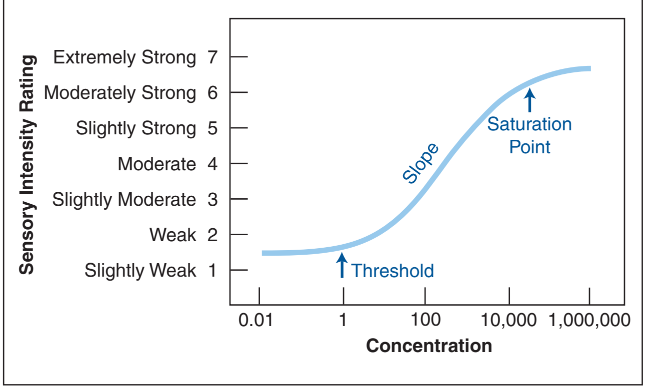

Figure 2. Three aroma chemicals with equivalent thresholds, but varying dose response curves

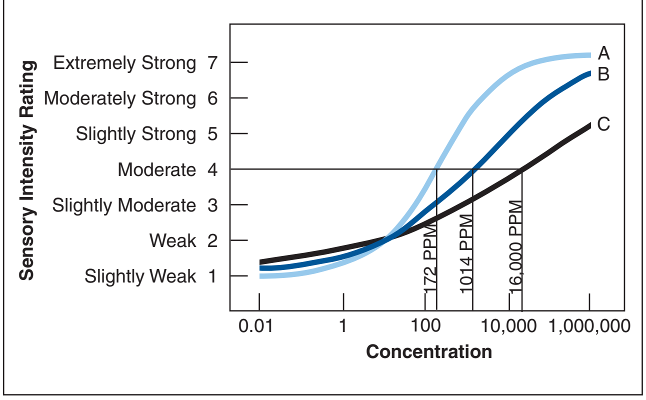

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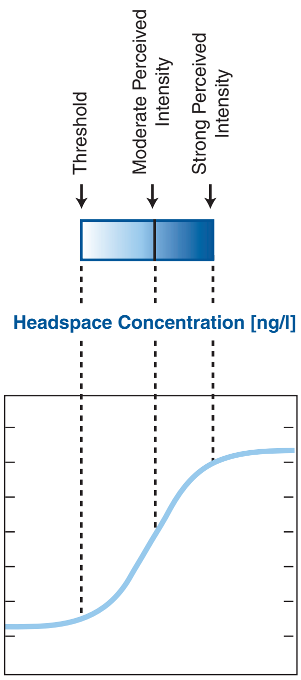
Figure 3. Sensory dose response bar



are needed for Compounds B and C, respectively. For Compound C, this is 36 times its threshold concentration. It is also interesting to note that at 1,000 ppm, Compound A is strongly perceived and near its saturation value, while Compound B is moderately perceived. Such differences can have profound affects on cost, construction and utility of a fragrance.

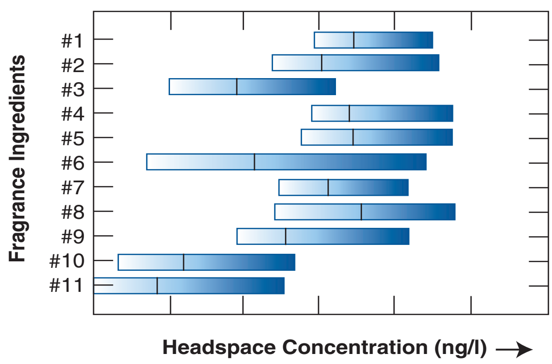
The saturation point is another important attribute provided within a sensory dose response curve. Knowing the point at which increasing the concentration of the aroma chemical no longer results in a significant increase in intensity can also affect fragrance cost and construction. For these reasons, we have decided to focus, beyond the important but limited threshold values, on the richer and more powerful dose response curves.

There are a number of ways to determine dose response curves. We use consumer sensory panels because, we believe, they provide a better olfactive representation of the population (as compared to expert odor evaluators) that ultimately purchases and uses the products. Panelists evaluate aroma chemicals in jars at various dilutions in a neutral, non-odorous solvent following the standard protocol of Marin et al.[1] We believe that this protocol has advantages over olfactometers, in that the simple act of sniffing from a jar more closely resembles the conditions under which a consumer experiences the aroma of a household (soap, detergent, etc.) or personal care (shampoo, deodorant, etc.) product.

Analytical headspace measurements: Quantitative headspace instrumental techniques provide a linkage of important psychophysical information contained within sensory dose response curves with analytical performance measures of aroma chemicals at various product performance stages.

In our research, we express dose response curves in nanograms/l in the vapor phase. This enables the linkage of sensory and analytical data at various product performance stages. We can then predict consumer perception of the intensity of each aroma chemical in the fragrance at each performance stage. We use this tool to more quickly and effectively create fragrances that perform well throughout the entire product use cycle.

Figure 4. Sensory bar plotting hypothetical laundry detergent



Resultant Technology

Our analysis technology, short for intensity plot, is a visual representation that simultaneously displays psy–chophysical sensory and analytical headspace data. The two main elements we employ are sensory dose response bars and headspace concentration "dots". When these two features are combined, they provide a concise way to visually present performance data for the many, typically 50-100, aroma chemicals that comprise a func–tional fragrance.

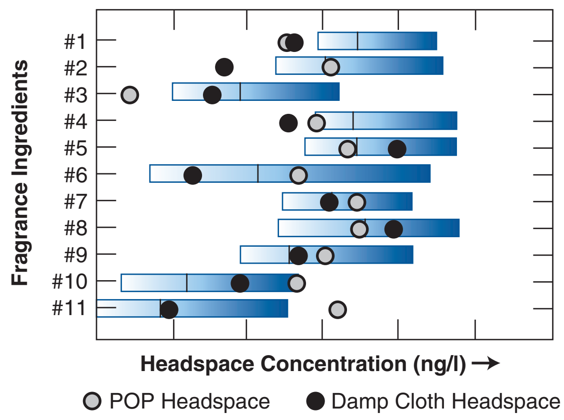
For fragrance formulations containing more than a few aroma chemicals, it would be confusing to display all of the dose response curves in a single chart. We have, therefore, developed a less confusing way to present the data that captures all of the essential sensory information for each aroma chemical into a sensory dose response bar, as illustrated in Figure 3. Our sensory bars represent psychophysical properties of an aroma chemical, so once it is determined it is fixed for all future intensity plots.

Figure 4 shows the sensory bars of one of our intensity plots representing a hypothetical laundry detergent fragrance. A review of the sensory bars of this fragrance provides important information about the psychophysical properties of the 11 aroma chemicals. First, the three ingredients with the lowest thresholds are aroma chemicals 6, 10 and 11, while those with the highest are aroma chemicals 1, 4 and 5. Second, the length of a sensory bar provides information about the rate of return value of each aroma chemical. For example, larger increases in the dosage of aroma chemical 6 are needed, compared to aroma chemical 7, to achieve an equivalent degree of sensorial intensity change. Finally, in addition to the threshold and rate of return values, the sensory bars also indicate the maximum effective dosage level for each aroma chemical. The intensity plot bars provide important psychophysical data to perfumery in a concise format.

To us, the real value of our system is in linking sensory dose response data to the analytical headspace data obtained during various product utilization stages. For example, for our hypothetical laundry detergent (Figure 5), intensity plots can be constructed for the fragrance intensity levels at the point of purchase and on damp cloth. As discussed above, the sensory dose response bars represent the psychophysical properties of the respective aroma chemicals and therefore remain constant in each plot. However, the concentration of each aroma chemical within the headspace can vary at each stage. A complete intensity plot is constructed when the analytically determined headspace concentrations for each aroma chemical in the fragrance, represented by dots, are simultaneously plotted with the corresponding sensory dose response bars.

The resulting plot is a graphical representation of fragrance intensity at that specific product utilization stage. The location of the dot with respect to the bar indicates its likely perceived odor intensity by an average consumer. Dots to the left of a sensory bar are below the threshold value (for an average consumer) of that aroma chemical and are therefore not expected to be perceived. The location of a dot within a sensory bar indicates the expected intensity contribution (e.g., threshold, moderate or strong) of that aroma chemical to the overall fragrance intensity. Dots to the right of the bar are above the saturation point and are expected to be perceived at the strong intensity level; that is the same as if the dots were on the right end of the bar.

Figure 5. Various fragrance performance features at point of purchase and on damp cloth



Fragrance performance measurement tool: Each performance stage has its own unique intensity plot. Therefore, in order to understand the performance of a fragrance more fully, plots must be constructed for each performance stage. The plots shown in Figure 5 represent the fragrance performance features at point of purchase and on damp cloth, illustrating that dots that are to the right or left of a sensory bar in one performance stage can be within the bar during another stage, and vice versa. Care must be taken not to draw conclusions about the contribution of an aroma chemical to a fragrance based on an intensity plot of only one performance stage.

Our perfumers have found this plotting system to be useful in designing, understanding and adjusting fragrance performance. Although primarily used for performance enhancements, intensity plots may also be used to adjust odor character. For example, if a perfumer wanted to enhance a green note, a fragrance modification could be made based on an assessment of the green notes within the plot. The perfumer could increase the amounts of those aroma chemicals associated with the green note or replace some of them with materials, within the green odor category, with lower thresholds or better performance features. All of these sensory performance features can be determined from sensory dose response or intensity plot data.

Our discussion of fragrance intensity has been limited to the contributions of the individual aroma chemicals. We, of course, recognize that certain synergies can exist between aroma chemicals and that the intensity plots, as presented here, do not take them into account. Odor mixture studies, however, show that such synergies are limited;[2] our experiences with intensity plots likewise support limited synergies.

Summary

Intensity plots are a useful tool for assessing fragrance performance and predicting sensory response in products at each performance stage. They are also useful for understanding changes in fragrance performance resulting from compositional changes in the product base. Likewise, intensity plots can also be utilized to make modifications to a fragrance formulation to improve a performance attribute or to adjust performance to compensate for compositional differences between product bases.

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Address correspondence to Michael Incorvia, IFF Inc, Corporate Research and Development, Union Beach, NJ 07735.

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