Fragrance Formulation

Once perfumers have determined the basic ingredients they will use, they must combine them in the appropriate proportions. The pioneers of perfumery formulated primarily by trial and error, mixing materials together until they discovered a pleasant combination.

Over time, they developed a more systematic, scientific approach, based on the volatility of fragrant materials. In this method, a fragrance is described by its' top, middle and bottom notes.

Notes: The top note, made of the most volatile materials, is the first element smelled when a fragrance is applied. Citrus notes are common top-note ingredients.

The middle note, or body of a fragrance, is composed of somewhat less volatile material. These components come more into play after the top notes have dissipated. Floral scents, such as violet or tuberose, are typical middle notes. The bottom, or base, note is made from the least volatile materials. Examples include musk scents, woods and vanillins. This portion is the longest lasting of the fragrance.

In recent years, fragrance suppliers have developed a new technology that allows them to create fragrances that closely match the aroma of living flowers. Generically known as "head-space analysis," this technology analyzes gases in the air above a living flower to synthetically match a flower's true scent.

Fragrance Testing

Before submitting their creations, perfumers typically conduct a series of evaluations. At this stage, the formulator of the personal care product will often provide the perfumer with an unfragranced product base. The fragrance house can then perform instrumental analysis, physical product testing and subjective consumer evaluations.

Instrumental evaluations, such as gas chromatographic or infrared analysis, may help establish fragrance quality. Physical product testing, such as emulsion stability testing, ensures that fragrance components do not adversely affect the product, such as causing separation or discoloration. Conversely, it is important to note that a product can cause the fragrance to deteriorate, as with high pH formulations that may be difficult to perfume.

Consumer testing: Subjective evaluations by selected groups of consumers may also establish whether a fragrance properly masks a product's base odor and creates the impressions desired. One way to obtain such information is by "mall intercept testing," in which samples are shown to a relatively large number of people (typically about 50) who fit the consumer profile specified by the formulator. Their responses provide the perfumer with information on the fragrance's performance.

Ideal consumer evaluations are done under actual-use conditions. Thus, many fragrance vendors have specially designed test rooms to mimic the conditions under which consumers actually smell the fragrance; soap may best be evaluated in a small shower chamber where the fragrance can interact with warm water.

When a fragrance has successfully passed all of these tests, a perfumer can have some degree of confidence that the fragrance and product are working together properly. The fragrance may then be submitted to a product-development chemist for further evaluation.

Further Evaluation

Upon receiving fragrance submissions, the formulating chemist determines if they meet the project requirements. This determination is no small task since a large number of fragrances may be submitted. While some companies work with a small number of houses or their own in-house perfumers, others may deal with a relatively large number of outside houses—as many as eight or 10. If each house submits multiple fragrances, the total number of samples can be great.

Steps and samples: The evaluation process involves several steps. First, it helps to determine how well the submissions fit the general profile. For example, those submissions not meeting cost considerations may be eliminated. Similarly, if the brief specifies that single-fruit notes should not be included, yet one submission smells like a strong green apple, the formulator may reject it.

Once the formulator has screened the submissions to a manageable number, samples of the actual product must be made with the appropriate amounts of fragrance. These samples are also evaluated for general acceptance by the product manufacturer and may be tested to ensure that the fragrance does not negatively interact with the base.

Finally, some form of consumer evaluation is, once again, helpful to determine fragrance suitability. To facilitate this process, many companies use employee panels to screen fragrances. Larger consumer studies may also be conducted to determine which fragrance best supports the product.

Ultimate fragrance selection is often done in conjunction with other members of the product-development team, such as the marketing departent. It is wise to select a backup fragrance in case problems arise with the first choice.

Stability testing: Once a fragrance has been selected, more detailed investigations can take place. For example, stability testing of the fragrance in the actual product base is a critical step. Whenever possible, testing should be performed in the final packaging, including caps and labels. Although fragrance houses often conduct their own (cursory) stability testing, formulators should conduct their own (more detailed) evaluations. Stability testing at higher temperatures can provide information about long-term fragrance stability quickly.

An industry rule-of-thumb roughly equates eight weeks at 45°C to one year at room temperature. In other words, if the fragrance still smells good after exposure to high temperature and the product shows no significant defects, such as discoloration or separation, the fragrance and the product base are probably compatible. If negative effects arise, the fragrance house may be asked to revise the fragrance and correct the problem. If the suitability of the final fragrances is eventually confirmed, the product can be produced for the marketplace. Consumers then decide for themselves if the formulator has done a good job in fragrancing the product.

Safety and Regulations

Safety has always been a crucial aspect of fragranced products. The industry has been self-regulating since the 1960s, but the current regulatory climate has complicated the situation. First, the California Air Resources Board placed significant VOC restrictions on many products. The European Union mandated labeling of 26 alleged allergens (see Schnuch for a review of the data) making many customers reluctant to accept them in fragrances (**Table 19.1**). The simple division of fragrances products into two categories, leave-on and rinse-off, was elaborated into 11 categories (**Table 19.2**). Safety testing was historically done on skin, but it is now evident that little is known about the environmental fate or respiratory effects of fragrance, issues that are now being addressed. The fragrance industry faces many new challenges as the world heads to global harmonization of safety standards.

Table 19.1. EU Allergens

Amylcinnamic alcohol	Farnesol
α-Amylcinnamic aldehyde	Gernaniol
Anisyl alcohol	α-Hexyl-cinnamic aldehyde
Benzyl alcohol	Hydroxycitronellal
Benzyl benzoate	HMPPC*
Benzyl cinnamate	Isoeugenol
Benzyl salicylate	Lillial
Cinnamic alcohol	Limonene
Cinnamic aldehyde	Linalool
Citral	Methylheptin carbonate
Citronellol	γ-Methylionone
Coumarin	Oak Moss
Eugenol	Tree Moss

* Hydroxymethylpentyl cyclohexenecarboxaldehyde (Lyral)

Table 19.2. RIFM Fragrance Categories

Category 1	Lip Products, Toys, Insect Repellents
Category 2	Deodorants/Antiperspirants
Category 3	Hydroalcoholic Products for Shaved Skin, Men's Facial Creams & Balms, Tampons
Category 4	Hydroalcoholic Products for Unshaved Skin, Hair Styling Aids & Sprays, Body Creams
Category 5	Women's Facial Cream/Facial Make-up, Hand Cream, Facial Masks, Wipes/Refreshing Tissue for Hands, Face, Neck, Body

Table 19.2. RIFM Fragrance Categories

Category 6	Mouthwash, Toothpaste
Category 7	Intimate Wipes, Baby Wipes
Category 8	Make-up Remover, Hair Styling Aids Non-spray, Nail Care
Category 9	Shampoo, Rinse-off Conditioners, Bar Soap, Feminine Hygiene Pads and liners
Category 10	Detergents, Hard Surface Cleaners, Diapers
Category 11	All Non-skin or Incidental Skin Contact Products

Conclusion

At first glance, fragrance looks like a simple material that adds esthetic appeal to a product. Closer inspection shows it to be a complex mixture of chemicals that demands the close attention of the formulator. The global marketplace has placed increased emphasis on the technical and regulatory aspects of fragrance. The Green Movement has also complicated the presence of fragrance in certified products. With challenges come new solutions, and surely the fragrance industry will evolve to enable us to continue to add value and pleasure to personal care products.

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Chapter 20

Microorganisms and Personal Care Products

A review of biological contaminants and the chemical preservatives inhibiting their growth.

key words: bacteria, yeasts, molds, biofilm, parabens, formaldehyde, phenols, pyridine

In the time it takes you to read the next few pages, you will encounter millions of tiny, alien-like creatures. No, this isn't science fiction, it's about microorganisms and how they can affect personal care products. These strange creatures are bacteria, molds and yeasts that hover in the air you breathe, rest on the things you touch, even live on your skin. Usually, they do not cause problems for cosmetic chemists. However, if enough of them get into product batches, they may cause trouble. Further all governemnts require cosmetics to be safe during their normal and foreseeable use. If these can grow in your product due to inadequate preservation, they can cause harm to the consumer.

What are these creatures? How do they get into our products? What happens when they do? Most important, perhaps, is how can we control them? We will discuss these microorganisms in the general environment, how they can contaminate personal care products, their growth and how we can protect against such contamination.

Microorganism Classification

These microscopic creatures cannot be classified as strictly animals or plants but according to their cellular structure. Biologists categorize those with a simple, unorganized nucleus as prokaryotes, members of the kingdom monera. Others with a well-defined cellular nucleus are eukaryotes—Greek for "true nucleus"—and belong to the kingdom protista. Certain eukaryotes, like fungi, are grouped separately in the kingdom mycetae. The main types of microorganisms affecting personal care products are bacteria, yeasts and molds.

Bacteria: Bacteria are single-cell prokaryotes whose cell walls are, for the most part, well-defined. They range from 0.5–10 µm in size and exist in a variety of shapes, such as spherical (coccus), rod-shaped (bacillus), spiral (spirillum) and comma-shaped (vibrio). Bacteria, which reproduce by cellular division, are classified as gram-negative or gram-positive, based on their ability to absorb and retain