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The Computer as the Perfumer's Helper

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Perfumery and computers are completely different, and therefore they compliment each other perfectly. Perfumery is a totally creative activity, not based on any known scientific or physiological rules or standards. Perfumery is truly a creative business where talent and experience count for everything.

Computers are the perfect idiot. They will never have an original creative thought, but they forget nothing and calculate perfectly. They can give back to you whatever you put in, nothing more and nothing less. By putting in the tremendous variety of detail that every perfumer must accumulate over many years of training and practice and retrieving it quickly, the computer makes the perfumer's job both easier and more efficient.

One of the major advantages of a computer-based formulating system is the retention of all formulation work done by the company, whether experimental or final formulas that are sold. This means that a formula file can be searched for odor characteristics, cost levels, stability data and application information. More than once I have seen perfumers searching frantically through old notebooks to try to find formula work previously done that was never properly filed or identified.

There are two basic elements in a computer system. First is a group of programs that are used to organize ingredients and to record the formulas as the perfumer's creative ideas and inspirations, and to save, retrieve, modify and otherwise manipulate previous formula work. Second is the database of materials that the individual or company chooses to include in the list of acceptable fragrance ingredients.

Programming for Perfumers

Database management systems are designed specifically to store, process and manipulate data. There are several well known computer database management systems available that cost a few hundred dollars. The two most popular are Lotus 1,2,3 and dBase, and have proved their value in thousands of different applications. There are certainly millions of people who have mastered these systems and who run thousands of applications in every conceivable area of human activity.

Several perfumers are among this group that more than ten years ago started constructing perfumery databases to run on standard programs. Any individual who takes the time to learn one of these programs, and to key in the data on materials can get excellent results.

This is the cheapest way to get into a computer program (cheap in money, not in time). It is well suited to an individual perfumer who works independently, whether inside or outside a perfumery company.

There are severe limitations to this system when more than one perfumer is to work with the same data, and expansion is not practical beyond the single user. The problems of security, supervision and control as well as functions like combining formulas, screening formulas for various safety, stability and regulatory purposes, etc. are really too cumbersome and time consuming to be practical.

Specially written programs are the answer, and several major companies have followed this route to privately written perfumery programs.

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This leads us to the few commercially available computer programs that I know of specifically written for perfumery use.

PERFORM by XICIS Corporation

William Brugger, a chemist working several years ago at IFF, and personally involved in computer programming, became part of a team to prepare a program for the IFF Perfumery Department.

Shortly after completing the job, he left to work on other computer program development dealing with chemical reseach and synthesis. He was then approached by industry people who had experience with his perfumery programs while at IFF and was asked to produce a commercial program for the industry. The result was the "PERFORM" program, first released in 1989 and subsequently used by some of the largest perfumery companies in the world.

INFORM Computer Program

Robert Maleeny, who has had many years of experience in this industry, started the development of a computer program for formulation work in flavors and fragrances eight years ago. It has since then been in constant use and development in his own company, Flavor & Fragrance Specialties.

INFORM II is a PC-operated computer system whose primary functions are to create, edit and price formulas, generate work orders, and maintain a perpetual inventory system. It is written in dBase—with INFORM the user can also purchase a materials database and a vendor database.

Central to the INFORM II program is an inventory database containing more than 3,500 ingredients with their prices, vendors and reference product code. This inventory is divided into 22 categories, such as essential oils, extracts, botanicals, chemicals, solvents, bases, etc. Each entry also has a number of optional fields where such information as FEMA number, CAS number, odor and flavor descriptors, GC retention times, etc. may be entered.

A vendor database is also included with names, addresses and other details on sources for these materials.

A formula database is a third file that contains all of the company's formulas for flavors, fragrances, bases and accords and provides such information as cost, yield, physical characteristics and manufacturing information.

INFORM II is an integrated system where additional modules produce work orders to manufacturing which interacts with the perpetual inventory system to indicate materials that must be re-ordered.

A complete file of sample activity is also maintained so that a record is kept of all samples of each formula sent out to various customers, as well as a record of all customer sales.

A new module giving retention times of aroma chemicals has just been completed and may be accessed by the retention time on carbowax column or silicone column or alphabetically.

FORMPACK

This is a formulation and manufacturing control system for the flavor and fragrance industry written by Mitron Computor Services in ZIM from Sterling Software, Inc. of Britain. It can run on a variety of computing platforms including IBM compatible PCs, IBM RS-6000, Data General, DEC VAX, and others.

There are three major operation areas in FORMPAK:

- Stock Items and Formulation Development
- Stock Control, Order Processing and Production Management
- Security and Maintenance

Stock items and formula development include the database of all materials and formulas in the system. When a formulation is created, modified or displayed, the following are shown on the screen:

- Total Concentration
- Component Concentration
- Formulation Unit Cost
- Component Unit Cost
- Component Cost per Unit of Formulation
- Component Cost Dates

Partial key selection is used throughout, and where applicable, a window of items appear on the screen that

match the partial code. The cursor is then moved to the required item and selected by a function key. This cuts down keyboard time and makes it very easy to select an item when the exact code is unknown.

Stock Control, Order Processing and Production Management are provided in a module that will produce orders, maintain stock inventory based on production orders, etc.

Operations of a Perfumery Program

All programs operate in generally the same way, so a general description of the operations of this type of program are given below. However, there are quite significant differences between these programs, and only a detailed review of the program at a computer terminal with one familiar with each particular system will give a true picture of the individual features.

A formula is constructed by entering materials from a list of materials in the Database of the system, and the number of parts for each material. The system will pick up the price listed for each product, and continuously give a cost of the formula as it is being developed. There may be more than one "book" of materials in the system, each one for special product types, special countries or parts of the world, or for other special purposes. Each such book will give only those materials approved for that purpose or area, and also the price applicable for that purpose.

As each material is added to a formula, automatic recalculations are made to show changes in the unit costs and total costs. It may be possible to have other formulas on the screen for comparision while working on a new formula. It may also be possible to add materials in dilution. At any time materials may be added, removed, and individual quantitites changed, with the cost figures reflecting these changes. The column of costs for each material may be given in:

1. money figures per pound or kilo,
2. percent cost in the formula,
3. percent weight in the formula,
4. actual cost in the formula, or
5. parts per thousand in the formula.

At any time the materials may be sorted on the screen by cost, alphabetically and sometimes by other criteria.

There is often a considerable amount of background information on each material in the database, and this can often be brought up to the screen during formulation work.

Most programs have a provision for using compounded bases in a formula. This requires the ability to "explode" the formula to be able to see all the individual ingredients in the formula.

It is usually possible to add personal notes to each formula.

Managing security for formulas, and for data used with them, is an obvious requirement for any system. A formula file is maintained for each perfumer, which can be entered for modifying and other purposes. Perfumery projects are organized and maintained. Formulas can be grouped by customer or by some company purpose.

Odor descriptions for each material should be a part of Database, and it is particularly helpful if this field can be used during the formulation process. The odor descriptors may be a combination of terms placed in the sytem for everyone to use, and one or more terms personal to the perfumer.

Materials Database

The database of materials is made up of all materials that management wishes to allow the perfumer to use, with related data on each material, such as cost, safety, regulatory considerations, customer or product screens, etc. All of this data must be laboriously keyed in by the company before any computer operation can begin.

The only published comprehensive list of fragrance materials is "Flavor & Fragrance Materials" from Allured Publishing containing about 3,700 materials. As far as actual different chemical molecules and derivatives of natural products is concerned, this list is probably at least 98% complete for even the largest company. The list includes all GRAS materials for flavor use, all those with a published RIFM monograph, and all natural derivatives of natural materials, as well as all materials that have been listed by known suppliers to the industry. This list is not available in computer form.

There is only one computer database of materials in our industry that I know of that is available for purchase. It is a part of "INFORM" and can be ordered as part of that program or separately. This has the great advantage of eliminating hundreds of hours of work in keyboarding in the data on thousands of materials. Even though this list will be specifically only of those materials in current use at Flavor & Fragrance Specialties, this will certainly contain the great majority of any company's list.

Fragrance materials not on published lists are primarily made up of captive chemicals developed and kept by the fragrance company for internal use, and natural materials processed to specifications particular to a customer for his exclusive use. Of course every company has bases created by perfumers for their own use, and often held for internal use or sold to a limited group of other fragrance houses.

The most specifically tailored database for perfumery is the one made up of the materials reviewed by RIFM in its safety evaluation program. This, together with the GRAS list of flavor materials compiled and reviwed by the FEMA expert panel will provide the perfumer with a great majority of perfumery materials.

"Flavor-Base," Leffingwell & Associates, is an extensive base of flavor materials principally that are GRAS (Generally Recognized As Safe) as determined by FEMA and the U.S. Government. Files include:

1. Over 1,750 natural and synthetic flavor materials including flavor descriptions and levels of flavor use. Threshold data is included on over 180 of these materials.

2. Natural essential oils and absolutes with composition data.
3. Foods and natural products with qualitative and quantitative occurrence of GRAS nature identical flavor chemicals.
4. Over 1,500 bibliographic citations to the flavor literature searchable by key subject words.

This database is in IBM PC compatible form and in dBase format.

Another useful database is produced by the TNO Research Group in Holland. For years they have compiled the most authoritative database in the world from over 3,000 literature references describing analytical work on food. This database, "Volatile Compounds in Foods," provides qualitative and quanitative data on the volatile compounds found in more than 300 foods and beverages. This database is a primary source used for identification of "nature-identical" flavor chemicals. This database is available on disk and in printed form.

Three databases have been prepared by Boelens Aroma Chemical Information Service (BACIS). FRM is a database of flavor raw materials containing over 2,400 flavor materials with related data on each. For each, there is an indication of the natural occurrence of flavor and its applications.

CNS is a database of perfumery aroma chemicals including chemical identity, commercial names, CAS numbers, and names of suppliers.

ESO is an essential oil database of over 800 essential oils with quantitative analysis, references to data and botanical names. Chemical names and CAS numbers of over 2,000 components are included.

There are a host of other computer-based databases that are more or less useful to perfumers depending on their method of working and their level of interest. An example is the database file named KOVATS.DB containing Kovats indices and principle MS fragment ions for essential oil components and other volatiles that are primarily flavor chemicals, written in the "Paradox" program. A separate file REF.DB contains references to the original documents. The data has been compiled from recent literature and contains about 4,300 entries (although many are multiple entries for different data on the same compound). Inquiries can be made on a range of Kovats indices and also by molecular weight or by the ion of greatest abundance. A name can also be searched: For instance, "germacrene" produced 31 answers.

Automatic Sample Weighing

As the creative work of the perfumer has been simplified and made more efficient, a single perfumer can now produce more creative work which then also requires more sample preparation for evaluation.

The bottleneck then moved "downstream" to the technician position and something is now required to apply the computer and automation to the production of perfume samples. Several companies have accomplished this step with a more or less automatic weighing of perfume samples.

The Henkel System

The system for automatically weighing out perfume samples was successfully started late in 1988 at the Henkel Fragrance Center in Krefeld, Germany. A central processor controls all of the weighing operations.

The fragrance materials that can be delivered in liquid form are arranged in rectangles in stainless steel receptacles from 0.5 to 5 liters. These are all under slight positive pressure of nitrogen and are connected by Teflon tubes to metering valve stations arranged in a circle below. The end of the tubes are capillaries of stainless steel, the diameter of which regulates the liquid flow capacity with great precision.

The containers receiving the perfume sample are bar coded and when placed on the weighing scale, the computer retrieves the formula and begins to pass the receptable underneath the delivery capillaries.

The receptacle pauses under each one where a fragrance component is to be deposited and the required valve opens, widely at first for a fast flow, and more restricted toward the end of the delivery quantity. The actual quantity delivered at each position is electronically recorded by weight for a final printout of the formula containing the required amount of each material and the amount actually weighed into the receptacle.

Dry ingredients or others that cannot flow through this system are added by hand afterward.

Sample receptacles with the required bar code are placed on the conveyor feeding this equipment and are stored on a conveyor after they have been completed. The entire operation continues automatically for 24 hours each day.

The Yamamoto System

A compact automatic weighing system has been developed by the Yamamoto Perfumery Co., Ltd. of Osaka, Japan. This is a small perfumery company that developed their own system and are offering it for sale.

Individual modules contain the controls for 40 individual materials. About 200 grams of materials are in a storage bottle behind the module feeding tubes through each module where valves are placed to control the flow. In principle, any number of these modules can be connected together, and the model at Yamamoto is now using five modules with a total of about 200 materials fed into five separate stations. Air pressure in each of the supply bottles powers the system.

The operator at a PC enters the formula which controls all of the valves on each of the lines.

After entering the system, a container is placed on the turntable which takes it to each of the five stations in turn.

The container rides on the turntable on the scale which records the actual amount of material placed into the container from each station. This gives a check on the actual formula in the bottle and allows the technician to make any necessary adjustments afterward.

Normally each formula will receive about 70% of the

materials required in this automatic system with the remainder being added by hand afterward.

It was found that the temperature in this room had to be kept very even in order to improve the accuracy of the weighing system.

The original machine was designed in 1988 with the installation in early 1989. The first prototype was actually in production in July 1989.

Dosilux—The Weighing Robot

Sistemas Industriales Aplicados, an engineering company belonging to the Electrolux Group, in cooperation with Lucta, the major Spanish perfume company, has developed an innovative system for the weighing of perfume samples.

Storage revolving modules with 60 containers of materials are combined into an integrated unit to provide 240 or more materials. The containers have been designed so that they are double, cylindrical and concentric. Various inner capacities with the same exterior volume result by modifying the diameter of the inside of the container. Capacities of normal containers are 200, 500, 1,000 or 1,500 millilitres. In this way, the system may be adapted to the volume and frequency of use, each material minimizing the length of time that they remain inside the machine, thus avoiding classic problems of quality due to aging of rarely used products.

A programmable algorithm implemented in the software allows a variable flow of the measure material under nitrogen pressure depending on the quantity to be allocated and the exactness required. An electronic precision scale (0.001 gr.) reports the actual weight of the dose to the control system.

The dosage process continues independently in each module of 60 containers into the bottle receiving the formula, which is situated on an electronic precision scale. The bottle moves from module to module until it has been completed.

The dosage algorithm controls the closed loop process taking into account the exactness required, the viscosity of the product and the weight to be allocated for each of the components.

A computer and two microcomputers run the various control levels of the modules which configure the system in real time.

One of the microprocessors is dedicated to the control of the peripherals, while the other deals exclusively with the positioning of the cylindrical storage containers and with the simultaneous dosage process of all the system's scales.

Van Wyk Engineering

A system of quite a different sort has been operational in a major company for several months. This system takes a rack of 99 sample bottles, and brings each supply bottle in turn to this rack. Any of the 99 samples requiring that component will receive the required amount, and the next component bottle will then be brought to the pipetting machine. When all the component bottles required by the

formulas in the rack are filled up, a new rack of 99 sample bottles is positioned for filling.

The pipet is based on the use of a capillary needle with a syringe which is really a high-precision piston pump. The pump sucks and delivers liquid through the needle. The contact of the needle with the liquid in the sample bottle allows the delivery of very small quantities with a reproducible accuracy of 0.001 grams. This pipet system permits the preparation of 50-gram samples with minor components with very high accuracy. A special cleaning station is used for the needle. Up to 2,028 component bottles can be used in this system.

What's in the Future?

An All Industry Data Base: It would certainly be very efficient and convenient if a single database arrangement were standard within the industry so that certain information could be communicated between suppliers, users and customers regarding flavor and fragrance materials. With the right kind of controls and planning, a database of flavor and fragrance materials could be based on a numeric system for identification and coordination.

The Chemical Abstract Service (CAS) number is ideal for aroma chemicals. However, there are serious problems with natural materials and bases as they would require the creation of phoney CAS numbers in order to accommodate all of the industry's products.

In publishing Flavor & Fragrance Materials, Allured has established a code number based on the FEMA number. This provides a four-digit number for each material for a total of 10,000 different possibilities.

However, it is quite obvious that this is simply not broad enough to encompass all of the flavor and fragrance materials, and their variations and combinations. However, it is very convenient since the FEMA number provides (via the supporting Scientific Literature Review) a regulatory and technical definition. Thus, lemon oil (FEMA No. 2625) is natural and GRAS for food use.

Since any database would have to accommodate variations, the four-digit number followed by a dash and a three-digit addendum would provide a total of 999 variations on each given product. Even for such proliferated materials as lemon oil and oakmoss extract—the 999 limit should provide more than enough possible variations.

Odor Descriptions

It seems inevitable that more extensive and sophisticated odor descriptors will be used in order to make the replacement of materials easier and quicker. While some of this is now being done, it will be far more important when much better understanding is gained of the structure/odor relationships of aroma chemcials.

The same might be done for perfume formulas where extensive odor characteristics combined with cost stability and other considerations could pinpoint a desired formula with great accuracy.

References

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