Computer-Assisted Product Development

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Synopsis–Initial steps in establishing an effective development program utilizing PERT (Program Evaluation and Review Techniques) and CPM (Critical Path Method) COMPUTER PROGRAMS are shown. Interactive computer-assisted FORMULATION of new NAIL LACQUERS is carried out using matrix programs. Analysis of completed formulas for specific parameters is performed. Stability analysis and statistical evaluation of the completed nail lacquers are handled by computers. Color formulation and batch correction of new pigmented nail formula are carried out under several light conditions in order to eliminate metamerism.

INTRODUCTION

Product development in the cosmetic industry consists of complex physical, chemical, and legal barriers which must be cleared before a new product can be marketed. The availability of minicomputers and time-share networks is permitting the research chemist to solve some of his problems. Our laboratory is currently using computer base data collection and analysis systems to handle several important development tasks. Computer programs handle project planning, analytical, stability testing, and color formulation for nail lacquers. Many of the concepts developed in this paper are generally applicable to other development projects.

PROJECT PLANNING

The ideas for new products can originate within the corporation or be obtained from outside sources such as inventors, suppliers, or advertising agencies. Project initiation by marketing is one of the most critical planning

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steps in the research organization. The systems used for assembling and screening ideas and the establishment of research projects need to be carefully analyzed. Responsibility and burden of program and project evaluation lie within research management. Planning activities should focus on the means of directing manpower, equipment, and cost factors in order to meet prescribed goals. Management is forced to choose among several worthwhile projects. The chemist who wishes to have his project accepted must be able to state his goals, his timetable for completion, and his manpower requirements (1).

One of the most widely used planning techniques available today is PERT, an acronym for Program Evaluation and Review Technique (2). PERT is a method of managing, a tool used by research management in planning and manipulating various laboratory resources to successfully attain the stated goal.

PERT was originally developed by the U.S. Navy to organize the development of the Polaris Missile system. The application of PERT is not limited to the development of missile systems, but can also be used for most laboratory research projects which meet two criteria: (a) definite objective to be attained; and (b) independent series of steps which must be successfully performed in sequence.

PERT is a network system which displays in graphical representation those ordered step-by-step actions which must be carried out in order to reach a specific objective. Before we begin, some basic definitions are in order.

Geometrically, the network is composed of two forms.

1. Event—A milestone of progress or accomplishment in the program plan depicting the start or completion of an activity which precedes or succeeds it. Usually represented by a circle.

2. Activity—A time-consuming element in a program plan; representative of work in progress or descriptive of a relationship between two events. Represented by a solid line.

3. Dummy Event—A nonexisting event in actuality, but occasionally inserted in a network to simplify the analysis of project status. Represented by a broken line.

The previous definitions permit us to extend PERT from a planning tool into a powerful control system by the simple expedient of applying time estimates to each activity. Estimates can be made in any unit, but all estimates in the network must be in the same unit. The unit most commonly used is weeks and tenths of weeks.

Some of the time involved for completion of a project is not definitely known by management due to unexpected delays or unpredicted speedups; PERT makes major recognition of uncertainty by placing it in a standard frame of reference, so that time estimates can be made with a predictable degree of success.

Three time estimates are made for each activity:

Optimistic Time (T_O)—Assume everything goes right. Small probability of being realized.

Most Likely Time (T_M)—What will occur in normal circumstances.

Pessimistic (T_P)—A large number of things go wrong.

Figure 1 shows the graph of probability of completion at any given time is assumed to be a skewed distribution, or beta distribution; the peak of which is the most likely time and the standard deviation is approximately ⅙ the range of T_P and T_O (2).
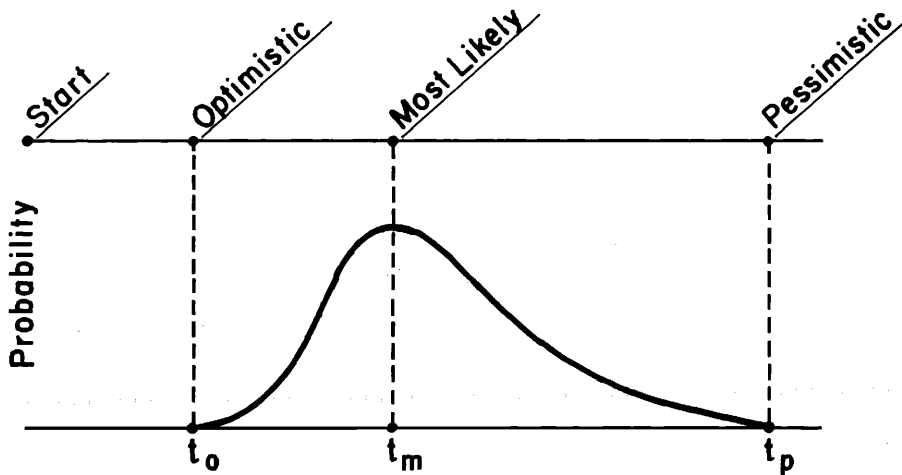

Figure 1. Probability of completion of an event

The expected time (T_e) is the mean time that divides the area under the curve. It is approximated by:

$$T_e = \frac{T_O + 4\,T_M + T_P}{6}$$

After this development of the basic definitions which apply to project planning, construction of a network flow sheet follows.

Figure 2 shows the initial planning steps from the sources of ideas to concept, Fig. 3 carries the network from the concept step through final product, and in Fig. 4 are shown the final stages of the network, from product to production.

Each of the events depicted in Figs. 2–4 have their own detailed PERT network. The R & D event depicted in Fig. 3 is expanded to show the separate events and activities in Fig. 4.

At this stage in the development project we can make time estimates for each activity in the flow sheet. The longest path, called the critical path, is
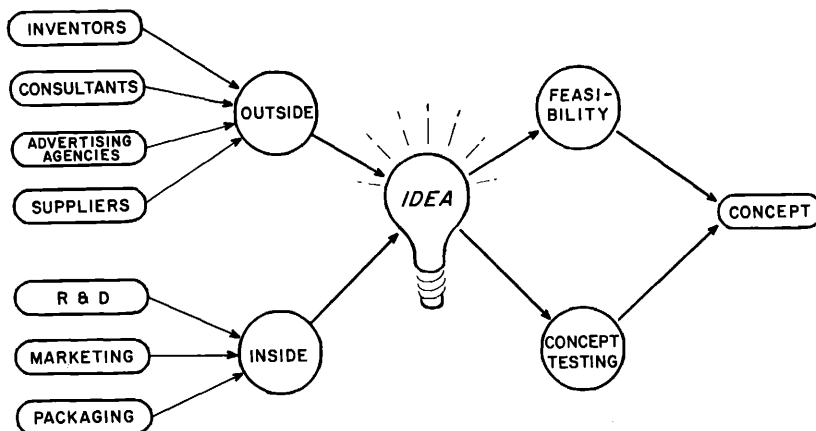
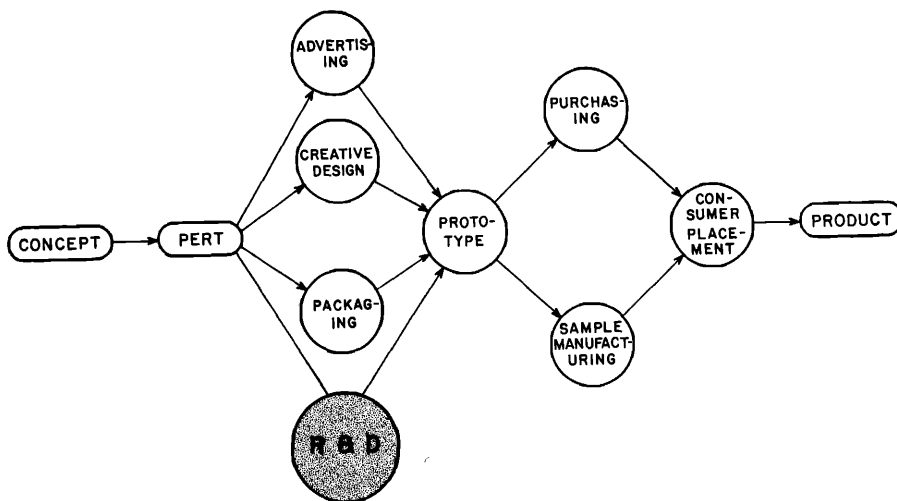*Figure 2.* Initial PERT network—sources of ideas to concept

Figure 3. PERT network—from concept through product stage

especially important since any delay along it will affect the completion of other activities. Any effort to speed up a project should be directed to those activities comprising the critical path.

The total network is upgraded when an activity is completed and an estimated time is changed to an actual time. This upgrading produces a considerable amount of calculations which lend themselves to computer processing.

The specific events (Fig. 5) are given identification numbers which simplify analysis of the network. Using the events and activities shown in Fig. 5, time

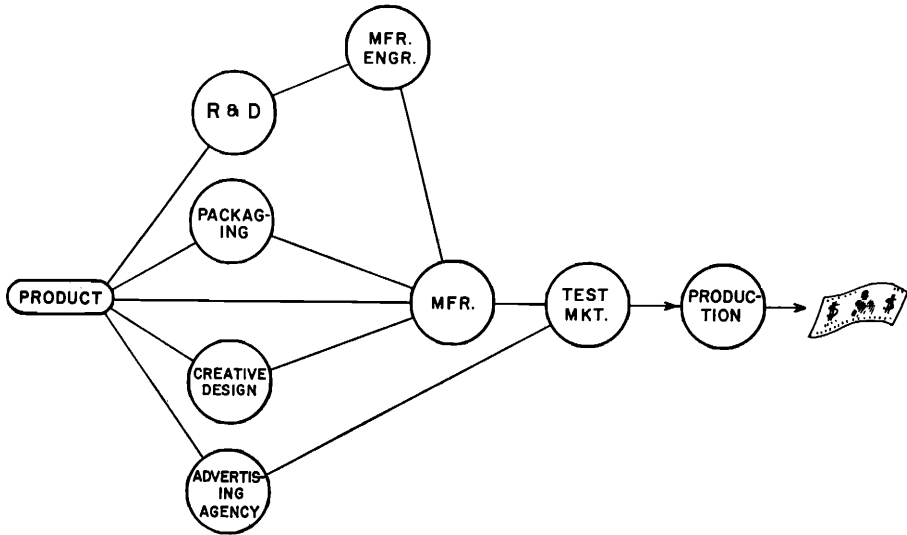*Figure 4.* PERT network—final stages—product through production
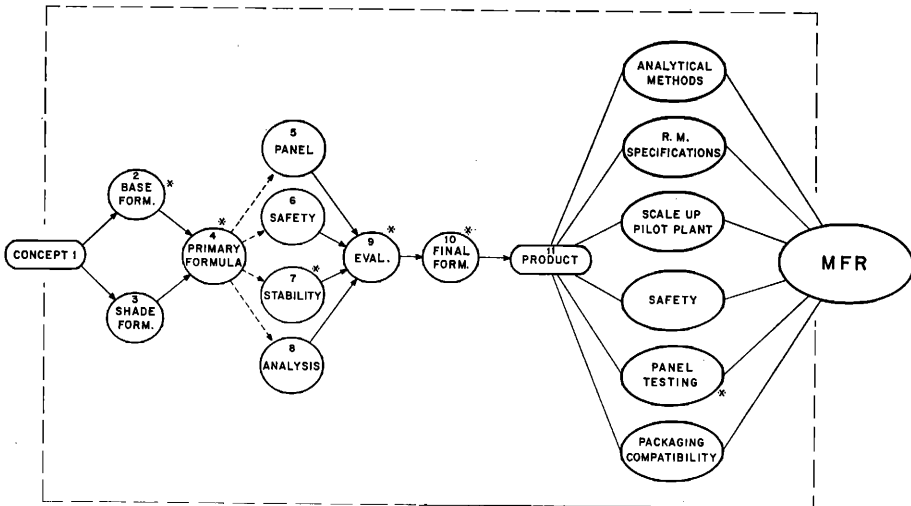

Figure 5. PERT network R & D functions—critical path analysis for nail lacquers

estimates for completion of the network have been established using the critical path method.

In the following sections of the paper, specific applications of computer techniques to product formulations, analysis, and color formulations are discussed.

The computer printout will be listed in the form of a table under the following headings (3);

S = starting event
E = ending event
D = duration of activity
ES = earliest start date
LS = latest start date
EF = earliest end date
LF = latest end date
F = maximum float factor
** = critical activities
RES = resources utilized (PD = product development)

The critical path method for a nail lacquer is illustrated in Table I. The float time of an activity is the difference between the earliest and latest starting dates. An activity is near critical if the float for that activity is equal to or less than some previously specified float factor.

Table I
Critical Path Analysis for Nail Lacquer Production[a]

	S	E	D	Cost	ES	LS	EF	LF	F	**	RES
Base formulation	1	2	10	600	12/12/72	12/12/72	12/18/72	12/18/72	0	CR	PD
Shade formulation	1	3	2	120	12/12/72	12/18/72	12/12/72	12/18/72	8		PD
Primary formula	2	4	2	120	12/19/72	12/19/72	12/19/72	12/19/72	0	CR	PD
Primary formula	3	4	2	120	12/13/72	12/19/72	12/13/72	12/19/72	8		PD
DUM	4	5	0	0	12/20/72	1/12/73	12/20/72	1/12/73	30		D
DUM	4	6	0	0	12/20/72	12/29/72	12/20/72	12/29/72	10		D
DUM	4	7	0	0	12/20/72	12/20/72	12/20/72	12/20/72	0	CR	D
DUM	4	8	0	0	12/20/72	1/12/73	12/20/72	1/12/73	30		D
Panel test	5	9	10	660	12/20/72	1/12/73	12/28/72	1/18/73	30		TS
Safety	6	9	30	1500	12/20/72	12/29/72	1/11/73	1/18/73	10		OS
Stability	7	9	40	240	12/20/72	12/20/72	1/18/73	1/18/73	0	CR	TS
Analysis	8	9	10	600	12/20/72	1/12/73	12/28/72	1/18/73	30		TS
Final formulation	9	10	2	120	1/19/73	1/19/73	1/19/73	1/19/73	0	CR	PD
Product	10	11	0	0	1/22/73	1/22/73	1/22/73	1/22/73	0	CR	MM

[a]Total number of activities = 14; total cost = 4080.

COMPUTER FORMULATION

In any product development laboratory, a given portion of work involves the formulation and reformulation of the product. Often, reformulation is required when either substitute ingredients or additives are introduced into a product, or when one mixture of ingredients replaces another mixture.

Both the old formula and the revised formula are then subjected to various types of tests and evaluations to determine whether a change in the product is warranted. In making such a change, it is important to know exactly how the final composition of the product is affected, since the change in the performance of the product may be reflected in a change in the percentage of a particular ingredient. Knowing the performance at several concentrations of the particular ingredient, the formulator can extrapolate the concentration yielding optimum performance. It is desirable to know the amount of each ingredient for the purpose of costing, and it is sometimes required that the exact composition of each product be available for legal and medical purposes.

Determining the composition of a product that is prepared by mixing several raw materials is simple. For example, the composition of a lacquer thinner that is the combination of three organic solvents is simply given by the weight percentage formula. But in a case where any of the main components added to the product at the final batch stage is a previously processed component, its formula must be substituted in the final formula where the composition is calculated. The process of determining the final composition becomes very complex when many preprocessed components containing common ingredients are involved, for the contributions of each ingredient from each component must be considered. Often, preprocessed components consist of preprocessed subcomponents, making the calculation of the final composition of the product all the more difficult and time consuming.

A program has been written that determines the composition of a lacquer containing several main components which break down into components, subcomponents, and finally ingredients. The computer program is not needed if one is dealing with pure ingredients which cannot be broken down. Our program utilizes a system of matrices that describes each breakdown step and allows quick changes to be made in the composition of any item that might occur in the product as new formulas are suggested. The chemist selects the formula of the product, and in a matter of minutes the final composition is printed out. At the request of the user, various analyses about the formula are determined and printed. Thus, before a single resin or solvent is mixed, the chemist has a good idea what the product will be like. In addition, these programs are adaptable to any kind of formulary work.

A matrix is required for each breakdown step of the formula (4). The matrix may be thought of as a table of the breakdown—along the left-hand column are the components and along the top row are the subcomponents contained in the components. The elements of the matrix are the coefficients or percentages of the subcomponents found in the components. The system requires first that the various breakdown steps be recognized, and that the components, subcomponents, and ingredients be recognized and assigned an identification letter. For example, let us consider the breakdown of a lacquer designated X. X is made from four main components: A_1 is a flow additive;

A_2, thinner; A_3, paint base; and A_4, a color concentrate mix. A_1 is a pure ingredient, purchased from the manufacturer as such and cannot be further broken down (except to chemical elements). A_2, A_3, and A_4, however, can be broken down further. The thinner is made from three solvents; the base from four solvents, two vehicles, and two plasticizers. The color mix is prepared from three color pastes; the pastes are each a combination of a dry pigment, a solvent, and a paint base A_3. As shown in Fig. 6, the lacquer X is broken down into four main components A's, six components B's, seven subcomponents C's, and finally 12 ingredient D's.
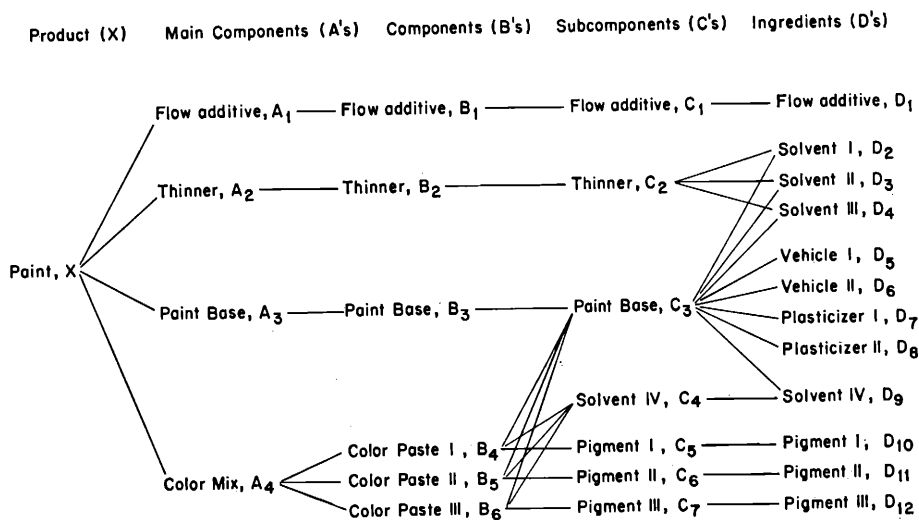

Figure 6. Breakdown of nail lacquer for formulation program

Notice that some of the main components are retained as components and subcomponents; any item must be re-entered at each level until it is actually broken down. A_1, the flow additive, cannot be broken down at all, hence it occurs as itself at each level. The paint base could have been broken down at matrix P; however, since it is a subcomponent contained in each of the components, B_4, B_5, and B_6, it is not broken down until after those components are. The thinner is not contained in any item A, B, or C; it is only contained in the lacquer X. Yet, it is not broken down until matrix S, simply to keep the number of components and subcomponents to a minimum. The matrix P describes the breakdown of the paint X, and has dimensions 1 x 4.

$$P = (P_{1,1} \ P_{1,2} \ P_{1,3} \ P_{1,4})$$

which may be interpreted as indicating:

$$X = P_{1,i}(A_1) + P_{1,2}(A_2) + P_{1,3}(A_3) + P_{1,4}(A_4)$$

where P_1,i indicates the percentage of Ai in X. The percentages must be expressed as decimals in order that the final composition of the paint totals 100% expressed as unity.

The matrix Q, dimensions 4×6, expresses the composition of the main components A_1 to A_4, each in a row:

$$Q = \begin{matrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & q_{4,4} & q_{4,5} & q_{4,6} \end{matrix}$$

which represents:

$$A_1 = B_1 + [0(B_2) + 0(B_3) + 0(B_4) + 0(B_5) + 0(B_6)]$$
$$A_2 = B_2 + [0(B_1) + 0(B_3) + ...]$$
$$A_3 = B_3 + [0(B_1) + 0 ....]$$
$$A_4 = q_{4,4}(B_4) + q_{4,5}(B_5) + q_{4,5}(B_6) + [0(B_1) + 0 ...]$$

Similarly, R is a 6×7 matrix expressing the composition of the six components B in terms of the seven subcomponents C; one can find the percentage of a given subcomponent C_j in a given component B_i by locating in matrix R the element $r_{i,j}$. The same holds true for the final matrix S, the rows of which express the composition of the seven components C in terms of the 12 ingredients D. If further breakdown steps had been necessary, more matrices could be written; the general formula is to put the compound items on the left-hand column and their constituents on the top row. Thus, the matrix will always have the dimensions $i \times j$ where i is the number of compounds and j is the number of constituents.

It is now necessary to reduce the matrices to a 1×12 matrix that expresses the lacquer in terms of 12 ingredients. This is accomplished in three steps. Let T be a 1×6 matrix that is the product of matrices P and Q, i.e., $T = P \times Q$. The lacquer is now expressed in T as the product of six components. Matrix $U = T \times R$ is a 1×7 matrix expressing the lacquer in terms of the 7 subcomponents, and finally matrix $V = U \times S$ has dimensions 1×12 and represents the composition of the paint in terms of the 12 ingredients, D_1 through D_{12}.

If we desire the final composition, we instruct the computer to print matrix V; if we desire any intermediate composition we ask the computer to print out the appropriate matrix. V will appear as 12 numbers in a row, representing the amounts, expressed as decimals, of each of the 12 ingredients. For display purposes, we might ask the computer to determine another matrix V^1 which is the transpose of matrix V. This would cause the data stored in V as a row of 12 elements to be stored in V^1 as 12 rows of one element.

If we ask the computer to print $V^1 \times 100$, the percentage amount of each ingredient in the lacquer will appear in a column. The computer then prints the

elements of a string numbering 12 ingredient names after each row of V^1 x 100. The output consists of the percentage followed by the ingredient name, one to a line.

By making each matrix larger than required, a new ingredient or subcomponent can be readily added when it does not occur in the original formula. The chemist needs only to enter zero or the percentage of the ingredients in the appropriate line of the matrix.

The formulation of a typical nail lacquer as shown in Table II is rapidly handled by the computer.

Table II
Computer-Formulated Nail Lacquer
(Typical Composition)

0.785481	Camphor
8.71251	Plasticizer
34.4034	Butyl acetate
15.2004	Ethyl acetate
9.05484	Isopropyl alcohol
19.8769	Toluene
9.241	Nitrocellulose
1.7625	Bentone 38 powder
0	Bentone 27 powder
0	D & C Red #7 Ca lake
0	Iron cosmetic oxide
0	Iron blue
0	D & C Yellow #5 Zr lake
0.705	Titanium dioxide
0.132062	D & C Yellow #6 Al lake
0	D & C Red #9 Ba lake
2.40428E-2	D & C Red #6 Ca lake
0	D & C Red #34 Ca lake

Do you want ratios and totals or stop?   YES
    Ratio—Modified Resins: Nitrocellulose = 0
    Ratio—Gellants: Resins = 0.1907
    Ratio—Pigments and Gellants: Resins = 0.283871
    Ratio—Resins: Solvents = 0.117682
    Ratio—Plasticizers: Resins = 1.03145
    Ratio—Gellants: Pigments = 2.04679

    Total Solids = 12.3007
    Total Pigments = 0.861105
    Total Gellants = 1.7625
    Total Solvents = 78.5355
    Total Plasticizers = 9.53289
    Total Resins = 9.24224

ANALYSIS AND EVALUATION

At this stage in the development project, the chemist will submit his product to the Technical Services Group for analysis, environmental and panel testing. Several computer programs have been written for detailed examination of nail lacquers. These programs are used to evaluate the data and write reports from a wide range of analytical instrumentation. The instrumentation, supported by data processing, covers the areas of rheology, DSC, tensile strength, particle size, and gas permeability (5).

Panel testing and laboratory evaluation for product likes and dislikes are statistically analyzed using stored programs available on the G-E Mark II System. Tests of significance and correlation are carried out in all panel studies in order to insure that the best prototype is selected (6).

Environmental testing of a product at several storage conditions seems to multiply at an enormous rate. Computers can be used to keep track of stability studies, store data regarding sample formula, project name, components, and packaging material involved. The computer program will print out the actual analytical data for several lots stored at various temperatures.

Using the Van't Hoff-Arrhenius Stability approach, the analytical data and temperature relationships are plotted according to zero, first, and second-order equations. These equations permit the chemist to estimate the time required to meet minimum acceptable concentration.

COLOR FORMULATION

An area where computers have made significant progress is in the field of color formulation and color matching. Our laboratory is currently using a series of color programs called Chroma-Pac®* which contains seven color programs (7). The programs and a brief description of their functions are found in Table III.

The color standard to be matched is measured on a suitable spectrophotometer interfaced to an ASR-33 Teletypewriter. The automated measurement and data collection steps eliminate a considerable amount of man-hours and substantially reduce errors. The measured data are next entered into the program called PMAT, *via* the teletype.

The PMAT program requires the following data at the time of execution:

User ID Code—4-5 character code which corresponds to the instrument and reference used.

Name of Standard—Arbitrary name, assigned by the user.

Pigments/Comb., Field Size & Sub. ID#—User supplies three numbers, the first specifies how many pigments are desired, the second, number of pigments per combination, the third number is the identification number of the TIO_2 substrate to be used.

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* Trade mark of Applied Color Systems, 221 Nassau St., Princeton, N.J. 08540.

Table III
Chroma-Pac Computer Programs

PCAL is a pigment calibration program. It accepts reflectance data for one or a number of concentration levels for individual pigments, along with the pigment cost, name, and an identification number. These data are processed and stored in a specified file in the correct format for use by the other programs in the package.

PMAT is a formulation program. It is single-constant in the sense that the absorption and scattering coefficients of each pigment are used as a ratio (K/S) rather than as separate values. PMAT uses the combinatorial technique in that it attempts to match the target shade with all possible combinations of ND colorants taken N at a time, where ND is the number of candidate components and N is the number of pigments desired in each formula. PMAT uses tritsimulus theory, incorporating data on the 2° standard observer, and is available with a number of illuminants.

PCOR1 is a formula correction program. It may be used to correct the color of material now in production, to correct a laboratory formula, or to produce initial matches of superior accuracy by correcting a library sample formula to match the target shade. PCOR1 automatically corrects for production variables using internally calculated correction factors. PCOR1 requires reflectance input for both the sample and the standard.

PCOR2 is similar to PCOR1 in that it is a correction program, but is somewhat more limited in use because it accepts tristimulus data as input rather than reflectance data. It is meant primarily for use in the production environment where simplicity of operation and speed of correction are the primary requirements.

UNKNWN has many of the features of PMAT, but is specifically designed to produce production formulas incorporating a maximum of "waste" material while maintaining product quality. It not only allows the user to "work-off" such material, it also shows how to accomplish this as rapidly as possible and at the lowest cost.

FMC is a color difference program incorporating Friele-MacAdam-Chickering mathematics. It accepts reflectance, tristimulus, or ratio data as input and prints CIE tristimulus values, chromaticity coordinates, and color differences as outputs. When reflectance data are entered, tristimulus integration may be done under any of a number of illuminants.

LISTER is a utility program used to prepare a log of all the primary information stored. It serves a record-keeping function and the logs are useful when entering input data to other programs in the CHROMA-PAC I series.

File Name and Pigment ID's—Identification number of the pigments used.

Standard % R's—User supplies 16 reflectance values (400-700 nm) at 20-nm intervals for the color to be matched.

The PMAT program prints out, in addition to the actual per cent composition of the color match, the color difference under Illuminant A and Illuminant C. A typical printout for a paint formula is shown in Table IV.

This selection process allows the user to select those color formulas which are of particular interest, whether they be low in cost, low in metamerism, or both.

SUMMARY

A data collection and analysis program which is used to aid the product development chemist has been described. It allows user interaction at the criti-

Table IV
Typical Printout of Paint Formula

User ID Code: BILL
Name of STD.: TEST STD. C
Pigments/Comb., Field Size, & Sub. ID#: 3 5 380
File Name and Pigment ID#S: Test 1 2 3 4 5
Standard % R's: 26 • 235 • 736 • 235 • 034 • 434 • 434 • 534 •
        735 • 638 • 340 • 340 • 840 • 640 • 239 • 939 • 6

| | | Formulas for Test Std. C | | |
Pigments	Amount	DEA	DEF	Cost
Prim. Yellow	3.062			
Oxide Red	6.289			
Phthalo Blue	0.227			
TiO₂	90.422	4.6	1.4	9.58
Prim. Yellow	1.601			
Oxide Red	3.652			
Lamp Black Lt.	0.468			
TiO₂	94.280	1.0	0.4	5.72
Oxide Yellow	2.925			
Oxide Red	5.446			
Phthalo Blue	0.245			
TiO₂	91.385	2.9	1.6	8.62
Oxide Yellow	1.515			
Oxide Red	3.113			
Lamp Black Lt.	0.485			
TiO₂	94.887	0.0	0.2	5.11

cal decision making steps. In addition, control of the test parameters and data reduction steps permit rapid analysis of physical and chemical data.

Experience with this simple system should enable one to develop more intelligent planning and broader uses for this valuable tool.

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REFERENCES

(1) Faust, R. E., Research planning, *Drug Cosmet. Indus.*, 111, No. 1, 42 (July 1972).
(2) Walck, R. Organizing the small research project with PERT, *Chem. Tech.*, 334–9 (June 1972).
(3) *Critical Path Scheduling—Users Guide, Mark II*, General Electric Co., Information Service Dept., 7735 Old Georgetown Rd., Bethesda, Md., 1968.
(4) Gere, M. J., and Weaver, William Jr., *Matrix Algebra For Engineers*, D. Van Nostrand Co., Inc., N.J., 1965.
(5) Kaplow, R., and Posn, H., Online computer analysis and control of experiments, *J. Appl. Phys.*, 40, 4948 (1969).
(6) *Numerical Analysis Routines—Users Guide*, General Electric Co., Information Service Dept., 7735 Old Georgetown Rd., Bethesda, Md., 1968.
(7) *Applied Color Systems Users Guide*, Princeton, N.J., 1972.