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Formulation with Fillers

There are several reasons for formulation development:

- A new product
- Product improvement
- Cost reduction
- Raw material substitution
- Raw material alternatives
- Process engineering

All of the above are components of the product cycle from creation to discontinuation or replacement. These reasons for formulation development may be treated as separate events which become important when urgently needed. Or, they can be a part of a continuous search for better, more economical products. It goes without saying that in many organizations the first option is a frequent choice. These are organizations which are driven by external events, such as

- We do not have product to sell
- Competitor has better product
- We are too expensive
- Raw material production was discontinued and has to be imported from another continent
- Raw material supplier increased price
- Our equipment breaks down every month because material is too viscous to mix
- etc.

It also goes without saying that this is not the type of organization to be in, considering that events should be driven primarily by predictions and planning during product cycles. The methods of formulation have an important influence on the *modus operandi* and *modus vivendi*. The discussion below analyzes components of an organized, planned formulation.

The reasons for formulation development have an impact on the data required to make such a process successful. New product development is always considered a jewel in the crown since it may open new opportunities, and it is usually associated with the conquest of new territory. It is also the most risky undertaking considering the probability of success, patent barriers, health and safety regulations determining the availability of raw materials and rights to produce, and frequently required investment in the new process and equipment. Even this short list of hurdles shows that the development effort is a multifunctional one since it requires not only the input of specialists in all these areas but also the understanding of the market, the competition, product requirements, and all components which convince people to use this product.

In new product development, the general term associated with an excellent solution is *invention*. There is very little guidance as to what this *invention* really means and how one arrives at an inventive solution. One dictionary says that the inventive person is "able to invent things". The archaic definition of invention is "the act of finding". Rather than analyzing various programs created to increase the inventiveness of inventors, let us concentrate on the root of the matter and analyze what this "act of finding" means in the case of formulating with fillers. It is very difficult to imagine that the "act of finding" can be based mostly on imagination without data; rather, the results of one's work suggest that certain properties or functions can be achieved with a particular set of observed properties or that this set of certain properties can be useful to enhance the properties of some product. This stresses a need for data as a stimulant of inventiveness. For example, it would not be possible to design conductive plastics if neither conductive polymers nor conductive additives were available. But the very fact that one can readily get many materials of this kind does not constitute an immediate solution for the problem.

There are examples in this book of fillers which have magnetic properties, but somebody in the act of inventiveness came to the conclusion that such material can be used for removing materials from their solutions and designed a composite which contains magnetizable particles attached to the various materials (e.g., selective adsobent of a particular material). By mixing this composite with a solution of material, material is adsorbed by adsorbent and removed from solution by a simple magnet. A new analytic technique was created which is very useful in pharmaceutical and biochemical research.

It has been known for about a century that the crystallization of material is affected by the concentration of solution and admixtures, but only recently have scientists come to the conclusion that if implants are to be compatible with a particular organism they have to be crystallized in the environment in which they later perform and from which they should not be rejected. This creates a new field of activities dealing with the development of bone materials that are compatible with real conditions of their performance.

Are these two examples inventions or the products of observation of previously generated data? They are both because previous knowledge and data were required to conclude that they can be useful in their applications and there was somebody who made these important conclusions. There are a large number of people involved in research but only some ever contribute new products. This is related to their ability to see ahead to the remedies for the full list of obstacles which separate the beginning of research from its successful conclusion. Applied chemistry is a complex subject involving the interference and interplay of numerous parameters – some sufficiently quantified and some known only by a general description. All of these parameters are important and must be included in an initial experimental plan. It is thus important to consider a sufficient number of these variables in order to increase the probability of success (or better yet to decrease the probability of obstacle which cannot be overcome with a formulation that is almost complete but not sufficient to proceed to the next phase – production). All of this discussion was designed to show the importance of data.

Let us now analyze what kind of data are needed for the various reasons of formulation listed in the beginning of this chapter. We may begin with new product development since it is so crucial to progress, easier life, and business. The development of a new product begins with an idea regardless of how this idea was generated. The idea can be generated by analysis of needs which were not fulfilled so far, or it may be conceived based on association of an observed property of some material with its possible application. It might be the result of development of a new raw material which has properties not available before and which creates new opportunities, or it may simply occur, as it happens sometimes, by coincidence. Some ideas are more conventional than others and thus they will be considered as incremental improvement. A few ideas are simple but so useful that they are considered breakthroughs. In each case there must be

- A need for product
- A cost/performance ratio acceptable in the market place
- A material means for its development
- Work leading to this development
- A successful conclusion – product implementation
- Communication of the success to the potential users.

If any of the above is missing, the undertaking fails to achieve its goals. From the technical point of view, the following data are needed to fulfill the above requirements:

- A detailed list of product properties
- Quantification of product parameters
- A concept of product design
- A list of materials required to formulate product which meets requirements
- Understanding of the roles which components play in fulfilling requirements
- Understanding of interactions between components of the formulation
- The effect of variation in each component on product properties
- The effect of processing parameters on product properties

In addition to these groups of information, many other data are very useful or sometimes very important. They include: health and safety regulations affecting the use of components, production of intermediates and final product, limits of existing equipment which can be potentially used for production, professional level of operators, precision of production, the effect of environmental conditions on product quality (e.g., variations in humidity, temperature, temperature of cooling water, etc.), cost performance ratios of existing solutions, features of the new product which can be easily communicated to customers to get them interested, size of the market, the effect of production scale on the cost of raw materials and production, product patentability, patents which might be infringed on by the new product, and packaging requirements and storage conditions to obtain the required shelf-life. It is important to stress that all components of this list have some price tags which should be closely monitored throughout the process of development; otherwise good product might be too expensive for buyers.

This makes a list which seems impossible to fulfill, but it is rarely realized that behind every product there was a person or a group of people who had sufficient perception of these requirements that the product was introduced into the market and performed for many years. It is also not fully realized that there has to be a person with vision and imagination who early in the development stage understands the interaction of all these parameters which are critical to the end-effect. It is important to consider that a particular raw material (e.g., filler) does not have only one function in the formulation; rather, affects numerous parameters important for product properties. The more these interactions are understood, the more chances exist that useful product is developed, and the shorter the development time.

Let us now consider the next reason for formulation on the list – product improvement. If in the very first stage of product development, sufficient time was spent on

- Understanding of the roles which components play in fulfilling requirements
- Understanding of interactions between components of the formulation
- The effect of variation in each component on product properties
- The effect of processing parameters on product properties

there is available a lot of useful information for reformulation. If the product was developed by a trial and error process, no such background information exists, which makes the task of product improvement similar to that of development of a new product; in addition, it is burdened by the requirement that it should frequently resemble features of existing product so that it would not be recognized by customers as a new product. Such lack of data is quite typical of older products which makes their improvement very costly and difficult.

It is very easy to show that whether it comes down to cost reduction, raw material substitution, raw material alternatives, or process engineering, well organized data become invaluable. Such data not only help to achieve goals quickly, at low cost, and successfully, but also help to build a process which organizes the present and future work and contributes to continuous progress.

The next question arises as to how such data can be generated? There are numerous examples in the literature on how such data are presented and utilized,[1-13] and many books were written on the approaches to the data processing.[14-20] The most common form of information on the performance of additives is the so-called "starting formulation". These formulations are prepared by the manufacturers of raw materials to demonstrate the performance of their additives. This work is done by the raw material manufacturer alone or in the cooperation with some other parties such as, for example, the leading manufacturer of products which make use of the additive. In some instances, such starting formulations are used for the production of real products, but typically they are not suitable for direct application, considering that products should be unique, well engineered, and economical. Some information is given in the format which shows the most important parameters of the raw material (e.g., particle size, shape, color, etc.) vs. the effect of this property on product performance (e.g., with particle size decreasing reinforcement increases). These are useful directions for selection but only as a starting point because in the technological development, these influences have to be quantified. There are patents and research publications which show the results of studies and which usually contain sufficiently detailed descriptions of conditions of material preparation that the experiment can be verified. The literature search, and scientific monographs are invaluable resources of information used to

- Formulate the concept of product design
- List materials required to formulate product
- Understand the roles which components play in fulfilling requirements
- Understand the interactions between components of the formulation
- Understand the effect of processing parameters on product properties

Still, data from the literature is not a substitute for data generated in the development process. Data from the literature save development time by directing effort to meaningful activities and by frequently suggesting inventive solutions.

The ultimate goal of product development is to describe the properties and functions of the product in form of an algorithm – a functional relationship which includes all essential variables and allows one to generate simple relationships of influence of one parameter on another or on the product property (humans are thought to comprehend better the relationship of two variables). Such an ultimate goal is too difficult to reach, but the sets of relationships relevant to the performance of the product are commonplace. And, these form a very good starting point in the quest to describe properties in the quantitative manner, which brings understanding closer to the ultimate algorithm or model.

There are numerous tools which were designed to help formulators cope with the large amount of data. These include relational databases with graphic capabilities, statistical methods of data validation and evaluation, programs to design experiments, process optimization, worst case analysis, safety analysis, quality control analyzing methods and programs, robust design, screening designs, computer aided formulation, multiple goal decision methods, experts systems, and more. These tools are helpful if they are not used to replace human logic, which is paramount to the successful conquest of the complexity of nature.

The so-called experimental design is the most frequently abused tool because of the lack of understanding of chemistry, technology, and mathematics. The most frequent use of this method is by selecting the ranges of concentration of materials, measuring a few properties of the product by crude methods and projecting results of "mathematical analysis" in the form of usually tridimentional graphs which supposedly offer information on how to regulate process or design material.

This book shows that one filler introduced to the formulation affects many different parameters characterizing the product. In typical formulations of finished products 5-30 raw materials are used, each playing some role and potentially interacting with the remaining components. If the entire direction of formulation is predicted based on a crude measurement of the most common product indicators in specification, the entire principle of mathematics is neglected because a sufficient amount of information does not exist to solve equations in a realistic way.

The computerized system which helps most in product development resembles more the so-called expert system, which is a set of relationships quantified by an experiment for the purpose of similar products. Such systems are increasingly more effective with the amount of data (information) increasing. Considering such need, this book will have in the future a companion CD-ROM containing a base of available data which will be periodically updated to build an incremental wealth of information serving two purposes: material selection and data processing for the needs of the formulator.

This chapter, in the view of some readers, may contain information too general to be useful. At the same time, it is very important to stress that the development of high technology products requires adequate effort from the formulators. Fillers produced today are no longer just low cost filling materials but are sophisticated multifunctional additives. They can contribute to a decreased total cost of final products but only if the functions which they were designed for are fully utilized in the product design. This requires sufficient effort and data to produce results.

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