Chapter 1

Raw Materials for Surfactant Preparation

Background

Formulators in the personal care field realize that there are a vast number of surfactants from which to choose in the preparation of new products. There are nonionic, cationic, amphoteric and anionic surfactants available. Within each class there are numerous individual surfactants. A neophyte formulator might ask, "Why are there so many types of surfactants?" The answer is clear: The structure of the surfactant determines its functionality.

Chart 1 shows some of the properties of the major types of surfactants. Selection of the kind of surfactant for use in a particular formulation is a challenge to formulators.

Once this is done, ensuring that the surfactant chosen is the same from lot to lot and manufacturer to manufacturer is quite another challenge. As formulations become more complicated, the need for salient specifications becomes more critical. Salient specifications are defined as those values established for specific chemical analysis that define whether a chemical raw material will function in a given formulation. When a good set of salient specifications for the raw material is clearly defined, products will work more consistently in a given formulation. To understand the salient specifications, one needs to understand not only the chemistry of the surfactant but also the chemistry of potential by-products and residual raw materials.

This work seeks to shed some light on these variables and to provide some guidance on the kind of analysis recommended for each class of product.

Surfactant Classification

One important way to classify surfactants is by the kind of ionic charge present. An example of this kind of classification is as follows:

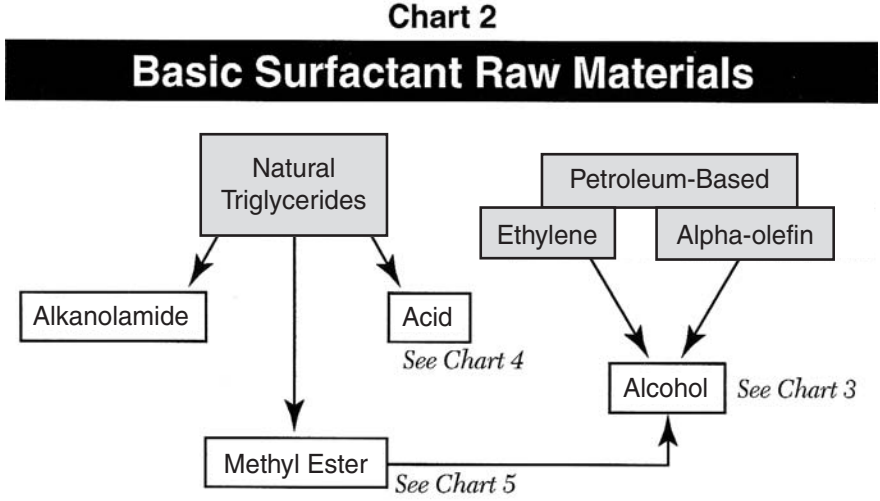
Class	Example	Charge
Anionic	Phosphate ester	Negative
Nonionic	Nonyl phenol ethoxylate	None
Cationic	Stearyl dimethyl benzyl ammonium chloride	Positive
Amphoteric	Cocamidopropyl betaine	Variable

Another way to classify surfactants is by function. This kind of classification is helpful to formulators. Chart 1 shows such a classification system.

Chart 1

PRODUCT CLASSES	RELEASE AGENTS	EMULSIFIERS	DETERGENTS	LUBRICANTS	SOFTENERS	WETTING AGENTS	LEVELING AGENTS	DISPERSANTS	CORROSION INHIBITORS	SOLUBILIZERS	COUPLING AGENTS	FOAMING AGENTS	FOAM STABILIZERS	DISINFECTANTS
Alcohol Alkoxylates		◆ ◆	◆ ◆	◆		◆ ◆		◆					◆	
Agricultural Surfactants														
Alkanolamides (1:1)														
Alkanolamides (2:1)		◆	◆ ◆	◆ ◆	◆	◆	◆		◆			◆		
Alkanolamide Ethoxylates				◆ ◆										
Alkylaryl Sulphonates		◆	◆		◆	◆	◆		◆				◆	
Alkylphenol Ethoxylates														
Amine Ethoxylates		◆ ◆	◆ ◆			◆	◆ ◆	◆	◆ ◆	◆		◆		
Amine Oxides														
Amphoterics														
Benzyl Quats		◆				◆	◆ ◆	◆	◆	◆				
Block Co-polymers			◆									◆		
Fatty Acid Ethoxylates														
Glycerol Esters		◆ ◆ ◆	◆	◆ ◆	◆ ◆									
Higher Alcohol Ethoxylates														
Imadazolines														
Imadazoline Quats		◆ ◆ ◆	◆	◆	◆ ◆							◆		
Lower Alcohol Ethoxylates														
Phosphate Esters		◆	◆	◆ ◆ ◆		◆				◆ ◆	◆ ◆			
Polyethylene Glycols														
Polyproylene Glycols														

FUNCTIONS



Raw Materials

The possible number of surfactants useful in formulations is truly staggering. To bring some organization to the surfactant world, we will start with the raw materials. The basic raw materials from which surfactants are prepared find their most basic origins in triglycerides, propylene and ethylene. The process of converting these very basic materials into acids, alcohols or methyl esters is shown in Chart 2.

Acids, alcohols and methyl esters are basic building blocks from which surfactants are derived. Charts 3, 4 and 5 show the various pathways from which these basic raw materials can be transformed into surfactants.

A very important concept that one must understand is that various analogous and homologous series of surfactants are available to formulators.

Analogous series surfactants differ only in the functional groups present. For example, sodium laureth-2-sulfate and sodium laureth-2-phosphate are two analogues. Their common raw material is lauryl alcohol with two moles of ethylene oxide. The substantial difference in properties between these analogues is due only to the different functional groups.

However, if one varies the carbon chain in the group, a series of homologues is prepared. Such a homologous pair is sodium lauryl (C12) sulfate and sodium behenyl (C22) sulfate. The differences in the properties of these two surfactants are due to the differing number of carbon atoms in the molecules.

It is often advantageous for formulators to take into account such differences as these to select a surfactant. The process becomes even more complicated when one considers modifications that change both functionality and carbon chain distribution.

The selection of the surfactant hydrophobe has a profound effect on the functional properties of the molecule and, consequently, the performance of the formulation. In addition, other formulation components influence the performance of the surfactant chosen. The importance of surfactant interaction in preparing formulations is often overlooked by new formulators.