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chemical formulation

AN OVERVIEW OF SURFACTANT-BASED PREPARATIONS USED IN EVERYDAY LIFE

TONY HARGREAVES

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An Overview of Surfactant-based Preparations Used in Everyday Life

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advancing the chemical sciences

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Preface

My first experience of the chemistry of surfactant-based formulations was when I was working on analysis of solvent blends by Gas Chromatography (GC) back in the early 1980s. In addition to GC work our laboratory would also carry out comparative studies of surfactant formulations like shampoos and related products.

Instrumental methods such as GC or Infra-red (IR) were out of the question because of the disproportionate amount of preparation required to make the sample, or a part of it, 'instrument ready'. As such many of these comparative studies were confined to quick and simple tests: pH, conductivity, solids, ash and indicator tests for surfactant type.

From time to time we would be asked: Can you test this and give an idea of how to make an equivalent? Although cautious of trespassing on someone else's intellectual property we would often take up the challenge of making and matching formulations based on surfactants. It was an interesting diversion: instead of the analytical approach of breaking down formulations we could go in the opposite direction and build them up.

It was then that I began to appreciate the difficulty of getting even a basic understanding of what goes into formulations, the amounts used and how each component functions. For a start the raw materials were commercial products with commercial names and often it was a problem knowing what the chemistry was. Although there were many formulations provided by chemical suppliers for us to study there seemed to be few, if any, guidance rules. It was only after a lengthy exercise of studying formulations, basic surfactant chemistry and discussions with surfactant manufacturers that I was able to form a generalised picture of what was going on.

This book is a summary of the chemistry and technology that was pulled together in the attempts to see more clearly what chemicals go into everyday preparations, how those chemicals function and some related aspects such as environmental effects. Hopefully the book will be of value for those with an interest in household chemicals, others who may

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wish to consider making such products as a commercial venture and students with an interest in applied chemistry.

In preparing this book I have used many formulations provided by surfactant manufacturers and to them I wish to express my gratitude. In particular I wish to thank Nick Challoner and Rebecca Webster at Croda Oleochemicals for permission to use their formulations and for the many helpful suggestions to ensure that what is reported is as up-to-date and accurate as possible. I would wish to extend my thanks to Chris Howard at Stepan UK and to Simon Nicholson at Huntsman Surface Sciences for their kind assistance.

Abbreviations Used

AG	Alkylpolyglucoside
ASTM	American Society for Testing Materials
BHA	Butylated hydroxyanisole
BHT	Butylated hydroxytoluene
BOD	Biochemical oxygen demand
BS	British Standard
CAS	Chemical Abstracts Service
CDE	Coconut diethanolamide
CFC	Chlorofluorocarbon
CI	Colour index
CMC	Critical micelle concentration
COD	Chemical oxygen demand
CoSHH	Control of Substances Hazardous to Health
CTFA	Cosmetics Toiletries and Fragrance Association
DEA	Diethanolamine
DSP	Disodium phosphate
DTPA	Diethylenetriaminepentaacetate
EDTA	Ethylenediaminetetraacetate
EO	Ethylene oxide
GC	Gas chromatography
GWP	Global warming potential
HCFC	Hydrochlorofluorocarbon
HEDTA	Hydroxyethylethylenediaminetriacetate
HFC	Hydrofluorocarbon
HFE	Hydrofluoroether
HLB	Hydrophile lipophile balance
HPLC	High performance liquid chromatography
INCI	International Nomenclature of Cosmetic Ingredients
IPA	Isopropyl alcohol
IR	Infra-red
ISO	International Organization for Standardization
IUPAC	International Union of Pure and Applied Chemists

LABS	Linear alkylbenzene sulfonate
LCA	Life cycle assessment
LCI	Life cycle inventory
MALDI	Matrix Assisted Laser Desorption Ionization
MEA	Monoethanolamine
MS	Mass spectrometry
MSDS	Material Safety Data Sheet
MSP	Monosodium phosphate
NMR	Nuclear magnetic resonance
NTA	Nitrilotriacetate
o/w	Oil-in-water (emulsion)
ODP	Ozone depletion potential
PEG	Polyethylene glycol
PO	Propylene oxide
PVC	Polyvinyl chloride
SCMC	Sodium carboxymethylcellulose
STPP	Sodium tripolyphosphate
TEA	Triethanolamine
TKPP	Tetrapotassium pyrophosphate
TOFA	Tall oil fatty acids
uPVC	Unplasticized polyvinyl chloride
UV	Ultra-violet
VOC	Volatile organic compound
w/o	Water-in-oil (emulsion)

Contents

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Introduction

Chemical formulations go so far back in time that we must turn to the archaeologist for examples. As long ago as Mesolithic times when people were hunter-gatherers they attached worked flint arrow heads to shafts by means of a blend of resin extracted from birch bark and made plastic with beeswax to produce a substance that had the best properties for the job.

Resin alone, once set, produces a brittle mass but when blended with just the right amount of beeswax it provides not only a strong adhesive but also has sufficient flexibility to withstand the mechanical forces imposed on a weapon such as an arrow.

Found only in certain limestone deposits flint was scarce and often was brought from far and wide. And so it seems reasonable to assume that a great deal of care went into any experiments of which it formed a part. Quite simply, a lost arrow point demanded a replacement that took a skilled person some time to make and required a fairly large chunk of that valuable material.

One can imagine that the process would follow the lines: theory, experiment, result, interpretation, new theory, new experiment, new result and so on until performance was optimized. Those stone-age experiments were in fact an early application of plasticizing a polymer – the beeswax was the plasticizer. The product must have been used as a hot melt adhesive which, on cooling, left the flint arrowhead firmly, but flexibly, bonded to its pine shaft.

The very same principle of plasticizing a polymer is used today to turn rigid uPVC (unplasticized PVC) into pliable PVC. Yes, we use a ten thousand year old discovery to take the 'u' out of uPVC. There are other examples from antiquity but the beeswax/resin example is of particular significance in a scientific context as it would have called for a good deal of quantitative experimental work to optimize the properties of the blend.

Eventually the hunter-gatherer lifestyle gave way to living in settled communities as a result of early agriculture. Now, instead of travelling far and wide to catch animals the task was simplified with much time and effort saved. With the animals in their pens and people living in settled communities two very favourable conditions, the availability of spare time and permanent work space, provided for a basic knowledge of materials to be developed.

The interest in materials led to the discovery of many chemical reactions that were to mark the onset of materials technology. Thus the foundation was laid for the high temperature chemistry that turns sand and clay into pot. The importance of recognizing essential properties was being learnt: quality of raw materials, proportions to blend together to achieve certain effects, estimation of kiln temperature, rate and duration of firing.

Later on, other high temperature reaction based processes were discovered, studied and refined to give rise to a new technology based on chemical reduction of a greenish rock to produce bronze. Still later, the iron-age, based on turning brown iron ore into iron developed. Thus, chemical technology was well established in times of antiquity. Much of the chemistry involved was brute force chemical reaction, high temperature stuff.

In general, chemistry is recognized in its ability to bring about reactions to effect a permanent change from one substance to another; the latter bearing no resemblance to that from which it was made – just like the green rock to bronze referred to above. However, the chemistry involved in making the plasticized resin did not involve chemical reactions to create new substances but was the practice of making chemical mixtures. It is the preparation of mixtures that is the essence of formulation work.

The properties of mixtures reflect the properties of the substances from which they are made and the mixtures can, by means of simple techniques, be split into their component substances. Often, to the frustration of the chemical formulator, a prepared mixture separates out on its own.

So, now to consider some simple two-part mixtures; some of these are natural and others are man-made ones:

Components	*Type of mixture*	*Example*
Solid in solid	Powder blend	Facial make-up powder
	Solid solution	Bronze
Liquid in liquid	Solution	Alcohol in water
	Emulsion	Mayonnaise

(*Continued*)

Components	*Type of mixture*	*Example*
Gas in gas	Perfect mixture	Air
Solid in gas	Smoke	Cigarette smoke
Gas in solid	Solid foam	Pumice stone
Liquid in gas	Aerosol	Fog
Gas in liquid	Foam	Shaving foam
	Solution	Sparkling water
Solid in liquid	Solution	Salt water
	Suspension	Milk of magnesia
Liquid in solid	Solid solution	Mercury gold amalgam
	Paste	Clay

Some everyday materials, particularly those that form parts of living systems, go even further and involve combinations of the above types in some incredibly complex mixtures. In the formulations discussed in the following pages the mixtures are relatively simple: solutions, emulsions, suspensions and foams. But just because a mixture is simple in terms of the number of components does not mean it is simple at the molecular level.

The aim in making formulated preparations is to take readily available substances (man-made or natural) to arrive at a preparation that is tailor-made for a specific task, a task that cannot be effectively carried out by a single substance working on its own. This requires a good deal of applied science and much of that is chemistry. In addition to the technical aspects of putting a preparation together there will also have been a study of many of the other aspects that are essential if a preparation is to be a commercial product.

Each of the following all have a role to play: formulation recipe, chemicals information, reactivity considerations, blending method, testing and analysis, stability trials (physical/chemical/microbiological) and shelf-life, health and safety, environment resources and waste, quality control, packaging and container interactions, labelling and user instructions and warnings as to adverse effects.

In all of this there is a big responsibility to ensure the product is fit for its intended purpose. This extends to an awareness of how the chemical blend may interact, physically or chemically, with the materials with which it comes into contact during use.

For example, a cleaning preparation based on ammonia may well have excellent performance on most surfaces but failure to point out that it should not be used on marble surfaces could turn out to be embarrassing, as could the fact that an acid-based metal brightener when in contact

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