Surfactants, soaps, and detergents

Case study # 3
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October 1st, 2010

Materials included in reading package:

1. Manahan, S., E. (2011). *Water chemistry.* CRC Press. Tylor and Francis Group. Boka Taton, FL, US

2. Bunce, N. (1994) *Environmental Chemistry.* 2nd Ed. Wuerz Publishing Ltd. Winnipeg, Canada.

3. *Sodium Laureth sulfate and SLS* (01 April, 2003). National Industrial Chemicals Notification and Assessment Scheme (NICNAS).
http://www.dweckdata.com/Research_files/SLS_compendium.pdf

4. Westgate, T. (17 Aug 2006). *Switchable surfactants give on-demand emulsions*. Royal Society of Chemistry. http://www.rsc.org/chemistryworld/News/2006/August/17080602.asp

5. Matthew, J.S. (3 Aug 2000). *The biodegradation of surfactants in the environment.*

6. J. A. Perales, M. A. *Linear Alkylbenzene Sulphonates: Biodegradability and lsomeric Composition.* Bull. Environ. Contam. Toxicol. (1999) 63:94-100. Springer-Verlag New York Inc.

Further reading:

1. Tadros, T., F (2005). *Applied surfactants: principles and applications.* Wiley-VCH.

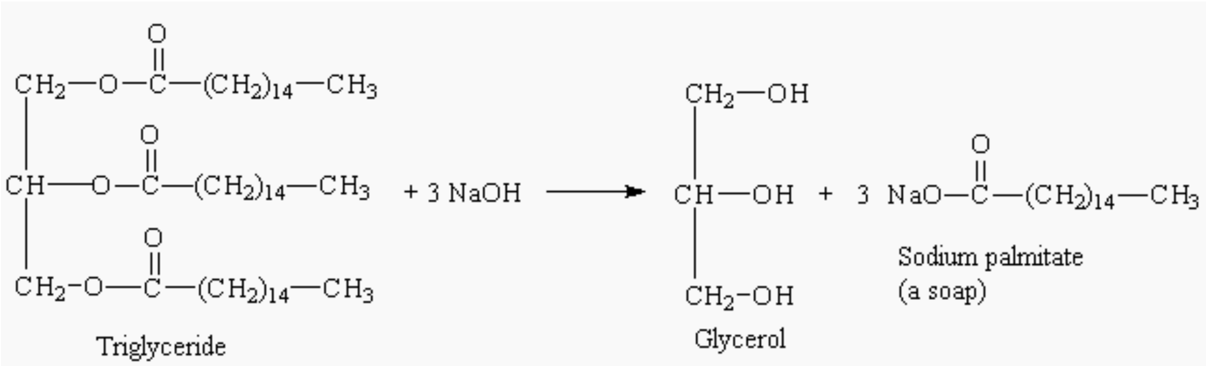
*2.*Cosmetic ingredient review (1983). *Final Report on the Safety Assessment of Sodium Lauryl Sulfte and Ammonium Lauryl Sulfate*. International Journal of Toxicology, Vol 2, No. 7, p. 127-181

3. Y, Liu et. al. (2006). *Switchable surfactants.* Science, Vol 313, p. 958-960

4. Coghlan, A. (17 August 2006). *Oil and water mix and un-mix on demand.*
http://www.newscientist.com/article/dn9781

5. Staples, C., J et. al. (2001). *Ultimate biodegradation of alkylphenol ethoxylate surfactants and their biodegradation intermediates*. Environmental Toxicology and Chemistry, Vol. 20, No. 11, pp. 2450–2455

Saponification – production of natural soap



Cross-section of a micelle

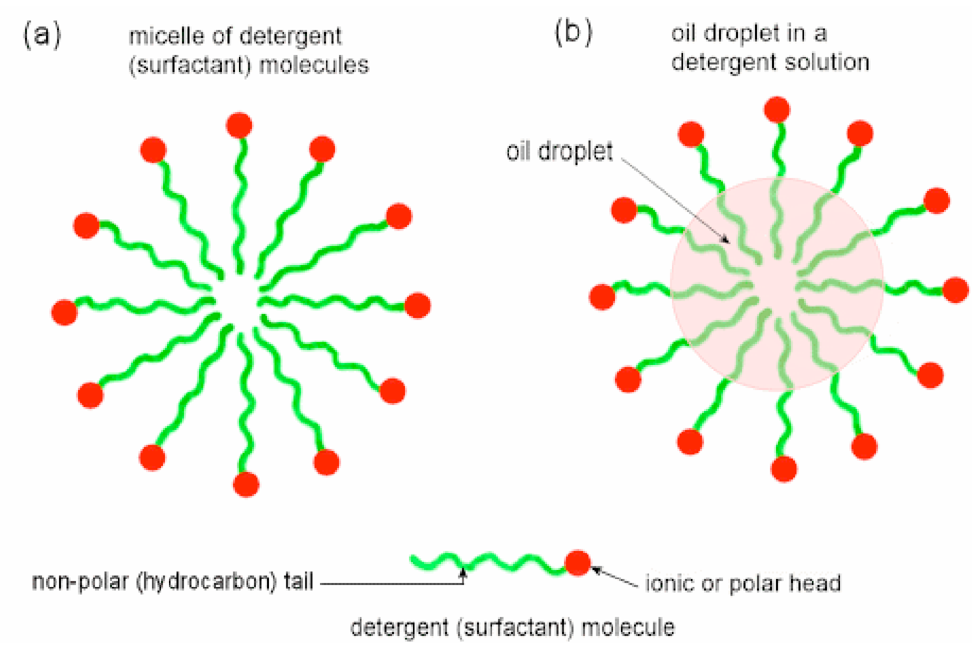
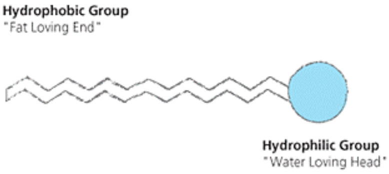
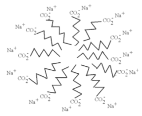
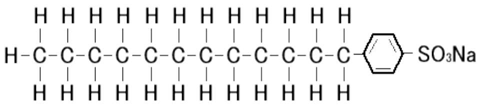
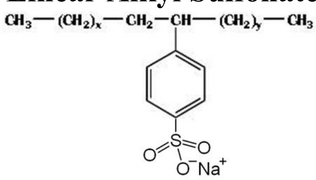
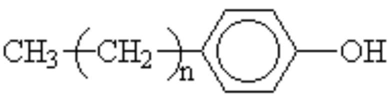
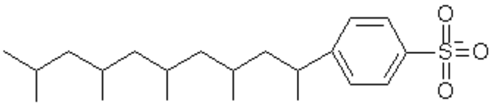
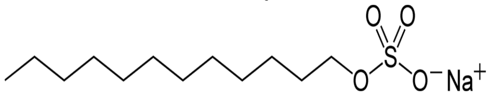


Table 1. Soapy definitions

Surfactant 	= "Surface active agent". A molecule that reduces the surface tension of water. It has a hydrophobic (non-polar, "fat-loving") tail and a hydrophilic (polar, "water-loving)) head. Works as a foaming agent, emulsifier and dispersant.
Micelle 	An aggregate of molecules forming a colloidal particle. Important in the chemistry of surfactants. See Picture on page 1.
Soap 	Mixture of sodium salts with naturally occurring fatty acids (vegetable or animal origin). Produced through base catalyzed ester hydrolysis. Head is a carboxyl group. Conjugate acids are weak acids.
Detergent 	Contain synthetic surfactants, a builder and other additives (i.e. bleach, enzymes, water softeners). Head is a sulfonate group. Conjugate acids are strong acids.
Types of detergents: **1. Cationic** **2. Nonionic** **3. Amphoteric**	1. Ammonium group (NH_4^+), used as anti fouling agent (prevents algae grow, and corrosion) 2. Often have chains of ether groups (can wrap around ion, works as chelator. Proton acceptor. No charge, but is polar. 3. Often used for oil dispersant, expensive.
Saponification	Base catalyzed ester hydrolysis. i.e., convert ester into an alcohol and a metal salt by alkaline hydrolysis (turn fat/oil into soap by reaction with an alkali element).
Builder	Builders help to bind cations in the water, which in terms lets the detergent work more efficiently and eliminates the creation of unwanted precipitate. (DOESN'T FORM PPTE, but prevents it from forming.
LAS – Linear Alkyl Sulfonate 	- An anionic surfactant - Biodegrades
APE – Alkyl Phenol Ethoxylate 	- A non-ionic surfactant - Primary degradation - APEs break down in series of intermediates, such as, ethoxylates, ether carboxylates and alkylphenol groups

ABS – Alkyl Benzene Sulfonate 	- An anionic surfactant - Used until 1960 - Non biodegradable - Foam on weirs and waterfalls on rivers downstream from sewage treatment plants
SLS – Sodium Lauryl Sulfate 	Anionic synthetic surfactant used in many personal care products and detergents for its foaming, emulsifying and dispersing properties.

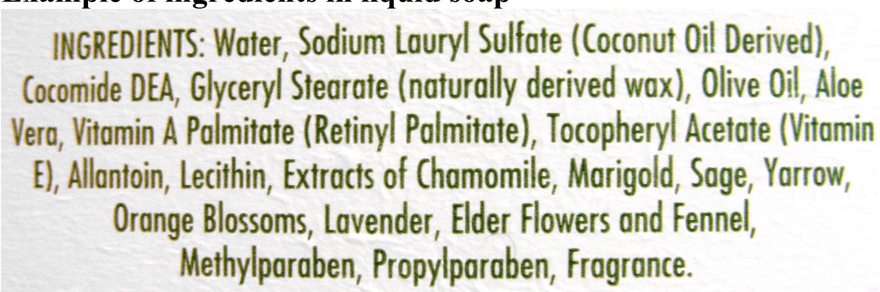
Sodium Lauryl Sulfate – is it safe?

Information circulating around the Internet has raised questions about the safety of SLS (Sodium Lauryl Sulfate). The cosmic ingredient review has fully assessed the safety of this ingredient and found it to be safe. CIR is an independent organization established to thoroughly review and assess the safety of ingredients used in cosmetics in an open, unbiased and expert manner, and to publish the results in the open scientific literature. The organization has a Panel comprised of seven experts in dermatology, pharmacology, chemistry, and toxicology.

SLS is a commonly used cosmetic ingredient that exerts emulsifying action, thereby removing oil and soil from the hair and skin. The Panel wishes to point out that SLS produces eye and/or skin irritation in experimental animals and in some human test subjects; irritation may occur in some users of cosmetic formulations containing the ingredient under consideration. The irritant effects are similar to those produced by other detergents, and the severity of the irritation appears to increase directly with concentration and time of exposure.

Although SLS is not carcinogenic in experimental animals, it has been shown that it causes severe epidermal changes to the area of the skin of mice to which it was applied. This study indicates a need for tumor-enhancing activity assays.

Example of ingredients in liquid soap

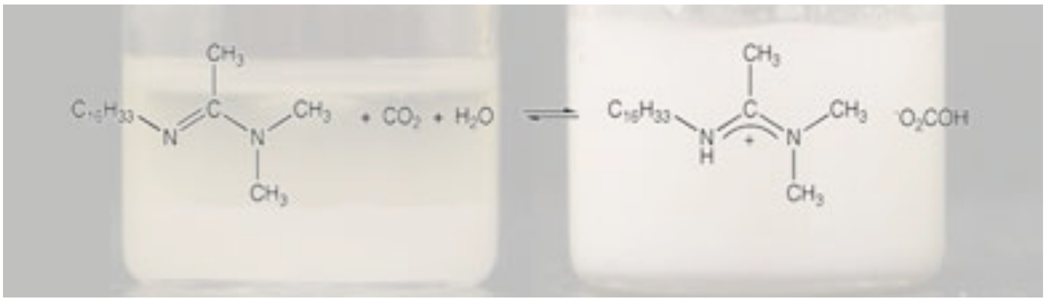


Switchable surfactants give on-demand emulsions

Oil and water can now be mixed or separated simply by bubbling carbon dioxide or air through the blend, thanks to a molecule developed by Canadian chemists.
Dispersions of oil droplets in water are called emulsions, and are used in numerous processes in the chemical industry. In order to prevent the oil and water separating into two layers, the droplets are stabilised by surfactants. These molecules, which usually have a charged end attracted to water and a hydrocarbon chain attracted to oil, self-assemble at the oil-water interface and prevent droplets combining into a distinct phase.

But these emulsions are very stable, so separating the two components again can be a real problem, explains Philip Jessop of Queen's University, Kingston, Canada.
Jessop and his co-workers now think they may have the answer. They have developed a molecule whose surfactant properties can be switched on and off by a simple, reversible reaction, they report in the journal Science.

Hubble bubble
The scientists found that bubbling carbon dioxide through a solution of a neutral amidine molecule made it react to form a positively charged group at one end. Bubbling air through the solution returned the molecule to its original form. Jessop's team successfully used this chemistry to form and break emulsions of the hydrocarbon hexadecane and water.



The switchable surfactant may be useful in the oil industry, said Jessop. High-pressure water and carbon dioxide are often used to pump oil out of oilfields. The presence of natural surfactants in the crude mix means 'there's a good chance you get an emulsion out the other end', Jessop said. If the amidine was added with the carbon dioxide and water, it would be much easier to break up the emulsion to separate oil from the mixture, he predicts.

“We haven't done the tests with real oil in real ground, but we have proved the chemistry does everything we wanted and more” he said. Tests on crude oil mixtures in the lab have shown that the neutral amidine can indeed break up emulsions formed by the natural surfactants.

Surfactant chemist Bernie Binks, of the University of Hull, UK, says that industrial chemists are likely to take an interest in the work. 'It would be nice to see what other chemical structures could possess this behaviour,' he added. Jessop now intends to develop the technique further and plans to make the molecule biodegradable by modifying the chemical structure of the hydrocarbon tail.