Household Chemicals

Soap and Detergent

“Old” way of making soap: Animal fats or vegetable oil + lye

\[
\begin{align*}
\text{Tripalmitin} & : \quad \text{CH}_2\text{O}\text{CCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \\
\text{Sodium hydroxide (lye)} & : \quad 3 \text{NaOH} \\
\text{Sodium palmitate} & : \quad 3 \text{Na}^+\text{O}\text{CCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \\
\text{Glycerol} & : \quad \text{CH}_2\text{OH} \quad \text{CHOH} \quad \text{CH}_2\text{OH}
\end{align*}
\]
How Soap Works

\[ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{Na}^+ \]

Hydrocarbon end
(dissolves in oils)

Ionic end
(dissolves in water)

Hydrophobic

Hydrophilic
How Soap Works
Advantages and Disadvantages of Soap

Relatively non-toxic
From renewable resources
Biodegradable

1. Animal fats or vegetable oil + lye (NaOH): excess NaOH

2. \[
\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{COO}^- \text{Na}^+ + \text{H}^+ \rightarrow
\]

A soap

\[
\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{COOH} + \text{Na}^+
\]

An acid

A fatty acid

3. \[
2 \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{COO}^- + \text{Ca}^{2+} \rightarrow
\]

Soap anion

\[
(\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{COO}^-)_2\text{Ca}^{2+}
\]

Bathtub ring
( insoluble)
Water Softeners

1. Washing soda: \( \text{Na}_2\text{CO}_3 \cdot 10\ \text{H}_2\text{O} \)

\[
\text{CO}_3^{2-} (\text{aq}) + \text{Ca}^{2+} (\text{aq}) \rightarrow \text{CaCO}_3 (\text{s})
\]

Another benefit: Keep water basic:

\[
\text{CO}_3^{2-} (\text{aq}) + \text{H}_2\text{O} (\text{l}) \rightarrow \text{HCO}_3^{-} (\text{aq}) + \text{OH}^{-} (\text{aq})
\]

2. \( \text{Na}_3\text{PO}_4 \)

\[
2\ \text{PO}_4^{3-} (\text{aq}) + 3\ \text{Ca}^{2+} (\text{aq}) \rightarrow \text{Ca}_3(\text{PO}_4)_2 (\text{s})
\]

Another benefit: Keep water basic:

\[
\text{PO}_4^{3-} (\text{aq}) + \text{H}_2\text{O} (\text{l}) \rightarrow \text{HPO}_4^{2-} (\text{aq}) + \text{OH}^{-} (\text{aq})
\]
Water Softening by Ion Exchange
**Synthetic Detergents**

\[
\begin{align*}
\text{CH}_3\text{CHCH}_2\text{CHCH}_2\text{CHCH}_2\text{CH}_3 + \text{SO}_3^- \text{Na}^+ \\
\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{SO}_3^- \text{Na}^+ \\
\end{align*}
\]

An ABS detergent (Alkylbenzenesulfonate)

An LAS detergent (Linear alkyl sulfonate)
Typical Detergent Components

**INGREDIENTS:** Cleaning agents (anionic and nonionic surfactants), buffering agent, brightening agent, perfume and colorant. Ultra “all” with Double Bleaching Action contains no phosphorus or chlorine bleach. The surfactants in Ultra “all” with Double Bleaching Action are biodegradable and safe for septic tanks. “all” bottles contain 25% or more post-consumer recycled plastic.
Surfactants

Anionic surfactants: so far the best (~65%)
Nonionic surfactants: best for cold water (more soluble) (~25%)
Cationic surfactants: may kill germs
Builders

Builders: any substance added to a surfactant to increase its detergency (~ softeners)

Na₅P₃O₁₀: banned in some states

Na₂CO₃: common

Zeolites: complex aluminosilicates most promising

\[ \text{Na}_2\text{Al}_2\text{Si}_2\text{O}_8 \text{ (s)} + \text{Ca}^{2+} \text{ (aq)} \rightarrow \text{CaAl}_2\text{Si}_2\text{O}_8 \text{ (s)} + 2 \text{Na}^+ \text{ (aq)} \]

Certain cationic complexes:

\[
\begin{align*}
\text{CH}_3\text{(CH}_2\text{)}_{14}\text{CH}_2\text{--N}^+\text{--CH}_3 \\
\text{Hexadecyltrimethylammonium chloride (a cationic surfactant)}
\end{align*}
\]

\[
\begin{align*}
\text{CH}_3\text{(CH}_2\text{)}_{16}\text{CH}_2\text{--N}^+\text{--CH}_3 \\
\text{Dioctadecyldimethylammonium chloride (fabric softener)}
\end{align*}
\]
Water Softeners

1. Washing soda: $\text{Na}_2\text{CO}_3 \cdot 10 \text{H}_2\text{O}$

   $\text{CO}_3^{2-} \text{(aq)} + \text{Ca}^{2+} \text{(aq)} \rightarrow \text{CaCO}_3 \text{(s)}$

   Another benefit: Keep water basic:

   $\text{CO}_3^{2-} \text{(aq)} + \text{H}_2\text{O} \text{(l)} \rightarrow \text{HCO}_3^{-} \text{(aq)} + \text{OH}^{-} \text{(aq)}$

2. $\text{Na}_3\text{PO}_4$

   $2 \text{PO}_4^{3-} \text{(aq)} + 3 \text{Ca}^{2+} \text{(aq)} \rightarrow \text{Ca}_3(\text{PO}_4)_2 \text{(s)}$

   Another benefit: Keep water basic:

   $\text{PO}_4^{3-} \text{(aq)} + \text{H}_2\text{O} \text{(l)} \rightarrow \text{HPO}_4^{2-} \text{(aq)} + \text{OH}^{-} \text{(aq)}$
Brighteners

Blancophor R

Visible light
Ultraviolet light
Visible light
Blue light
Optical brightener
Optical brightener
Fabric
Others in Detergents

- **Bleach**
  - Classic bleach
  - Slow-chlorine releasing bleach
  - Oxygen-releasing bleach

- **Enzymes**

- **Perfumes**

- **Colorants**
1. Classic bleach:
   sodium hypochlorite, NaOCl, in solution
calcium hypochlorite, Ca(OCl)$_2$, in powder

effective, cheap, but rapidly release chlorine that may damages fabric

2. Slow chlorine releasing bleach:
symclosene

3. Oxygen releasing bleach:
   powder: sodium perborate: NaBO$_2$ $\cdot$ H$_2$O$_2$
sodium percarbonate: NaCO$_2$ $\cdot$ H$_2$O$_2$
liquid: hydrogen peroxide: H$_2$O$_2$

Requires higher temperature, higher alkalinity and higher concentration.
Powdered Oxygen
Releasing Bleach

**Sodium percarbonate:** \( \text{NaCO}_2 \cdot \text{H}_2\text{O}_2 \)
- has the highest solubility in water, used mostly in deck, carpet, household and laundry cleaning products

**Sodium perborate:** \( \text{NaBO}_2 \cdot \text{H}_2\text{O}_2 \)
- more storage stable in detergent formulations, used mostly in automatic dishwashing and laundry products as a hot water bleaching agent

**Advantages:**
- Little damage to fabric
- Longer shelf-life than liquid \( \text{H}_2\text{O}_2 \)
- Acts as a disinfectants
- can be mixed or used with other household cleaners
- Non-toxic to animals, plants and humans.
- Environmentally friendly

**Disadvantages:**
- Costs more
- Takes time to dissolve in water
- Takes longer to work
- Not suited for some finer grades of silk or wool

http://oxygenbleach.homestead.com
Powdered Oxygen Releasing Bleach

Ultra-Concentrated Oxygen Bleaches:
80-100% of oxygen

Concentrated Oxygen Bleaches:
40-70% of oxygen

Oxygen bleaches with additives and other cleaning agents:
20-40% of oxygen

Cleaning products that contain oxygen bleach as an ingredient:
< 25% of oxygen

http://oxygenbleach.homestead.com
1. Proteases: used most often
specialty detergent enzymes that hydrolyse proteins and break down them into soluble polypeptides or free amino acids. Such enzymes effectively removes protein stains like blood, sweat etc.

2. Lipases:
lipolytic enzymes capable of removing fatty stains like lipstick, frying fats, butter sauces and tough stains from collars and cuffs

3. Amylase:
starch hydrolysing enzymes used to remove residues of starchy foods like spagetti, mashed potato, gravies and chocolate. Liquid bioamylases can be used in dishwashing formulations for effective results..

4. Cellulase:
complex cellulase enzymes which effectively handle particulate and dirt stains. Imparts brightness, sheen and softness to the fabric

Cosmetics: articles intended to be rubbed, poured, sprinkled, or sprayed on, introduced into, or otherwise applied to the human body or any part thereof, for cleansing, beautifying, promoting attractiveness or alternating the appearance....

- Soap
- Toothpaste
- Lipsticks
- Vaseline (petroleum jelly)
- Antidandruff Shampoo

Drugs: must be proven to be safe and effective

Cosmetics: not necessary
Keratin: fibrous protein; moisture content: 10%
Melanocyte: produces melanin (tan) or melanoma (skin cancer)
Skin Care

Moisturizers: lanolin

UV-protection: sun screen

Ultraviolet rays result in melanin formation (a SLOW process)

UVA (320 to 400 nm): causes tanning and some damage
UVB (280 to 320 nm): causes damage in the form of sunburn
UVC (< 280 nm): filtered out by the atmosphere

SPF: skin protection factor: SPF of 30 = one can stay in the sun without burning 30 times as long as one could with unprotected skin (rated only for UVB protection)

http://travel.howstuffworks.com/sunscreens1.htm
Sunblocks

UVB protections:
- PABA (para-Aminobenzoic Acid) & Derivatives: Used extensively in the 1950's and 1960's, no longer a common ingredient in sunscreens
- Salicylates: Used mostly in waterproof sunblocks
- Cinnamates: not waterproof

UVA protections: Benzophenones, Dibenzoylmethanes

Physical Blockers: ZnO and TiO₂

http://www.sunscreens.net/
# Sunblocks

## Suggested SPF

<table>
<thead>
<tr>
<th>Type</th>
<th>Characteristics</th>
<th>Routine day</th>
<th>Outdoor Activity</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>Always burns easily, never tans</td>
<td>15</td>
<td>25-30</td>
</tr>
<tr>
<td>II</td>
<td>Burns easily, tans slightly</td>
<td>12-15</td>
<td>25-30</td>
</tr>
<tr>
<td>III</td>
<td>Sometimes burns, tans gradually and moderately</td>
<td>8-10</td>
<td>15</td>
</tr>
<tr>
<td>IV</td>
<td>Burns minimally, always tans well</td>
<td>6-8</td>
<td>15</td>
</tr>
<tr>
<td>V</td>
<td>Burns rarely, tans deeply</td>
<td>6-8</td>
<td>15</td>
</tr>
<tr>
<td>VI</td>
<td>Almost never burns, deeply pigmented</td>
<td>6-8</td>
<td>15</td>
</tr>
</tbody>
</table>

[http://www.sunscreens.net/](http://www.sunscreens.net/)
# Toothpaste

## Table 17.2  ■ A Typical Recipe for Toothpaste

<table>
<thead>
<tr>
<th>Ingredient</th>
<th>Function</th>
<th>Amount</th>
</tr>
</thead>
<tbody>
<tr>
<td>Precipitated calcium carbonate</td>
<td>Abrasive</td>
<td>46 g</td>
</tr>
<tr>
<td>Castile soap or sodium dodecyl sulfate</td>
<td>Detergent</td>
<td>4 g</td>
</tr>
<tr>
<td>Glycerol (glycerin)</td>
<td>Sweetener</td>
<td>20 g</td>
</tr>
<tr>
<td>Gum tragacanth or gum cellulose</td>
<td>Thickener</td>
<td>1 g</td>
</tr>
<tr>
<td>Oil of peppermint (or peppermint extract)</td>
<td>Flavoring</td>
<td>1 mL</td>
</tr>
<tr>
<td>Water</td>
<td>—</td>
<td>28 mL</td>
</tr>
</tbody>
</table>

CH₃CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH₂CH₂OSO₃⁻Na⁺

## Table 17.1  ■ Abrasives Commonly Used in Toothpaste

<table>
<thead>
<tr>
<th>Name</th>
<th>Chemical Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Precipitated calcium carbonate</td>
<td>CaCO₃</td>
</tr>
<tr>
<td>Insoluble sodium metaphosphate</td>
<td>(NaPO₃)ₙ</td>
</tr>
<tr>
<td>Calcium hydrogen phosphate</td>
<td>CaH₂PO₄</td>
</tr>
<tr>
<td>Titanium dioxide</td>
<td>TiO₂</td>
</tr>
<tr>
<td>Tricalcium phosphate</td>
<td>Ca₃(PO₄)₂</td>
</tr>
<tr>
<td>Calcium pyrophosphate</td>
<td>Ca₂P₂O₇</td>
</tr>
<tr>
<td>Hydrated alumina</td>
<td>Al₂O₃·nH₂O</td>
</tr>
<tr>
<td>Hydrated silica</td>
<td>SiO₂·nH₂O</td>
</tr>
</tbody>
</table>
Toothpaste

Fluoride:
- SnF$_2$ (+ calcium pyrophosphate): early use, but few used now
- NaF (+ hydrated silica abrasive): leading
- Na(FPO$_4$)$_2$ (sodium monofluorophosphate (MFP)): fair amount of use

Sugars to dextrans (Plaque) and to acids (lactic acid)

\[
(Ca_5(PO_4)_3OH + F^- \rightarrow Ca_5(PO_4)_3F
\]
Hydroxyapatite fluorapatite

- Fluoride concentrates in the growing bones and developing teeth of children, helping to harden the enamel on baby and adult teeth before they emerge;
- Fluoride helps to harden the enamel on adult teeth that have already emerged

Mike McCoy, C&E News, 79 (16) 42 (April 16, 2001)
http://www.colgate.com