# Formulated Product Industry

# Examples

- Food and Beverage Products
- Cleaning Products
- Pharmaceuticals and Healthcare products
- Coatings (and inks), Adhesives, Sealants and Elastomers (CASE)
- Personal Care Products/Cosmetics
- Lubricants (and many Transportation Fuels)
- Pesticides and Agrichemicals
- Composites
- (Can include concrete and ceramics although not typically considered)
- A range of specialised products
- Many other products contain formulated components *e.g.* batteries

**The value of formulated products industries is in excess of USD1.5 trillion**

**Value-Multiplier in the range of 3 to several hundred times the raw material cost**

# What is a Formulated Product?

**BASIC:**
**"a mixture prepared according to a specific formula for a specific purpose"**

**TECHNICAL:**
**"multi-component (commonly multi-phase) mixture used as a delivery vehicle which enables a specific function to be performed"**

- Typically the end result is a tablet, solution, gel or dispersion *e.g.* cream, lotion, paint
- Can involve chemical reactions and phase changes
- Heavy on the D in R&D
- Can and often does involve the R where existing technology is insufficient for the function being performed *e.g.*
    - New pharmaceutical excipients
    - New pigments (CASE industries)
    - New polymers (used in all previous examples)

# Formulation Science

**Multidisciplinary**

- Chemistry is integral to all formulated products
  - Design and Development
  - Synthesis
  - Production/Manufacturing
  - Quality
  - Testing and Analysis
- Computer modelling and statistics (and more recently machine learning)
- Physics
- Engineering
- Depending on the formulation, other disciplines become important *e.g.* biochemistry

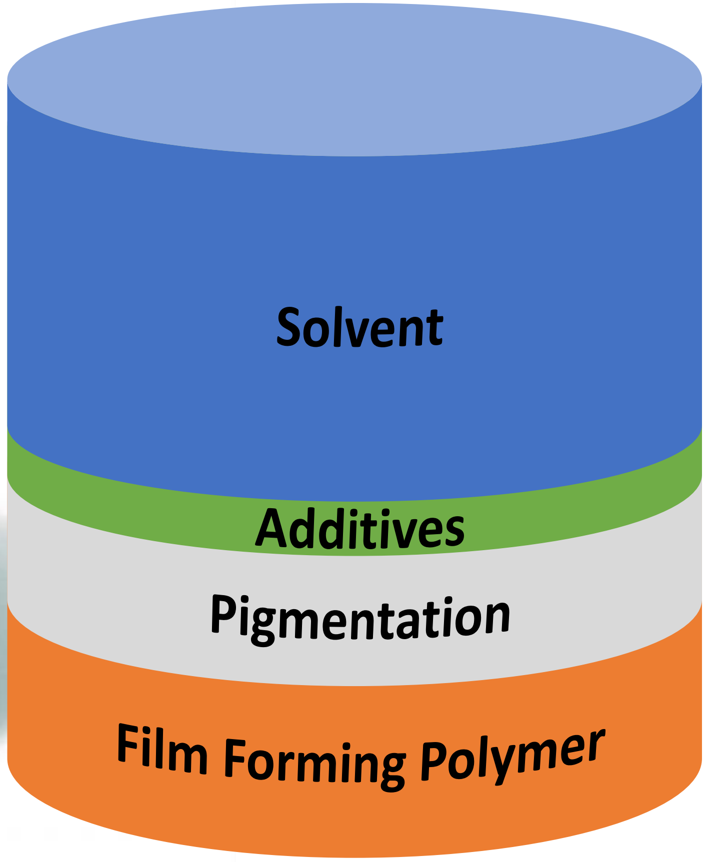
# Coatings

**Three general classes:**

- Delivered as solid
- Delivered as liquid
- Delivered as vapour/gas

**Resene produce liquid-applied coatings**

# What's in a can of paint?


**Organic Solvent or Water**
(hydrocarbon, ester, amide, glycol ether, alcohol….)

**Additives**
- Rheology modifiers
- Surfactant
- Dispersant
- Defoamer/antifoam
- Biocides
- *p*H control

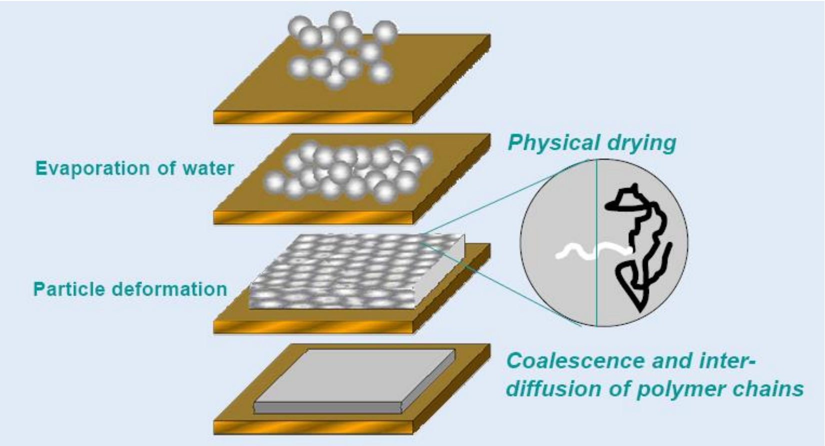
**Pigmentation**
- Titanium dioxide
- Phthalocyanines, azo and aromatic heterocyclic types
- Metal oxides
- Carbon black

**Polymer**
- Acrylic
- Polyester/alkyd
- Epoxy-amine
- Polyurethane

# Liquid-to-Solid (Film Formation)

**Two primary types:**

- Solution-based (commonly uses organic solvent soluble polymer)
  - Film formed slowly as solvent evaporates (shrinkage) and solid components are forced together – polymer is effectively precipitated
  - Other components *e.g.* pigments are trapped in the polymer matrix
- Dispersion-based (commonly uses aqueous polymer dispersion)
  - Film formation is more complex and requires deformable polymer particles to interdiffuse (only a few nanometres required) with neighbours (coalescence)
  - Other components *e.g.* pigments are trapped in the polymer matrix




- $T_g$ is important as it partly define the temperature at which sufficient deformation is possible
- Hydroplasticisation reduces film formation temperature
- Plasticisers can also be used to reduce film formation temperature (permanent or temporary)

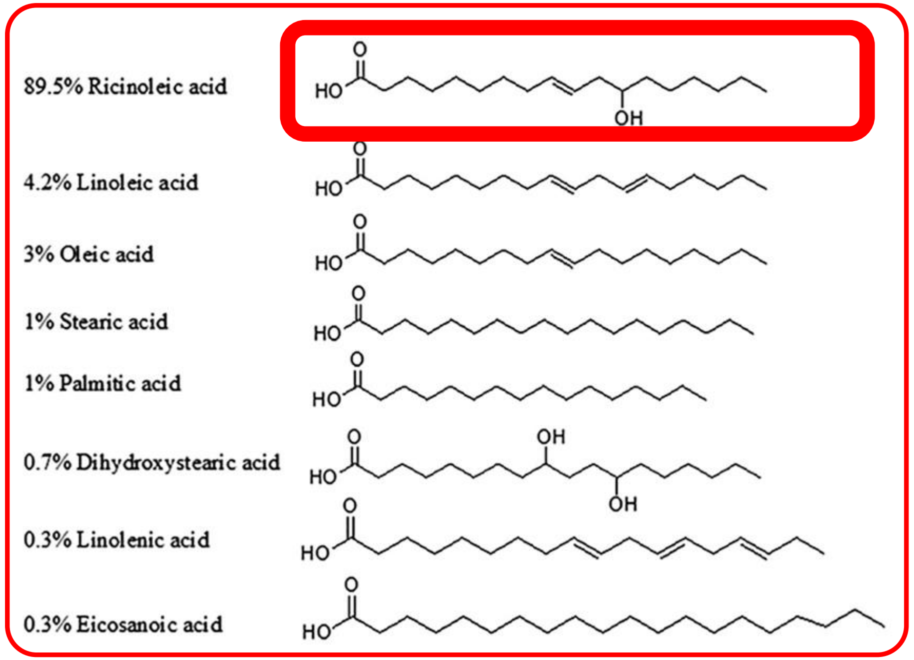
## Organics (AS91391 – C3.5)

- Organic compounds are limited to those containing one or more of the following functional groups: alkene, halo alkane, amine, alcohol, aldehyde, ketone, carboxylic acid, ester (including triglycerides), acyl chloride, and amide.
- Structure includes functional groups and isomerism (constitutional isomers and stereoisomers).

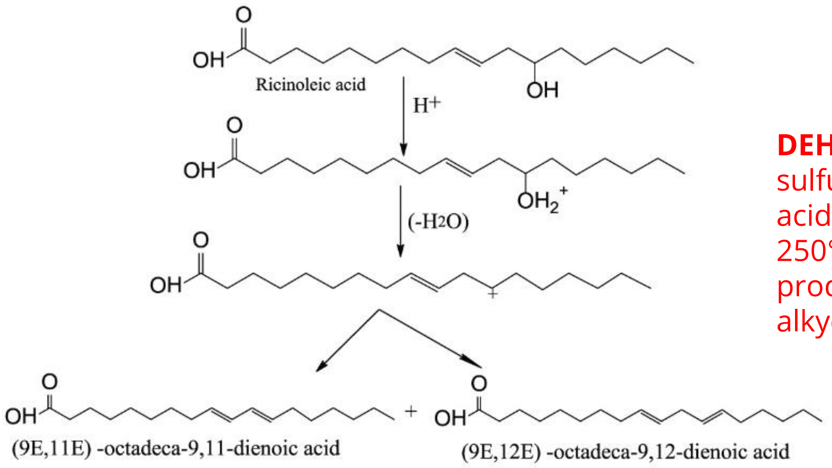
- Substitution reactions using the following reagents: concentrated HCl, HBr, $SOCl_2$, NaOH, KOH (in alcohol or aqueous solution), concentrated NH3, primary amines, primary alcohols/$H^+$, $H_2O/H^+$, $H_2O/OH^-$ (Substitution reactions include esterification, condensation, hydrolysis, and polymerisation.)
- elimination reactions using the following reagents: KOH in alcohol and concentrated $H_2SO_4$ (includes major and minor products from asymmetric alcohols and halo alkanes)
- polymerisation reactions involving formation of polyesters and polyamides including proteins

- **Alkyd polymers and the raw materials used in their production are good examples from the coatings industry**
- **The use of castor oil is particularly good since it touches many aspects relevant to the syllabus**

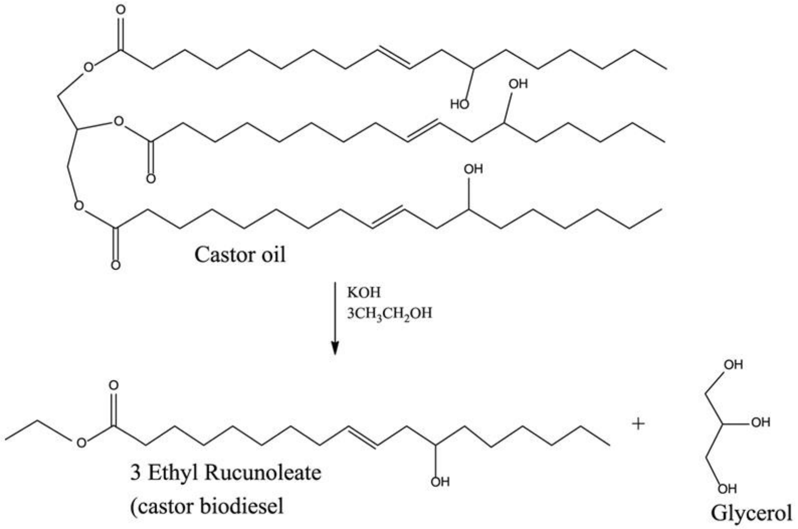
# Castor Oil



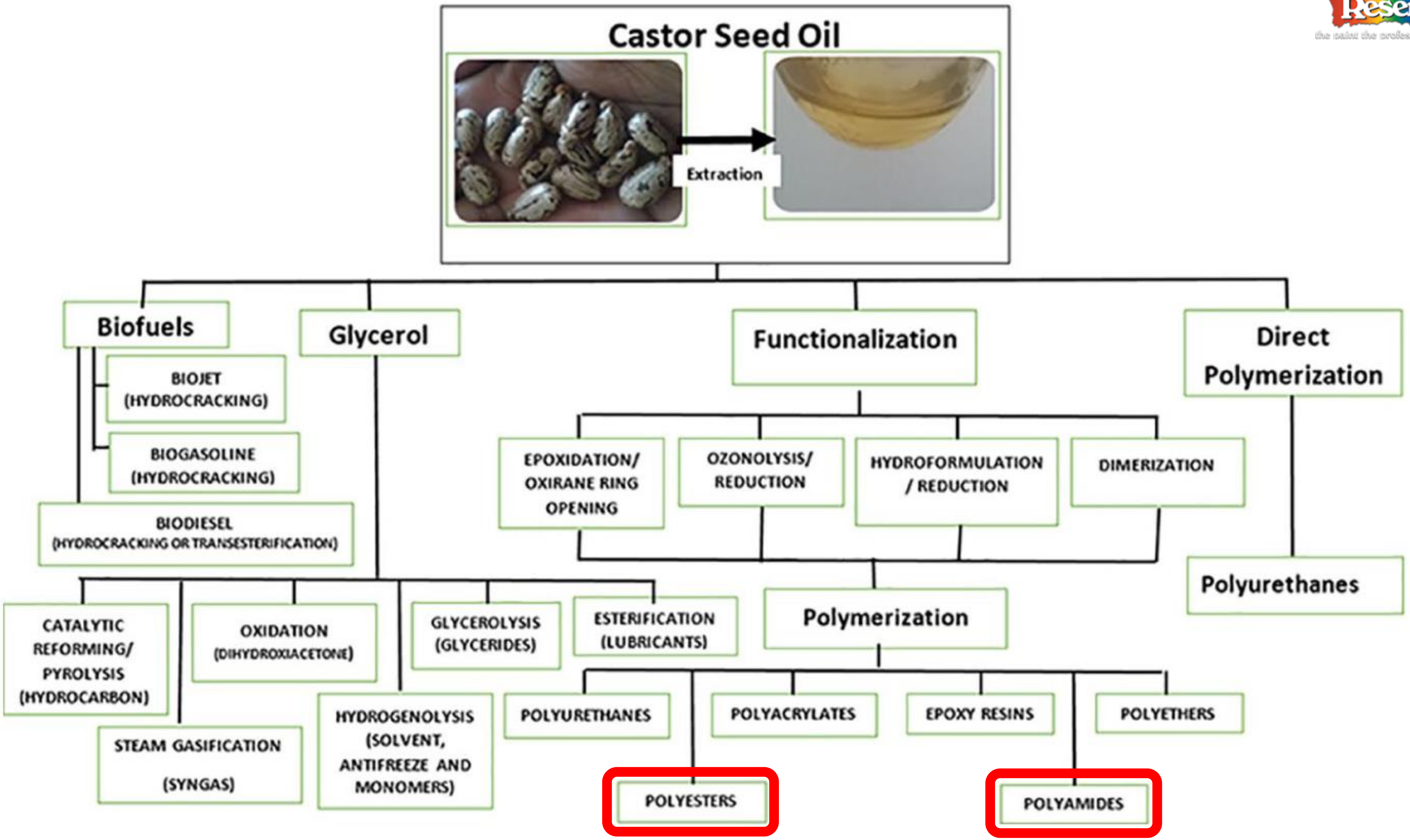

- A lot of renewed interest in bio-based feedstocks for various technical uses including polymers
- The ricinoleic acid component of castor oil can take part in useful chemistry and has a lot of industrial uses




**DEHYDRATION (elimination)**
sulfuric acid or phosphoric acid catalyst at approximately 250°C under vacuum. The product is used to prepare alkyd polymers



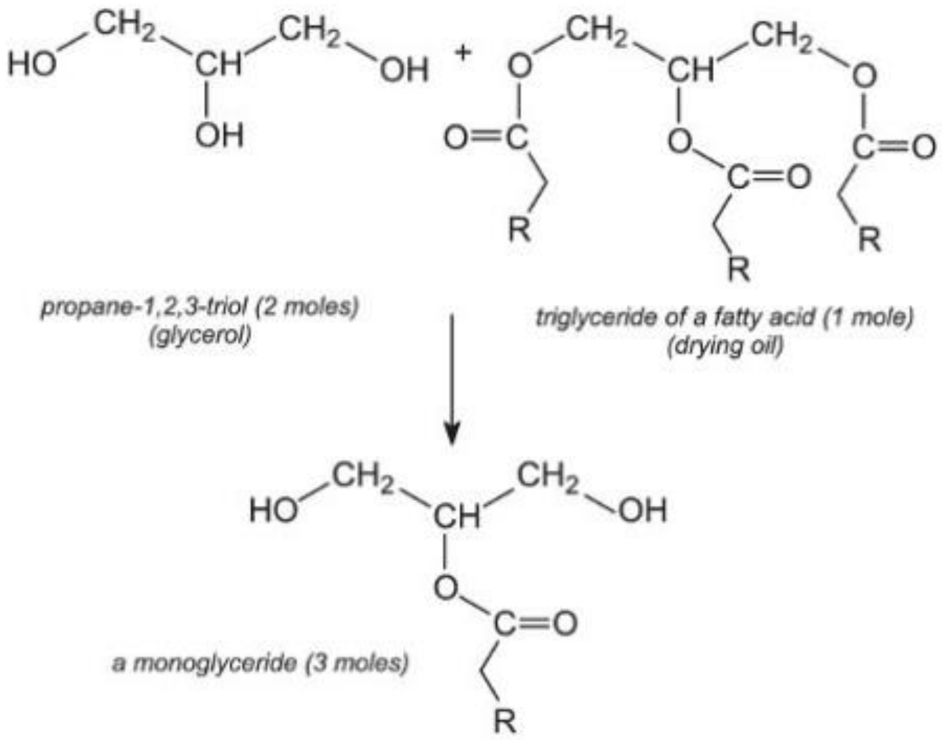

**TRANSESTERIFICATION**
Commonly potassium hydroxide and a low molecular weight alcohol.
Uses as fuels and lubricants

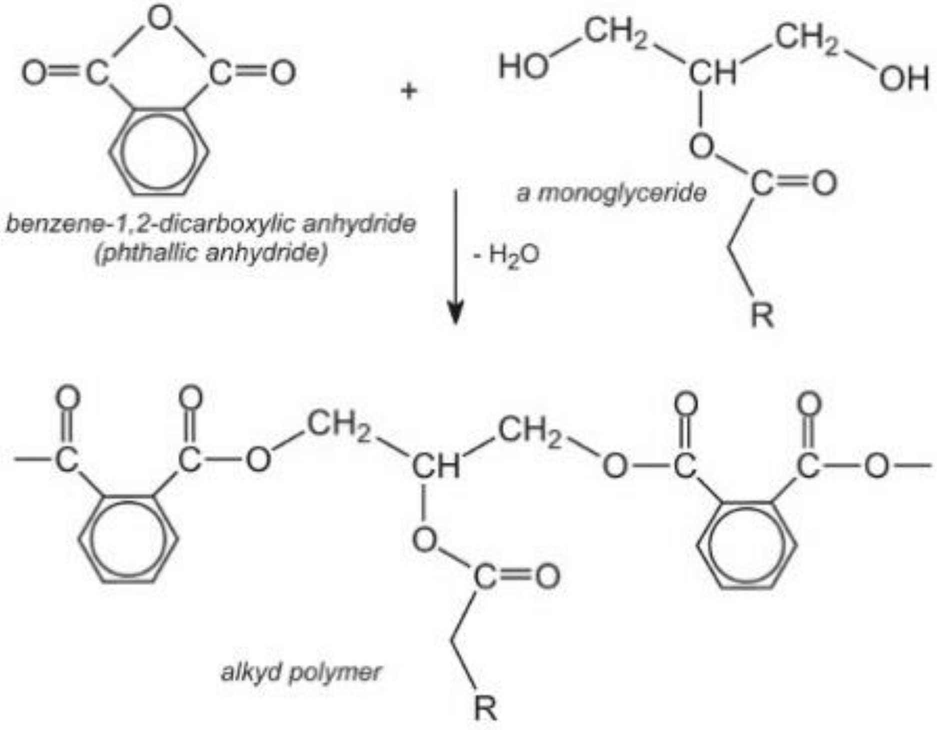



Resene
the paint the professionals use

# Alkyd

## (name derived from **Al**cohol + A**cid**)




Linoleic rich oils are commonly used

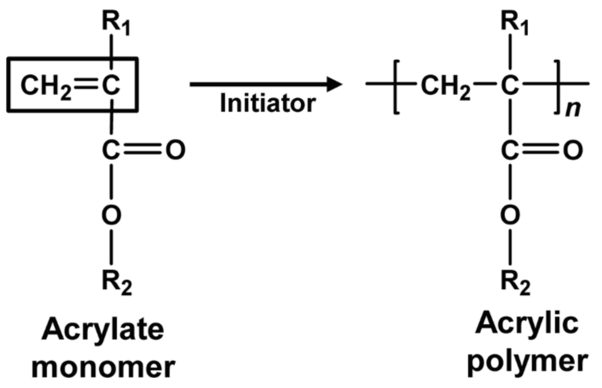

Catalysts (Co, Mn, Fe, V salts) required to accelerate film formation (hydroperoxide formation)

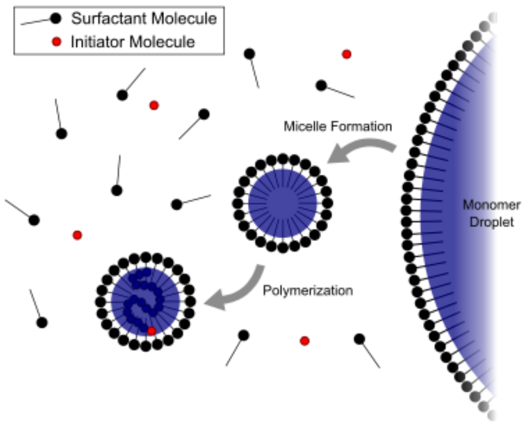
## Aqueous (AS91391 – C3.6)

- Sparingly soluble ionic solids are limited to AB, $A_2B$ and $AB_2$ types where neither of the ions A nor B reacts further with water.
- **Barium sulfate (and calcium carbonate although this doesn't quite fit the requirement) are common components of coatings**
- **Low water solubility and low cost are the desirable features**
- **Used for bulking formulations, increasing hardness, decreasing surface reflectivity (particle size effect) while maintaining transparency (refractive index is very similar to typical polymers)**

## Redox Chemistry

- Oxidation-reduction processes involve the use of the relative strengths of oxidants and reductants.
- **Redox systems are common in aqueous acrylic ester polymerisation – latex products used in coatings and adhesives as examples**
- **Peroxides and persulfates as oxidisers paired with ascorbic acid, sodium formaldehyde sulfoxylate or sodium sulfite/metabisulfite to generate free radicals (polymerisation initiators)**




- Radical process – peroxide or persulfate initiator, iron catalyst common
- Approx. 13 million tons p.a. acrylic emulsion production
- USD 35 billion p.a. global market

## Chemical processes in the world around us

- Links between chemical processes and the consequences of the chemical processes for the environment or people (e.g. ozone depletion, greenhouse effect, acidification of oceans, acid rain or pollution)

- **Many industrial coating processes releases organic solvent (VOC's) to the atmosphere**
- **Photochemical smog formation is one consequence**

- Chemistry involved in the development of new technology to meet a societal need (e.g. polymers, energy production, pharmaceutical or food production)

- **The chemistry in coatings, including in-situ reactive chemistry such as formation of epoxy and polyurethane polymers, are responsible for protection of vital infrastructure, buildings and vehicles against environmental damage and corrosion – direct link to improved sustainability**