CHEMISTRY & ISOLATION TECHNIQUES OF ESSENTIAL OILS

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Course name: **AROMATHERAPY**

Grade 4- Spring Semester 2023-2024

Course code: **PHAR 429**

Week 3 & 4

Essential oils

- ✓Volatile oils are fragrant compounds derived from both plant and animal origins. *They possess the unique characteristic of evaporating upon exposure to air at ordinary temperature and are hence known as volatile or ethereal oils.*
- ✓*These represent the essence of active constituents of the plant and hence are also known as essential oils.*

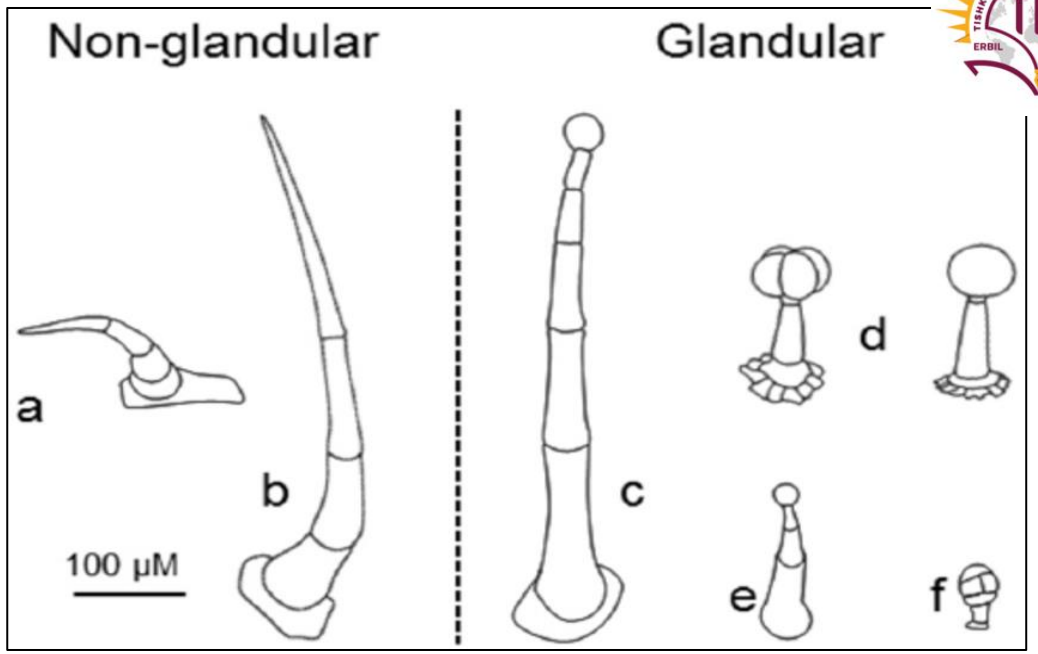
- The presence of volatile oils is important in various biological processes such as ***pollination, defense mechanisms, and communication with other organisms.***
- These oils play a crucial role in the ecology and physiology of plants and have been utilized by humans for medicinal, culinary, and aromatic applications.

- ***Schizogenous glands*** are specialized structures found in plants that produce essential oils. These glands are characterized by the formation of cavities or sacs within plant tissues, which contain volatile compounds. When these cavities rupture or release their contents, the essential oils are released into the surrounding environment.
- On the other hand, ***lysigenous glands, or schizolysigenous*** glands, are a subtype of schizogenous glands.

Storage

- These oils are often stored in specialized structures within plants, such as secretory cells, glandular trichomes, oil ducts, or resin ducts.
- **Secretory Cells:** Some plants contain secretory cells that produce and store volatile oils. These cells are often located in specific plant organs such as leaves, flowers, stems, or roots. Within these cells, biosynthetic pathways produce the volatile compounds, which are then accumulated and stored until needed.

- **Glandular Trichomes:** Many plants have glandular trichomes, which are *hair-like structures* found on the surface of leaves, stems, and other plant parts. These trichomes can secrete volatile oils directly onto the plant's surface, where they serve various functions such as attracting pollinators or deterring herbivores.



- **Oil Ducts:** Some plants have specialized ducts or channels that transport and store volatile oils. These oil ducts are often found in plant tissues such as the bark, leaves, or fruits. They can act as reservoirs for storing these volatile compounds.

- **Resin Ducts:** Certain plants produce resin ducts, which contain resinous substances along with volatile oils. These ducts are typically found in coniferous trees and other resinous plants.
- The volatile oils stored within resin ducts contribute to the characteristic scent of the resin and may also serve protective functions against pests and pathogens.

Physical and Chemical Properties

- These are chemically derived from terpenes (mainly mono and sesquiterpenes) and their oxygenated derivatives. These are made up of **isoprene units (C_5H_8)** and are usually, mono, sesqui, and diterpenes with empirical formulae as $C_{10}H_{16}$, $C_{15}H_{24,}$ and $C_{20}H_{32}$ respectively.
- These are soluble in alcohol and other organic solvents, practically insoluble in water,
- Lighter than water (except **Clove oil heavier**),
- Possess characteristic odor, have high refraction index, and most of them are optically active.
- Volatile oils are colorless liquids, but when exposed to air and direct sunlight these become **darker due to oxidation**. Unlike fixed oils, volatile oils neither leave permanent grease spots on filter paper nor are saponified with alkalis.

Clove oil has a specific gravity greater than 1, making it heavier than water. This means that if you were to pour clove oil and water into a container, the clove oil would sink to the bottom while the water would float on top.

➢ Pharmaceutical/ medicinal uses of volatile oils

- Volatile oils are used as **perfuming agents** in pharmaceutical **formulations, food, beverages and cosmetics.**
- These are also used as important medicinal agent for therapeutic purposes like:
  1. *Carminative*: e.g. Umbilliferous fruits (Coriander, fennel, dill etc)
  2. *Anthelminitic*: e.g. Chenopodium oil
  3. *Diuretics*: e.g. Juniper
  4. *Antiseptic*: e.g. Eucalyptus

5. *Counter irritant*: e.g. Oil of winter green
6. *Local anesthetic*: e.g. Clove
7. *Sedative*: e.g. Jatamansi
8. *Local irritant*: e.g. Turpentine
9. *Insect repellant*: e.g. Citronella
10. *Source of vitamin A*: e.g. Lemon grass

Classification of volatile oils: Volatile oils are classified on the basis of functional groups present

Groups	Examples of compounds	Drugs/ Plants
Hydrocarbons	Acyclic monoterpene: e.g. Myrecene Monocyclic monoterpene: e.g. Limonene, α and β-phellandrene, α-terpinene etc. Bicyclic monoterpene: e.g. α and β-pinene Sesquiterpenes: e.g. Zingiberene and Caryophyllene	Turpentine oil
Alcohols	Acyclic terpenes: e.g. Geraniol, Coriandrol etc. Cyclic terpenes: e.g. Menthol and borneol Sesquiterpenes: e.g. Santalol and Gingerol	Coriander Mentha and camphor Chandan and Ginger
Aldehydes	Acyclic: e.g. Citral, Geranial, Citronellal etc Cyclic: Cinnamicaldehyde, Cumin aldehyde, Safranal	Cymbopogon sp., Lemon Cinnamon, Cumin and Safron

Ketones	Monoterpene ketone (Monocyclic): e.g. Menthone, Carvone, Peperitone and Pulegone etc Diterpene ketone (Bicyclic): e.g. Camphor, Thujone and Jatamansone	Mentha, Caraway Spearmint and Dill Camphor, Jatamanshi
Oxides	Cineol and Ascaridol	Eucalyptus, Cardamom and Chenopodium oil
Phenolics	Eugenol, Thymol and Carvacrol	Clove and Thyme
Phenolic ethers	Anethol, Safrol, Myresticin and Dillapiol	Fennel, Anise, Nutmeg, Dill
Esters	Borneol acetate, Terpeneol acetate and Geraniol acetate Methyl salicylate Pyrethrines and Jasmolines	Common Oil of wintergreen Valerian Pyrethrum

Terpenoids

- Terpenoids are hydrocarbons of plant origin of the general formula $(C_5H_8)_n$ as well as their oxygenated, hydrogenated and dehydrogenated derivatives.
- Terpenoids are abundantly available in volatile oils. They consist of a complex mixture of terpenes or sesquiterpenes, alcohols, aldehyde, ketones, acids and esters. E.g. Menthol, Citral, Eugenol, Citronellol Geraniol, Limonene, etc.

Classification of Terpenoids

S. No.	Name of the class of terpenoids	No. of Isoprene units	Molecular formula	Examples
1	Monoterpenes	2	$C_{10}H_{16}$	Limonene, Pinenes, Myrcene
2	Sesquiterpenes	3	$C_{15}H_{24}$	β-Caryophyllene, Humulene, Germacrene D
3	Diterpenes	4	$C_{20}H_{32}$	Taxus, Carnosic Acid
4	Triterpenes	6	$C_{30}H_{48}$	Ursolic Acid, Oleanolic Acid, Glycyrrhizin
5	Tetraterpenes	8	$C_{40}H_{64}$	β-Carotene, Lycopene, Lutein
6	Polyterpenes	n	$(C_5H_8)_n$	Rubber, Gutta-percha, Rosin

Extraction of volatile oil

- **Solvent Extraction** This is the most used and economically important technique.
- Raw materials are submerged in a solvent that can dissolve the desired aromatic compounds. Fragrant compounds from woody and fibrous plant materials are often obtained in this manner.
- The technique can also be used to extract odorants that are too volatile for distillation or easily denatured by heat.
- Commonly used solvents for maceration/solvent extraction include **hexane** and **dimethyl ether**. The product of this process is called a "concrete”

Solvent Extraction

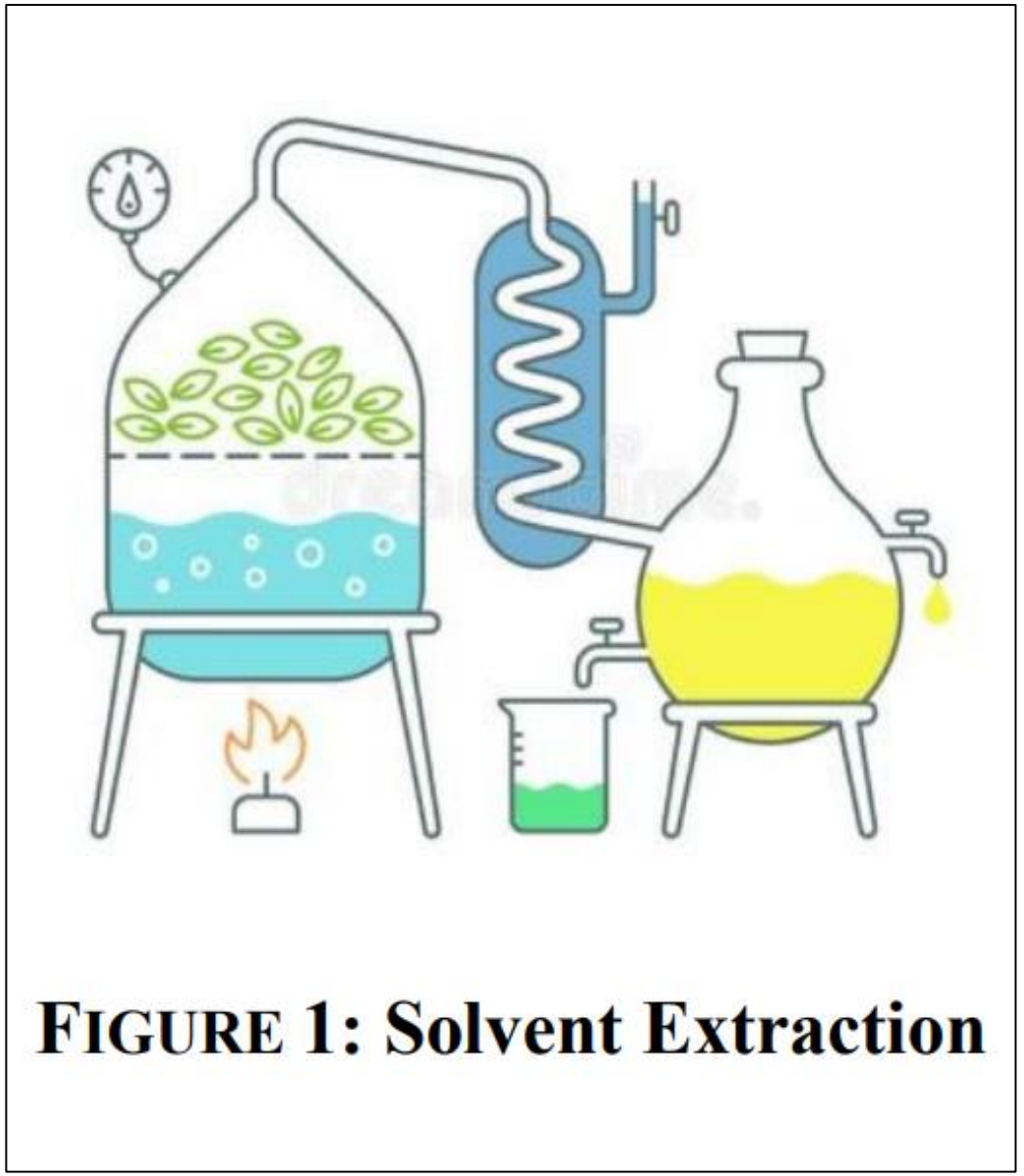
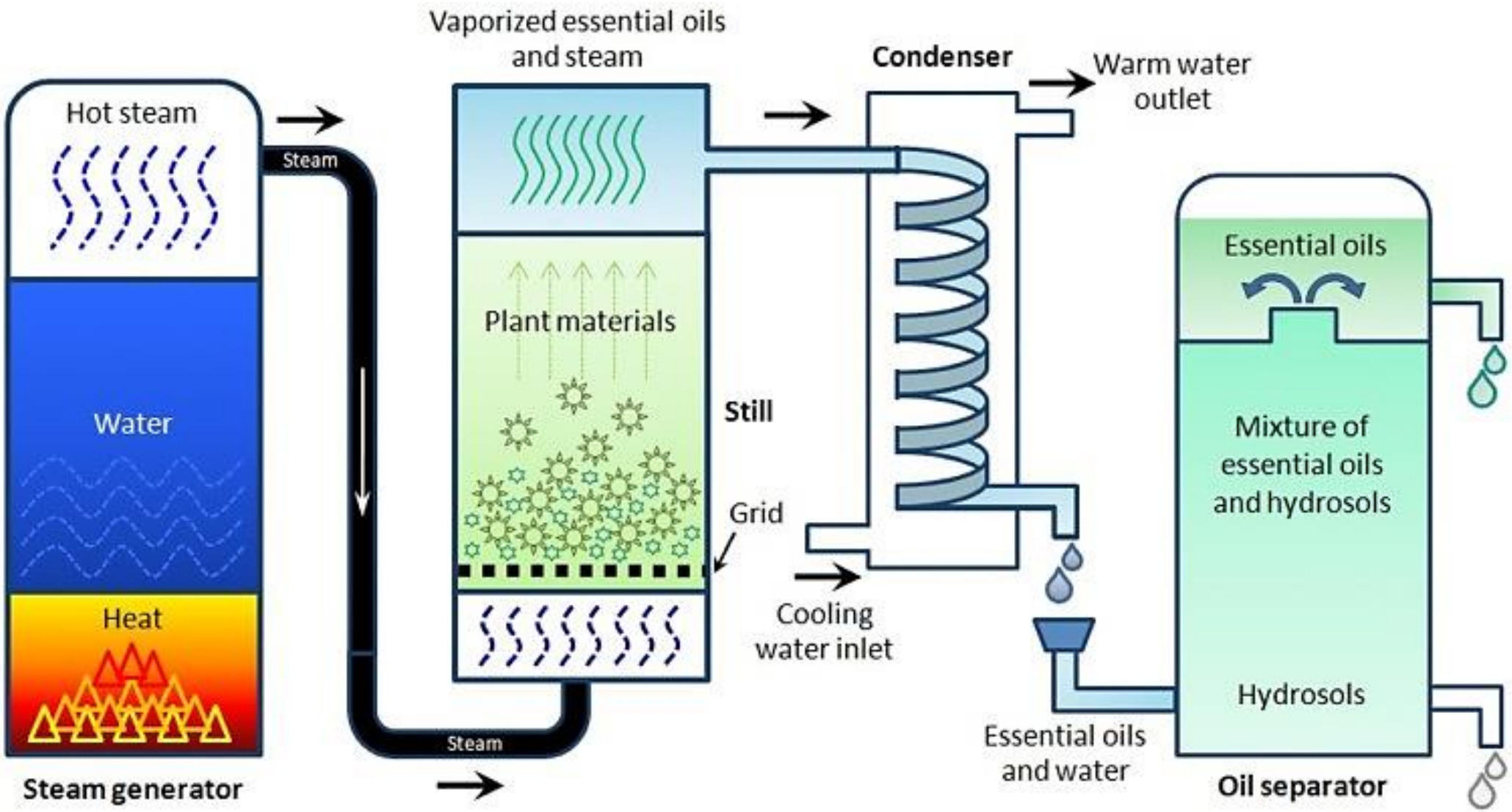


FIGURE 1: Solvent Extraction

Steam Distillation

- Steam from boiling water is passed through the raw material for 60-105 minutes, which **drives out most of their volatile fragrant compounds.**
- The condensate from distillation, which contains both water and the aromatics, is settled in a Florentine flask. This allows for the easy separation of the fragrant oils from the water as the oil will float to the top of the distillate where it is removed, leaving behind the watery distillate.
- The water collected from the condensate, which retains some of the fragrant compounds and oils from the raw material, is called hydrosol and is sometimes sold for consumer and commercial use. This method is most commonly used for fresh plant materials such as flowers, leaves, and stems.

Steam distillation



Enfleurage

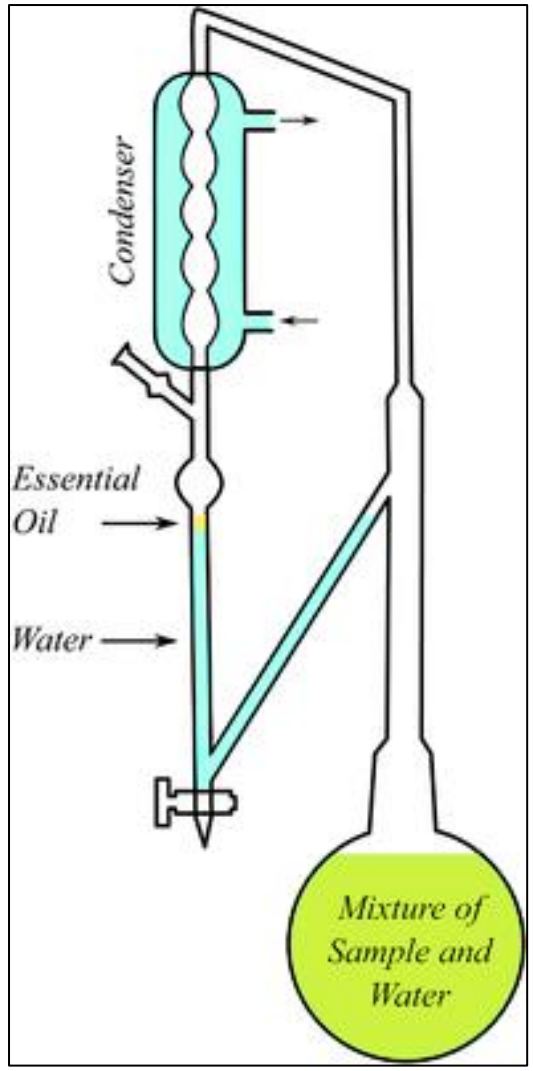
- This process involves absorbing aromatic compounds into **solid fat or wax,** followed by extracting the fragrant oil using ethyl alcohol.
- Extraction by enfleurage is commonly used when distillation is not possible because some fragrant compounds denature through high heat.
- Enfleurage is a two-step process during which the odor of aromatic materials is absorbed into wax or fat and then extracted with alcohol.

Enfleurage

FIGURE 3: Enfleurage

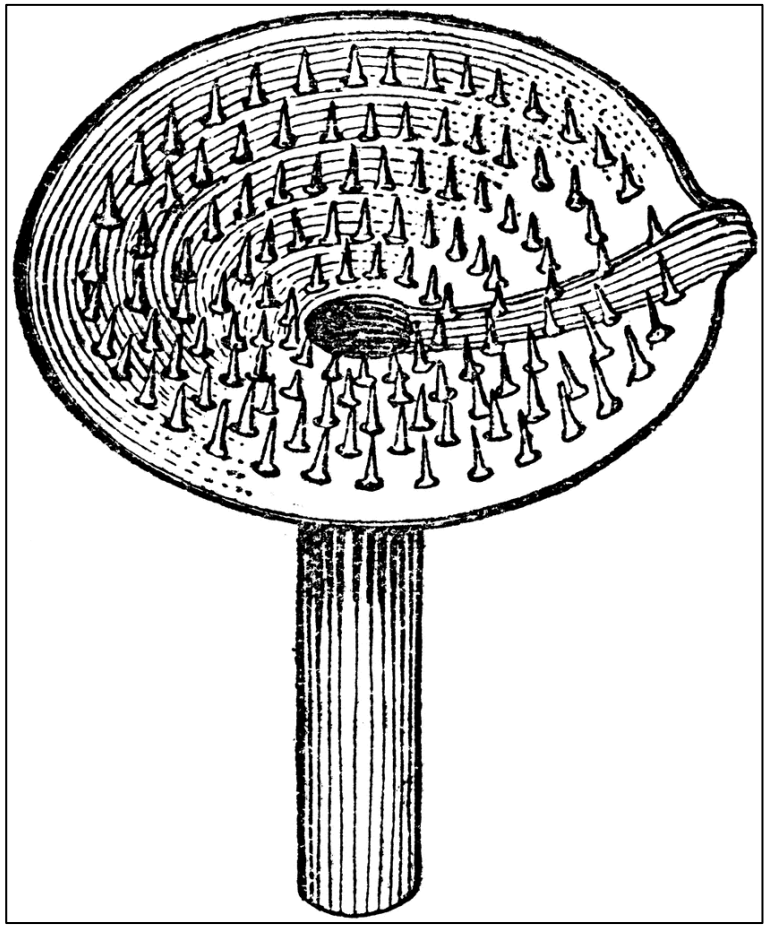
Hydro-distillation using a Clevenger Apparatus

- Hydro-distillation using a Clevenger apparatus is a common method for extracting essential oils from plant materials.
- The Clevenger apparatus, named after its inventor Friedrich Clevenger, is a simple distillation apparatus specifically designed for the extraction of essential oils.



Ecuelle method

It is used for extraction of **citrus oil**, wherein cells in the rind are ruptured mechanically using pointed projections by twisting raw material over them in a clockwise direction either mechanically or manually.



Chemical Tests of volatile oils

- To the thin section of drug, add an alcoholic solution of **Sudan III**. The red color obtained by globules indicates the presence of volatile oil.
- To the thin section of drug, add a drop of **tincture alkane**. The red color obtained by globules indicates the presence of volatile oil.

References

- Evans, W. C. (2009). Trease and Evans' Pharmacognosy. Elsevier Health Sciences.
- Price S, Price L. Aromatherapy for health professionals. 4th Edn., London: Churchill Livingstone; 2011.
- Lis-Balchin M. Aromatherapy Science: A guide for healthcare professionals. London: Pharmaceutical Press; 2006

Thank You