Vegetable and Paraffinic Waxes, the chemistry of candles

Derivatives

July 2011

PRESENTATION INDEX

- Introduction: Wax Definitions
- Origin and General Classification
- Origins of Petroleum Based Wax
- Crude Composition: Hydrocarbons
- Paraffin Wax Composition
- Manufacturing Process
- Principal Physical & Chemical Properties
- Paraffin Wax Classification
- Paraffins and Vegetable Waxes
- Candle Making Blends
- The Properties of Wax Blends

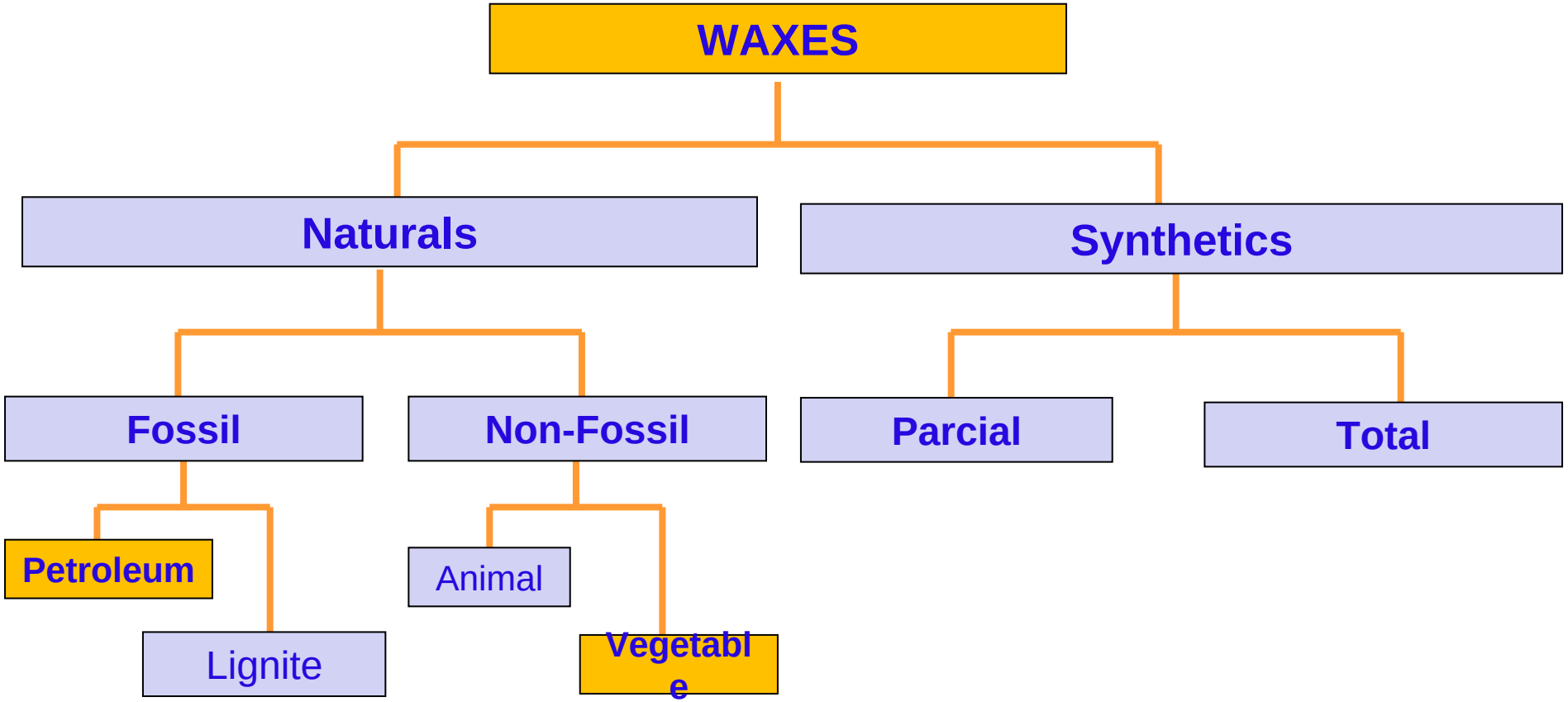
Introduction: Wax Definitions

What products can be called waxes?

The term “Waxes” includes materials of different origins and compositions.

Materials called “Waxes” are sticky solids that melt and show different levels of shine and plasticity.

General Classification and Origins



Origins of Petroleum Based Waxes

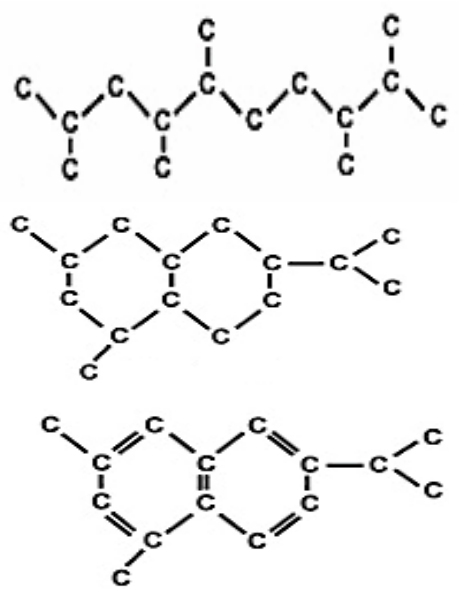
Paraffin waxes come directly from the vacuum distilation of petroleum crude.

Paraffin waxes can be refined, formulated, modified with additives and are offerd in packaged slabs, powder, chips, etc.

Crude Composition: Hydrocarbons

Petroleum crude is the raw material used to obtain paraffin waxes among other derivatives. Other hydrocarbons can also be found within its composition:

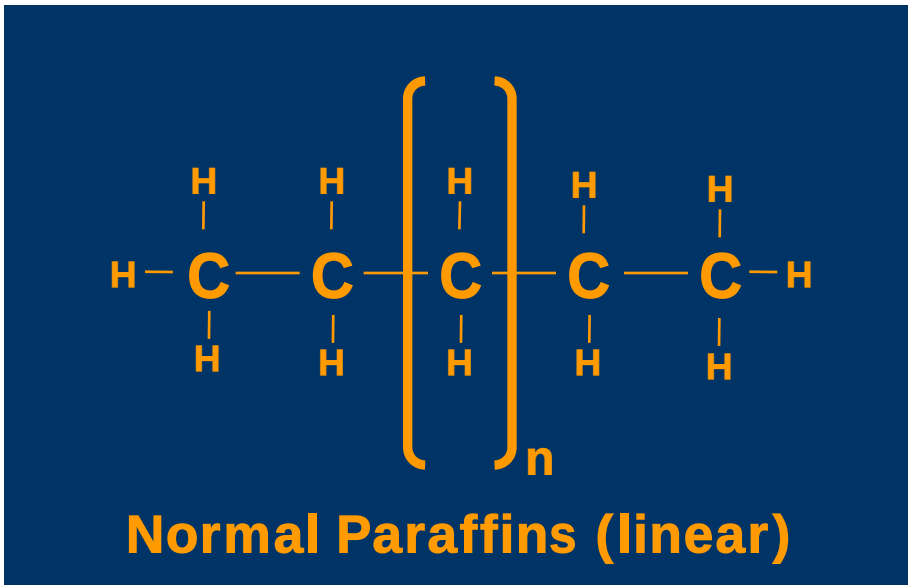
- **Normal & Branched Paraffins**
- **Naphthenic**
- **Aromatic**



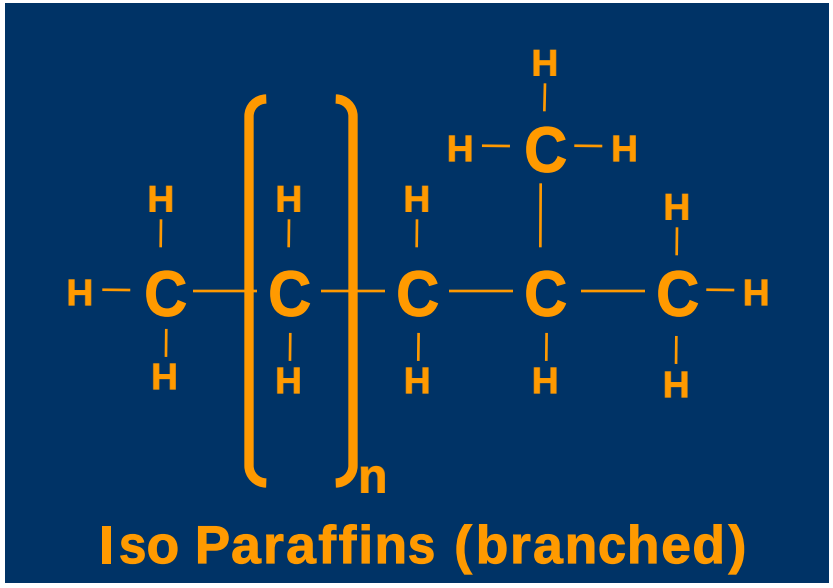
Paraffin Wax Composition

Paraffin waxes are made up of a blend of saturated hydrocarbons (alkenes) with a chain length from C20 to C60.

Depending on the structural shape of the chain, two different types of paraffins exist:

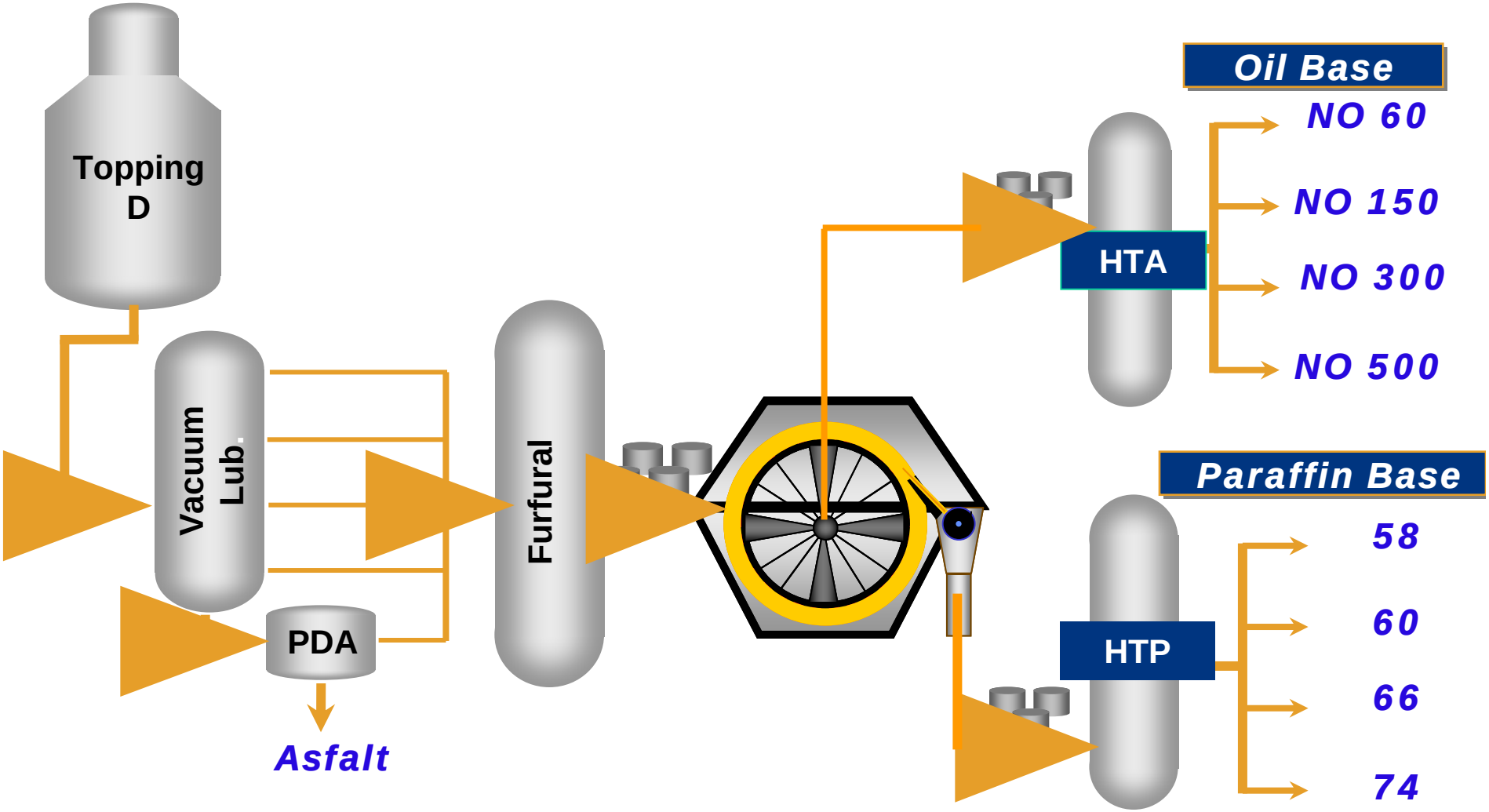


Normal Paraffins (linear)



Iso Paraffins (branched)

Paraffin Waxes: Manufacturing Process



Paraffin Waxes: Characteristics

- Solid at room temperature
- Poses a variable melt point
- Insoluble in water
- Antioxidants y antiozonants
- High fluidity
- Ease in recuperating its physicochemical characteristics

Paraffin Waxes: Characterization Tests

TEST	METHOD
Melt Point (° C)	ASTM D-87
Penetration (1/10 mm) max.	ASTM D-1321
Oil Content (% p), max.	ASTM D-721
Color Saybolt, min.	ASTM D-156

Paraffin Wax Testing

Testing

Melt Point

There are 3 methods that indicate the solid to liquid transition point of petroleum based waxes.

- ✓ Paraffin waxes are hydrocarbon blends with different molecular weights, that crystallize approximately at the same temperature forming a plateau. (ASTM D87)
- ✓ High viscosity and microcrystalline waxes do not present this plateau in their cooling curve. (ASTM D 127)
- ✓ The 3rd method is the congealing temperature. The congealing temperature is slightly lower than the melting point. (ASTM D 938)

Testing

Penetration
(ASTM D 1321)

Determines the paraffin wax hardness by needle penetration in standardized conditions.

A standardized dimension and weight needle is dropped with a 50 g weight over a paraffin wax sample at 25° C for 5 seconds. A measurement is taken on the depth the needle penetrated the wax in 0.1 mm increments.

Test significance: It relates to the composition and oil content of the paraffin wax.

Testing

Color (Saybolt)
(ASTM D 156)

Indirectly determines wax purity.

Paraffin wax is melted and subjected to halogen lighting. On a comparative scale, the color of the product is determined. The Saybolt scale ranges from -30 to +30.

Test significance: It is one of the critical parameters to identify the potential use of the paraffin wax. The higher the value is on the scale, the better the color is, as it means that it is whiter.

Testing

Kinematic Viscosity
(ASTM D 445)

Viscosity describes a fluid's internal resistance to flow and may be thought of as a measure of fluid friction (thickness). The “thicker” or more “viscous” the material is, the more difficult is its flow, harder to pump, decant, move around and handle.

Test consists in using “U” shaped pipettes in a temperature controlled water bath with bulbs and holes according to the range of viscosity to be measured.

Test significance: It is relevant in film (coating) applications.

Testing

Oil Content
(ASTM D 721)

- ✓ Indirect measure of the level of paraffin wax refinement
- ✓ Useful as a quality indicator.
- ✓ Fully refined paraffin waxes have an oil content under 1%

Testing

Oil Content

Description of methodology

This method is based on the insolubility of paraffin wax in Methyl Ethyl Ketone at a low temperature (MEK) - (ASTM D 721)

- ✓ The paraffin wax is dissolved in MEK solvent with heat.
- ✓ It is cooled and filtered to separate the paraffin wax from the MEK.
- ✓ The amount of oil is determined by weighing the filter after the solvent has been evaporated.

Testing

Compositional

What is chromatography

It is an analytic tool that allows to separate, isolate and identify the components of a blend.

The sample is distributed between two phases, one mobile and one stationary.

As the components move thru the mobile phase, they are retained by the stationary phase and then leave the column to be detected and identified.

Testing

What is Gas Chromatography?

The *stationary phase* is a microscopic layer of liquid on an inert solid support, inside a piece of glass or metal tubing called a column.

The *mobile phase* (or "moving phase") is a carrier gas, usually an inert gas such as helium or an un-reactive gas such as nitrogen.

Testing

Gas Chromatography in Paraffin Waxes

Allows to construct relational curves between the number of carbon atoms of its components and the percentage of them in the blend.

It consists of a simulated column distillation, where the paraffin is absorbed in a column and later separated by the different boiling point temperatures.

Test significance: Allow to characterize the paraffin wax and know its hydrocarbon chain composition to select it for different applications.

Paraffin Classification

Level of Refinement	Oil Content (% of weight)
Fully Refined	< 1
Semi Refined	1-3
Petrolatum	➢3

	Macrocrystalline	Microcrystalline
Melt Point	Medium (50-70° C)	High (70-90° C)
Molecular Weight	Medium C19-C42	High C25 - >C50
Crystals	Large and Regular	Small & Irregular
Flexibility	Low	High
Aspect	Brilliant	Opaque

New Waxes From Renewable Resources

Introduction

- Waxes, Fats and Oils are high carbon number carboxylic acid esters found in nature.
- Fats are solid or semi-solid at room temperature while oils remain liquid.
- Waxes, Fats and Oils are classified depending on their origin:
  - Vegetable
  - Animal

Waxes, Oils and Fats

Product	Origin	Caracteristics
WAXES	Vegetable Animal	Monohydric Alcohol Esters
FATS	Vegetable Animal	Glycerol Esters
OILS	Vegetable: Dry, Semi-dry, Non-dry Animal: Marine, Land	Glycerol Esters

Oils and Fats

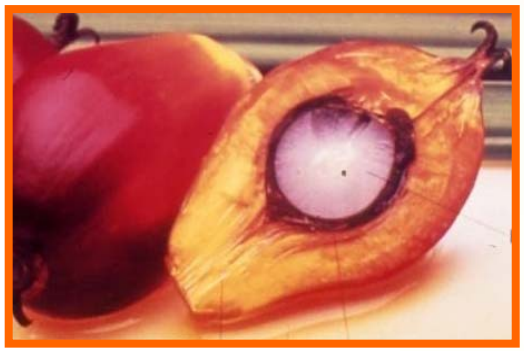
- Vegetable oils are triglyceride blends of several fatty acids.
- The composition of vegetable waxes varies with the origin of the product.
- On the next slide, the table shows the percentage of each fatty acid available in several vegetable oils and animal fats.
- The 2 numbers at the end of each column represent the number of carbon atoms and the double bonds (example, 16:0 means 16 carbon atoms and 0 double bonds on the large palmitic acid chain).

Typical Composition

Oil or Fat	Samponification Index	Iodine Value	Myristic %	Palmitic %	Stearic %	Palmitoleic %	Oleic %	Linoleic %
Coconut	*250-60*	*8-10*	*17-20*	*4-10*	*1-5*		*2-10*	*0-2*
Palm	*196-210*	*48-58*	*1-3*	*34-43*	*3-6*		*38-40*	*5-11*
Tallow	*190-200*	*31-47*	*2-3*	*24-32*	*14-32*	*1-3*	*35-48*	*2-4*
Olive	*185-200*	*74-94*	*0-1*	*5-15*	*1-4*	*0-1*	*69-84*	
Peanut	*185-95*	*83-98*		*6-9*	*2-6*	*0-1*	*50-70*	
Rapeseed	*172-5*	*94-106*	*0-2*	*0-1*	*0-2*		*20-38*	*10-15*
Corn	*188-93*	*116-30*	*0-2*	*7-11*	*3-4*	*0-2*	*43-49*	*34-42*
Cotton	*191-6*	*103-15*	*0-2*	*19-24*	*1-2*	*0-2*	*23-33*	*40-48*
Soy	*189-94*	*124-36*	*0-1*	*6-10*	*2-4*		*21-29*	*50-59*
Sunflower	*190-2*	*122-36*		*10-13*	*10-13*	*21-39*	*51-68*	
Sperm (whale)	*188-94*	*110-50*	*4-6*	*11-18*	*2-4*	*13-18*	*33-38*	

Palm Wax

- Palm oil is obtained from the fruit of a palm tree
- The hydrolysis of palm oil yields palmitic and oleic acids
- The process in obtaining a wax involves:
  - Gathering and Harvesting
  - Pressing
  - Distillation
  - Esterefication
  - Finishing and Packaging



Chemical Composition

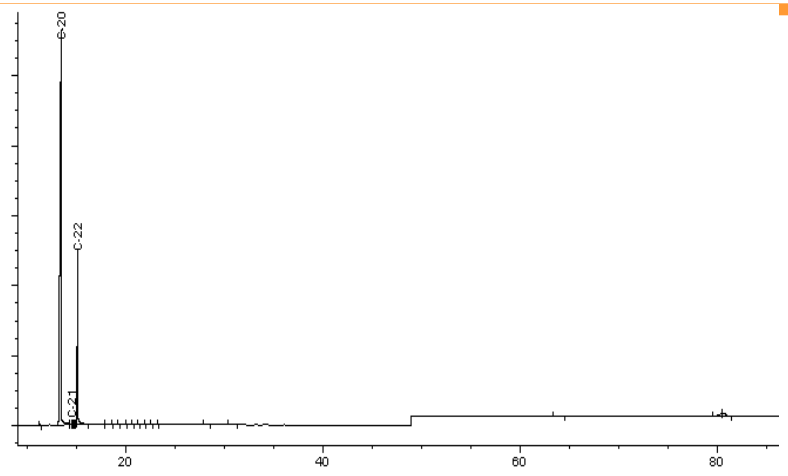
Palm Waxes

Mono, Di y Tri Glicerides

- $R1 - CO_2 - CH2$

  $R2 - CO_2 - CH$

  $R3 - CO_2 - CH2$

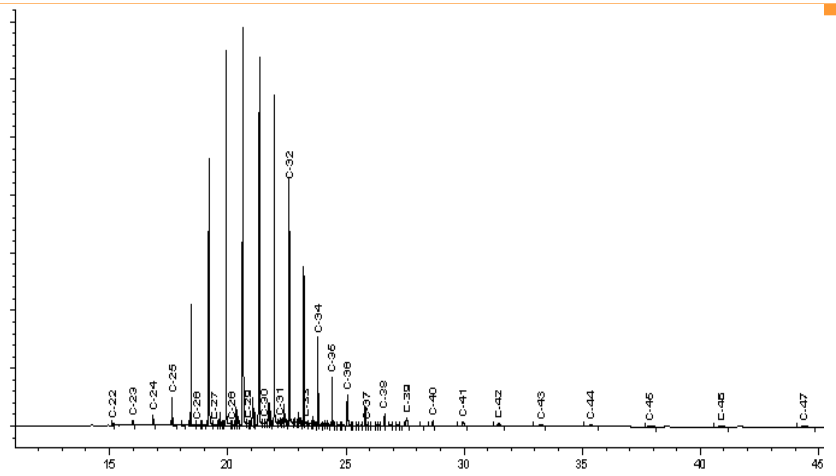


Petroleum Waxes

Normal & Iso Paraffins

- $R - CH_2 - CH_2 - CH_2 - R$

- $R - CH_2 - \underset{\displaystyle CH_3}{CH} - CH_2 - R$



Soy Wax

Soybean oil Fatty acids composition						
Fatty acids						
C 14:0	C 16:0	C 18:0	C 18:1	C 18:2	18:3	otros
0,1	10,0 - 10,5	3,5 - 4,5	23,5 - 25,5	52,0 - 54,0	7,0 - 7,5	0,4 - 1,4

Vegetable Wax Testing

YPF

Chemical and Physical

- Color (Lovibond) AOCS Cc 13j-97
- Peroxide Value AOCS Cd 8b-90
- Iodine Value AOCS Cd 1b-87
- Mettler Drop Point AOCS Cc 18-80

Wax Characterization

Properties	Wax 1 Vegetal	Wax 2 Vegetal	Paraffin Wax	Blend 1	Blend 2
Melt Point ° C	55.6	56.9	59	57.9	57.3
Penetration (mm/10)	17	22	14	16	17
Color	-16	-12	+30	10	3
Oil Content, % p/p	n/a	n/a	0.5	-	-
Acid Number	175	103	-	-	-
Iodine Value	9	8.3	-	-	-

Candle Evaluation

Comparative testing was performed in the laboratory on candles made with mineral waxes, vegetable waxes and blends between both:

- Color
- Compatibility with pigments
- Compatibility with fragrances

Candle Evaluation

The candle blends were evaluated for the following characteristics:

- Wax Contraction
- De-molding
- Combustion

Conclusions

- We have achieved very satisfactory results from the typical testing performed on candles, comparing results between the vegetable based, mineral and the blends.

- Given that vegetable waxes have a different chemical composition to the petroleum ones, we identified characterization testing and differential specifications for these products.

- Considering the blends between petroleum based products and vegetable waxes, we are also defining tests and specifications for these new hybrid products.