Effect of Chemical Treatments of Banana Leaf On The Physical Properties

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UNIVERSITI SAINS MALAYSIA

2015

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By

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Thesis submitted in fulfilment of the requirements for the Degree of Masters of Sciences

October 2015

ACKNOWLEDGEMENTS

First and foremost, thank you Almighty Allah for finishing my Master thesis work. Special thanks dedicated to my supervisor Assoc. Prof. Dr. Baharin Azahari for his valuable supervising, advising, comments and suggestions which lead me to learn much valuable information during the preparation of master project. I would like to express my deep appreciation to Ministry of Education for providing a funding under MyBrain15. I am also pleased to express my thanks to Syazwani, Nadirah, and others fellow labmates for their heartfelt assistance, guidance, helps and ideas. I am also grateful to Mr Azhar, Mr Basrol, Mr Munir, Mr Abu, Mr Ahmad, Mr Shamsul, Ms Hasni and Ms Aida for extending their help in technical and laboratory work. To all my fellow friend especially, Sobra, Fahmi, Ezwan, Asniza, Atiqah and Syafiq in Bio-Resource, Paper and Coatings Technology division, thank you for their support, friendships and great memories during my study. Last but not least, thank you to my parents and beloved family who always have strong faith in me and provide me with countless support in terms of time and morals. Thank you mama, Mazitah Binti Hussin. Thank you very much for all your helps and sacrifices.

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LIST OF ABBREVIATIONS

ASTM	American society for testing and materials
CC	Calcium carbonate
DFT	Density functional theory
FT-IR	Fourier transform infrared spectroscopy
GPa	Giga pascal
MMA	Merthyl methacrylate
MPa	Mega pascal
PMMA	Poly methyl methacrylate
PC	Polycarbonate
SEM	Scanning electron microscope
TAPPI	Technical association of the pulp and paper industry
TGA	Thermogravimetric analysis

LIST OF SYMBOLS

%	Percentage
ºC	Degree Celsius
cm	Centimeter
d	Thickness
g	Gram
J	Joule
kg	Kilogram
M	Mega
m	Meter
m	Mass
mg	Miligram
mm	Milimeter
ml	Mililiter
T_g	Glass Transition Temperature
V	Volume

KESAN RAWATAN KIMIA KE ATAS SIFAT FIZIKAL DAUN PISANG

ABSTRAK

Penyelidikan ini dijalankan untuk mengkaji kesan rawatan kimia ke atas sifat fizikal daun pisang. Filem dari daun pisang dihasilkan dengan merendamkan daun pisang sedia ada ke dalam nisbah larutan glycerol terhadap air yang berbeza kepekatannya iaitu 1:1, 1:2 dan 1:3 dimana 1 itu ialah glycerol serta masa rendaman juga berbeza iaitu 4,6,8,10 dan 12 saat. Suhu larutan glycerol dan air yang digunakan untuk rendaman juga berbeza sebanyak 40,60,80 dan 100 darjah celcius. Sifat daun pisang asal termasuklah kadar penyerapan air, kekuatan tensil dan modulus tensil telah dikaji sebelum daun pisang direndam kedalam larutan glycerol dan air. Filem yang terhasil dari hasil rendaman larutan glycerol dikaji sifat mekanikal dan fizikalnya. Filem hasil dari nisbah larutan glycerol terhadap air 1:3, suhu larutan 100 darjah celcius dan masa rendaman 10 saat menunjukkan peratusan penyerapan air yang rendah, kekuatan tensil, koyakan,dan ketahanan lipatan yang tinggi jika dibandingkan dengan filem yang lain. Kesan rendaman dalam larutan glycerol juga diperhatikan dengan menggunakan mikroskopi pengimbas electron (SEM). Filem yang terhasil dari rendaman glycerol akan melalui proses pemindahan resin acrylic melalui vakum dengan memaksa resin acrylic untuk masuk kedalam filem melalui perbezaan suhu sebanyak 100,130 dan 150 darjah celcius dan masa tekanan yang bebza iaitu 10,20,30,40,50 dan 60 minit. Berdasarkan kajian, didapati filem yang terhasil dengan resin acrylic menunjukkan penambahbaikan pada peratusan penyerapan air, kekuatan tensil, kekuatan koyakan dan ketahanan lipatan. Kesan

serapan pelarut dilakukan untuk mengetahui tahap kematangan resin acrylic yang terdapat didalam filem tersebut. Semakin banyak serapan terlarut, semakin rendah hubungan silang berlaku. Daripada keputusan yang direkodkan, didapati sifat ketahanan tensil yang mempunyai hubungan malar dengan kesan serapan pelarut.

EFFECT OF CHEMICAL TREATMENT OF BANANA LEAF ON THE PHYSICAL PROPERTIES

ABSTRACT

The study was conducted to investigate the effect of chemical treatment of banana leaf on the physical properties. Film from banana leaf were produced by soaking raw material banana leaf in to the glycerol solution with different ratio that is 1:1, 1:2, and 1:3 where 1 is the glycerol with different soaking time; 4,6,8,10 and 12 seconds. The temperature for the glycerol solution also ranged from 40, 60, 80, and 100°C. The properties of raw banana leaf including waster absorption, tensile strength, and young modulus was investigated before the banana leaf soaked into glycerol solution. The physical and mechanical properties of the film produce from soaking into glycerol solution were evaluated. Film produced from ratio 1:3, temperature of the solution 100°C and soaking time 10 seconds shows lower percentage of water absorption with higher tensile strength, tearing strength, and folding endurance compared other films. The effects of soaking into glycerol solution also were viewed using Scanning Electron Microscope (SEM). Another study was on the film that was produced from soaked glycerol solution will undergo Vacuum Assisted Resin Transfer Moulding to impregnated the acylic resin into the film from different temperature range from 100, 130 and 150°C and pressing time from 10, 20, 30, 40, 50 and 60 minutes. Based on the study, the film that was produced shows some improvement in term of water absorption percentage, tensile strength, tearing strength and folding endurance. Solvent uptake was to investigate the degree of polymerization of acrylic resin. More solvent uptake occurred shows

that less crosslinking happens. Based on the result, only tensile strength has a linear relationship with the solvent uptake of the acrylic resin.

CHAPTER 1 INTRODUCTION

1.1 General

In the last decade, the important of packaging within this system has increasing significantly. Packaging basically being used to protect the product. Normally, the material being used for packaging application such as paper and paper pulp based material, metal, wood, glass or combination of more than one material such as composite and its depends for its appearance and performance (Kirwan, 2012). Advanced researches have been conducted to look for alternative sources of natural fiber (Oliveira et al., 2006a). Crops and agriculture waste have been selected as the favorable raw materials for renewable natural fibers (Cordeiro et al., 2004). Renewable natural fibres have the compositions, properties, and structure that make them suitable for the fabrication of composite, textile, pulp and paper (Wan Nadirah et al. (2012).

Renewable sources of natural fibers are plenty and can be divided into two categories. There are primary fibre crops and secondary fibre crops. Primary fibre crops such as cotton, jute, hemp and kenaf are grown mainly for their fibre. Secondary fibre crops such as banana, sugar cane and palm oil are not grown for their fibre, but rather their fruits, oil, seed and leaves. The seasonal nature of some crops becomes the main factor in selecting the suitable renewable secondary fibre crops. Some crops such as hemp and rice husk have the potential to be used in paper and panel production, but they will create problems in term of costs in storage and seasonal supply (Bilba et al., 2007). On the other hand, crops such as banana and oil palm are harvested throughout the year, resulting a linear and uniformly steady constant supply of natural fibre (Oliveira et al., 2007). Banana was well known for its large production and many research has been conducted to explore the potential of banana (Mohapatra et al., 2010).

Banana is an edible fruit, contributing about 16% of the world's total fruit production and its among one of the world's most important crop of small and large scale production in more than 100 countries (Mohapatra et al., 2010). People from Latin America, Southeast Asia and West Africa based their economic importance on the banana industry. World production of bananas increased by 33 percent from 24 million metric tonnes to 36 million metric tonnes between 2000 until 2012. In banana commercialization plants, huge amount of wastes, including the leaf, pseudostem and stalk were generated.

Work done by Fernandes et al regarding an overview of banana, for every ton of banana plant harvested, 100 kg of fruit is rejected and approximately 4 tons of lignocellulosic wastes (3 tons pseudostem, 160 kg stalks, 480 kg leaves and 440 kg skins) were produced. Despite huge amount of lignocellulosic residue, banana leaf normally fed to livestock and these waste are spread over the soil as much as it can cover and left to decompose naturally to maintain the temperature and moistures of the soil and also can be used as organic fertilizer (Fernandes et al., 2013). Using back all these waste and turn them into something useable or transforming them into a commodity would increase the value to banana cultivation and reduce environmental pollution. Banana leaf can be considered renewable lignocellulosic biomass because it's coming in abundant, inexpensive and always available. Few researches has been done to utilize the banana waste such as biodegradable plastic (Liu et al., 2009) by mixing up the banana waste with resin. Acrylic resin is one of the resin that have many potential.

Acrylic resin or poly methyl methacrylate was widely known to be a clear plastic used as shatterproof replacement for glass (Björkner, 2000). When it comes to making windows, PMMA has another advantage over glass. PMMA is more transparent than glass. When glass windows are made too thick, they become difficult to see through. But PMMA windows can be made as much as 13 inches (33 cm) thick, and they're still perfectly transparent. This makes PMMA a wonderful material for making large aquariums, whose windows must be thick in order to contain the high pressure millions of gallons of water. In fact, the largest single window in the world, an observation window at California's Monterrey Bay Aquarium, is made of one big piece of PMMA which is 54 feet long, 18 feet high, and 13 inches thick (16.6 m long, 5.5 m high, and 33 cm thick). Many research has been done and recently, researchers found another usage of arylic resin in In orthopedic surgery, PMMA bone cement is used to affix implants and to remodel lost bone (Abar et al., 2015). It is supplied as a powder with liquid methyl methacrylate (MMA). PMMA has also been linked to cardiopulmonary events in the operating room due to hypotension (Khaled et al., 2010). Bone cement acts like a grout and not so much like a glue in arthroplasty. Although sticky, it does not bond to either the bone or the implant, it primarily fills the spaces between the prosthesis and the bone preventing motion (Mao et al., 2014).

The aim of this research was to study the potential of banana leaf for packaging application and to maximize the utilization of banana leaf, especially in increasing the strength and reducing the water absorption of the new modified banana leaf. In this research, banana leaf that has been modified with a glycerol solution undergoes several dipping time, temperature and ratio of the solution. The properties of acrylic resin blend with banana leaves will be investigate.

1.2 Objective of Research

The main objective to be achieved in this study area

- To study the effect of glycerol towards banana leaf film and evaluate the physical and mechanical properties of banana leaf.
- To study the effect of impregnation of acrylic resin on the physical, mechanical and morphological properties of the treated banana leaf film.

CHAPTER 2 LITERATURE REVIEW

2.1 Packaging

2.1.1 Introduction

Packaging is best described as a coordinated system of preparing goods for transport, distribution, storage, retailing, and use. It is a complex, dynamic, scientific, artistic, and the controversial business function, which in its most fundamental form contains, protects or preserves, transports, and informs/sells (Kirwan, 2012). The first paper packaging was recorded at 1035, when a Persian traveler found the spices and vegetables were wrap in a paper for customer in Cairo markets. Paper and paperboard packaging play well-dressed roles in world economy. Their printability is their main asset. They have been responsible for the dazzling graphic display in retail stores for the past century and advertising communications on bags, cartoons and labels. The roles played by corrugate fiberboard and kraft paper are less glamorous, but no less significant. Corrugated fiberboard boxes are the shipping container choice for the most products in many supply chains in the world. Today, advanced packaging technology has go further with a wide range of material used to produce cheap and strong packaging such as metal, glass, plastic, paper and composite; combination of more than one material.

2.1.2 Purpose of Packaging

Packaging is greatly utilized due to several objectives.

a) Physical damage protection	The objects enclosed in the package may require protection from, among other things, mechanical shock, vibration, electrostatic discharge, compression, temperature, etc.
b) Barrier protection	A barrier from oxygen, water vapor, dust, etc., is often required. Permeation is a critical factor in design. Some packages contain desiccants or oxygen absorbency to help extend shelf life. Modified atmospheres or controlled atmospheres are also maintained in some food packages. Keeping the contents clean, fresh, sterile and safe for the intended shelf life is a primary function.(Lee et al., 2008)
c) Convenience	Packages can have features that add convenience in distribution, handling, stacking, display, sale, opening, re-closing, use, dispensing, reuse, recycling, and ease of disposal.
d) Information transmission	Packages and labels communicate how to use, transport, recycle, or dispose of the package or product. With pharmaceuticals, food, medical, and chemical products, some types of information are required by governments. Some packages and labels

also are used for track and trace purposes.

e) Marketing

The packaging and labels can be used by marketers to encourage potential buyers to purchase the product. Package graphic design and physical design have been important and constantly evolving phenomenon for several decades. Marketing communications and graphic design are applied to the surface of the package and (in many cases) the point of sale display.

f) Security

Packaging can play an important role in reducing the security risks of shipment. Packages can be made with improved tamper resistance to deter tampering and also can have tamper-evident features to help indicate tampering. Packages can be engineered to help reduce the risks of package pilferage.

2.1.3 Packaging Categories

The type of material used to produce a packaging usually depends on the application of the product. There are three categories of packaging (Kirwan, 2012).

- Primary packaging — Usually the packaging product in single units at the point of sale or use, for example cartons
- Secondary packaging — Collections of primary packs grouped for storage, distribution and wholesaling such as boxes and cases
- Tertiary packaging — Packaging used for handling and distribution in bulk, for example heavy-duty fiber board packaging

2.2 Packaging Papers and Paperboards

2.2.1 Introduction

A wide range of papers and paperboards are commercially available to meet market needs based on the choice of fiber. The fibers are bleached or unbleached, chemically or mechanically separated, virgin or recovered fiber. The treatment and additives used at the stock preparation stage. Paper and paperboard based products can be made in a wide range of grammages and thicknesses. The surface finish (appearance) can be varied mechanically. Additives introduced at the stock preparation stage provide special properties. Coatings applied to either one or both surfaces, smoothed and dried, offer a variety of appearance and performance features which are enhanced by subsequent printing and conversion, thereby resulting in various types of packaging material (Abd Rahman and Azahari, 2012).

2.2.2 Types of Paper Packaging

2.2.2.1 Tissues

These are lightweight papers with grammages from 12 to 30gm $^{-2}$. The lightest tissues for tea and coffee bags which require a strong porous sheet are based on long fibers such as those derived from Manila hemp. To maintain strength during immersion in boiling water, wet strength additives are used. Heat-sealed tea and coffee bags require the inclusion of a heat-sealing fiber, such as polypropylene.

2.2.2.2 Label Paper

Usually this type of packaging may be coated either one side or both, such as machine glazed paper or machine finished using kraft papers in the grammage range 70–90 gm $^{-2}$. The paper may be coated on-machine or cast coated for the highest gloss in an off-machine or secondary process. The term 'finish' in the paper industry refers to the surface appearance. For example, machine finish type paper that is smooth but not glazed, water finish; where one or both sides are dampened and calendered to be smoother and glossier than machine finish; and supercalendered; which is dampened and polished off-machine to produce high gloss on both sides.

Depending upon the environment in which the label is to be used, various functional chemicals may need to be added, for example for labelling packages containing fatty products, grease-resistant chemicals, such as fluorocarbons, may be included.

2.2.2.3 Bag papers

'Imitation kraft' is a term on which there is no universally agreed definition; it can be either a blend of kraft virgin fibre with recycled fibre or 100% recycled. It is usually dyed brown. It has many uses for wrapping and for bags where it may have machine gloss and a ribbed finish. Thinner grades may be used for lamination with aluminium foil and PE for use on form, fill, and seal machines. For sugar or flour bags, coated or uncoated bleached kraft in the range 90–100gm $^{-2}$ is used.

2.2.2.4 Sack Kraft

Usually this is unbleached kraft pulp, though there is some use of bleached kraft. The grammage range is 70–100gm $^{-2}$. Paper used in wet condition needs to retain considerable strength, at least 30%, when saturated with water. To achieve this, resins such as urea-formaldehyde and melamine formaldehyde are added to the stock. These chemicals cross-link during drying and are deposited on the surface of the cellulose fibres making them more resistant to water absorption.

2.2.2.5 Solid Bleached Board

This board is made exclusively from bleached chemical pulp as seen in Figure 2.1. It usually has a mineral pigment-coated top surface, and some grades also coat on the back. This paperboard has excellent surface and printing characteristics. It gives a wide scope for innovative structural designs and can be embossed, cut, creased, folded and glued with ease. This is a pure cellulose primary (virgin) paperboard with consistent purity for food product safety, making it the best choice for the packaging of aroma and flavour sensitive products. Examples of use include chocolate packaging, frozen, chilled and reheatable products, tea, coffee, liquid packaging and non-foods such as cigarettes, cosmetics and pharmaceuticals.

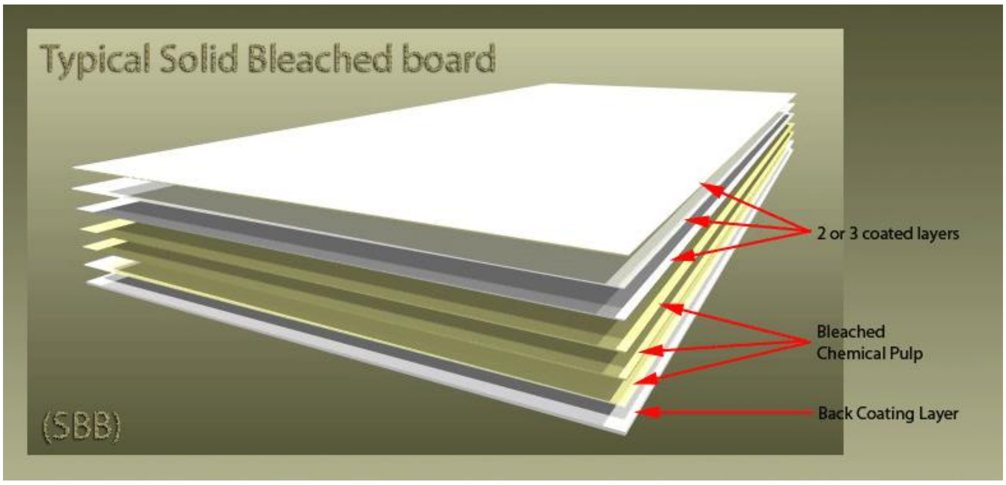

Figure 2.1 Example of solid bleach board

2.2.3 Paper and Packaging Industry in Malaysia.

The packaging industry is one of the most dynamic growth sectors within the Malaysian manufacturing sector. The paper packaging sector is the second largest sector for the packaging industry accounting for 45 per cent of the total industry output. Malaysia is currently a net exporter of packaging products. The total export of packaging materials, both flexible and rigid, increased by 7.7% from RM6.35 billion for 2007 to RM6.84 billion in 2008. Stronger performance in the export of paper packaging was due to higher demand from the EU and Chinese markets.

The establishment of the pulp and paper products as a dominant material in packaging has been running for many years in Malaysia and because of that in 2003, Malaysia was ranked eleventh in the world paper and paperboard production with a total of 1.3 million tones. United States has been the largest producer of pulp and paperboard production followed by China, Japan, Canada and others (Rosnah, 2011)

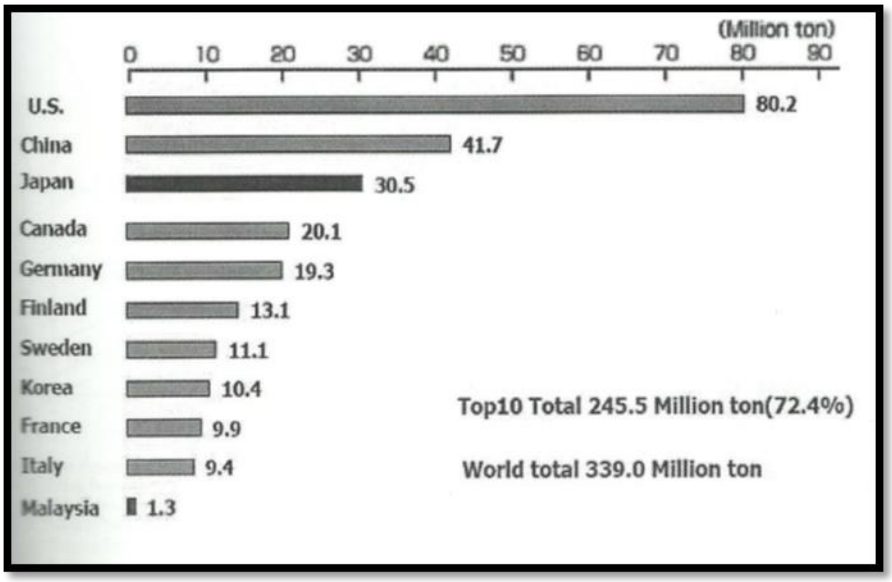

Figure 2.2 World paper and paperboard production in 2003 (Rosnah, 2011)

Although Malaysia has becomes one of the main producer in pulp and paper product among ASEAN countries, the production rate does not fulfill the domestic requirement (Figure 2.3). Due to this phenomena, half of the country needs was imported to cover the country consumption (Roda, 2006).

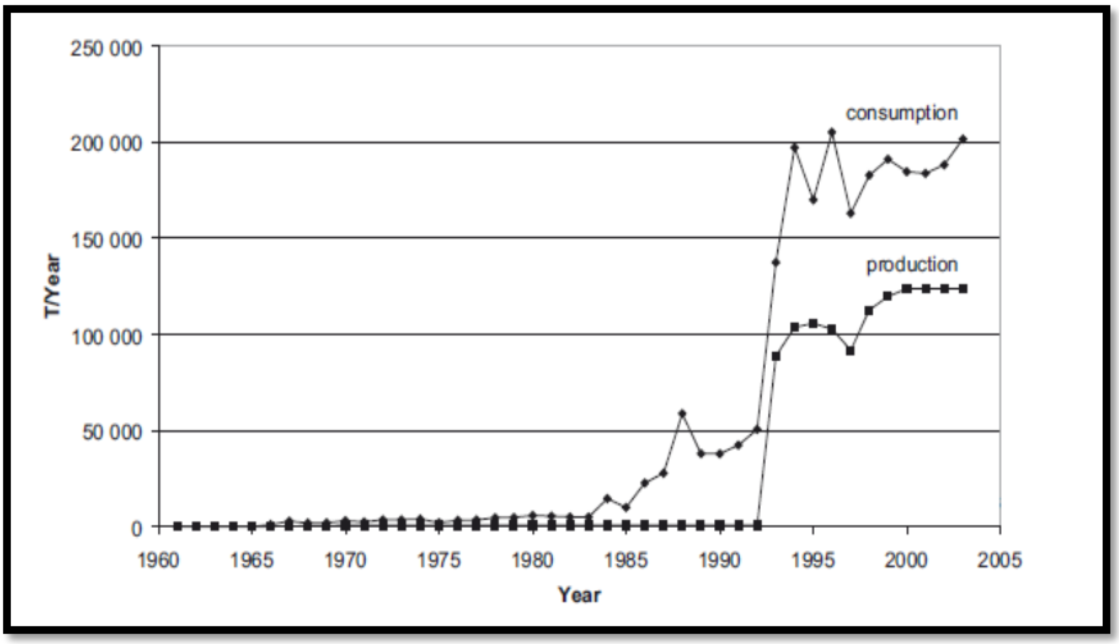

Figure 2.3 Malaysia pulp product and consumption ((N. Harijati, 2013)

Since Malaysia pulp and paper industry totally depends on imported fiber especially virgin pulp to maintain the consumption of the country, many researches have been done to find a new source of fiber to fulfill the demand. The utilization of agricultural residue and noon wood material such as oil palm leaf, empty fruit bunch, kenaf, banana residue and baggase can be utilize as other source of fiber.

2.3 Agricultural Waste/Non Wood

The byproducts of agricultural activities are usually referred to as "agricultural waste" because they are not the primary products. These wastes chiefly take the form of crop residues from plantation such as residual stalks, straw, leaves, roots, husks and animal waste. Agricultural wastes are widely available, renewable and virtually free, hence they can be an important resource. They can be converted into heat, steam, charcoal, methanol, ethanol, biodiesel as well as raw materials for animal feed. However, many of the agricultural wastes are still largely underutilized, and left to rot or openly burned in the field, especially in developing countries (Sirivasan, 2009).

Nonwood agricultural residues are highly abundant around the world and are becoming increasingly important as raw materials for energy and chemical feedstock production. The annual production of such biomass per area is much higher than in forests, and the payback time of nonwood plantations is much shorter than that of forest plantations. Wheat straw, rice straw, banana leaves and bagasse are the most well-known agricultural residue. The banana tree, an annual herbaceous plant that produces fruit all year around, could potentially serve as an inexpensive and readily available nonwood, renewable source of biomass. However, the characteristic and processing method for non-wood material are slightly different from wood (Selamat et al., 2014).

2.4 Banana Plant

Banana plants are the world's largest herbs and the stalk of the plant is made from long,green leaves or sheaths, which wrap around each other to form trunk like pseudostem. It belongs to a genus Musa in the family *Musaceae* and it originated from india and Eastern Asian region like Malaysia (Mohapatra et al., 2010). Most of the world's edible bananas are derived from *Musa acuminata* or naturally occuring hybrids between *Musa acuminata* and *Musa balbisiana*. Hundreds of different banana and plantain cultivars are grown for domestic consumption, but 'Cavendish' bananas dominate the world export trade. Although there is a rich diversity of plantains and East African Highland bananas, they are genetically very similar. This means all varieties tend to be susceptible to the same pests and diseases, such as the infamous Panama disease. Each plant just produces one stem of bananas, holding up to 200 bananas.

Banana plants consist of rhizome pseudo steam, sucker, petioles, leaf and fruits (Eagan, 2006) its shown in Figure 2.4. Cultivated banana plants vary in height depending on the variety and growing conditions. Most are around 5m (16ft) tall, with a range from 'Dwarf Cavendish' plants at around 3m (10ft) to 'Gros Michel' at 7m (23ft) or more (Ploetz, 2007). Leaves are spirally arranged and may grow 2.7 metres (8.9ft) long and 60cm (2.0ft) wide. They are easily torn by the wind, resulting in the familiar frond look. After harvesting the single bunch of bananas, a great amount of agricultural residues are produced. These residues are usually left in the soil plantation to be used as organic fertilizer (Oliveira et al., 2009).

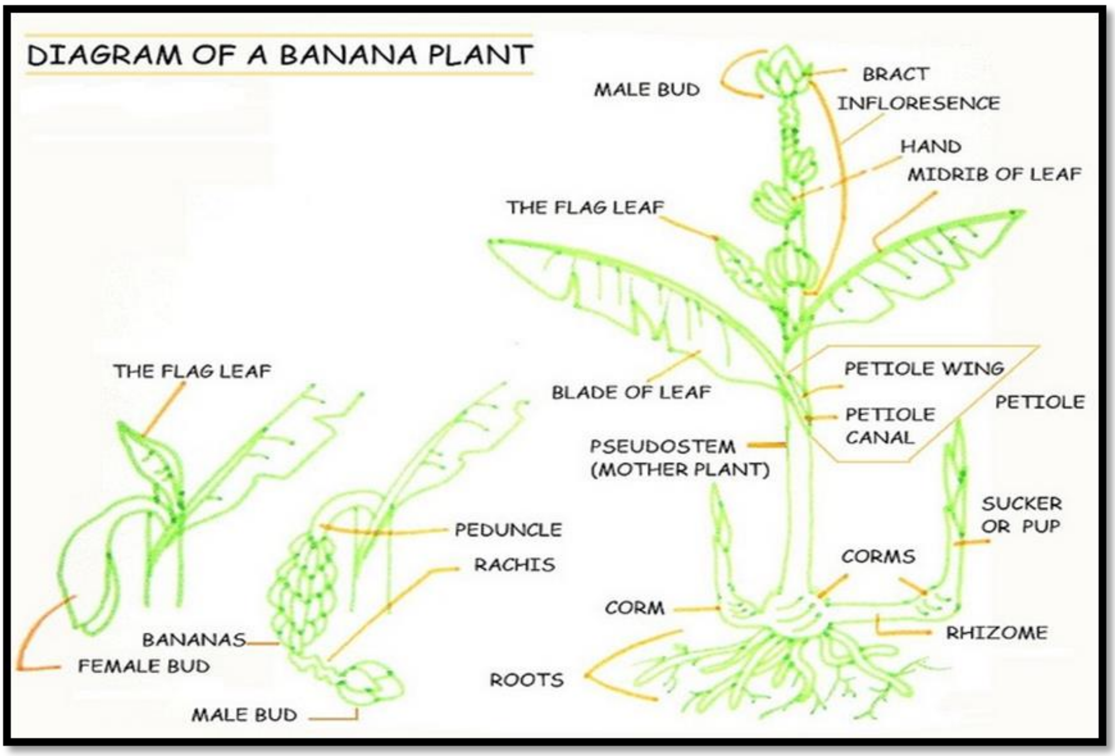

Figure 2.4 Diagram of banana plant (Oliveira et al., 2006b)

India has become the largest producer of banana contributing to 27% of world's banana production estimated around 16.8 million ton per year followed by Eduardo and Brazil with 5.4 million tonne per year and 5.3 million tonne per year, respectively (Mohapatra et al., 2010). In Malaysia, banana is the most widely cultivated fruit, covering about 33,495 ha with a total production of 357,745 metric tonne. Banana production has increased marginally for the 5 years from 2011-2013. From the banana production statistic reported by Department of Statistic Malaysia (2014) in year 2011 (Table 2.1), about 350,000 metric tonne of banana residue was created without utilize it as new resources for other industries such as paper and wood product industries.

Table 2.1 Banana production statistic in Malaysia in year 2011

Production	357,745 tonne
Export	30,0193 tonne
Import	678.2 tonne
Per capita consumption	9.2 kg/yr

2.4.1 Morphology and anatomy of Banana Leaf

2.4.1.1 Morphology

The leaf is the banana plant's main photosynthetic organ. It consists of the leaf blade and the leaf sheath, which contracts into a petiole. The modification of basal part of midrib was called pseudostem. The petiole had halfcircle-like shape and the adaxial part grooved. The petiole becomes the midrib, which divides the blade into two lamina halves. Lamina veins run parallel to each other in a long S shape from midrib to margin. Veins do not branch, which results in leaves tearing easily (Anonymous, 1996). The shape of the leaves usually oblong with flat tip. The surface of the leaves was protected by cuticle layer.

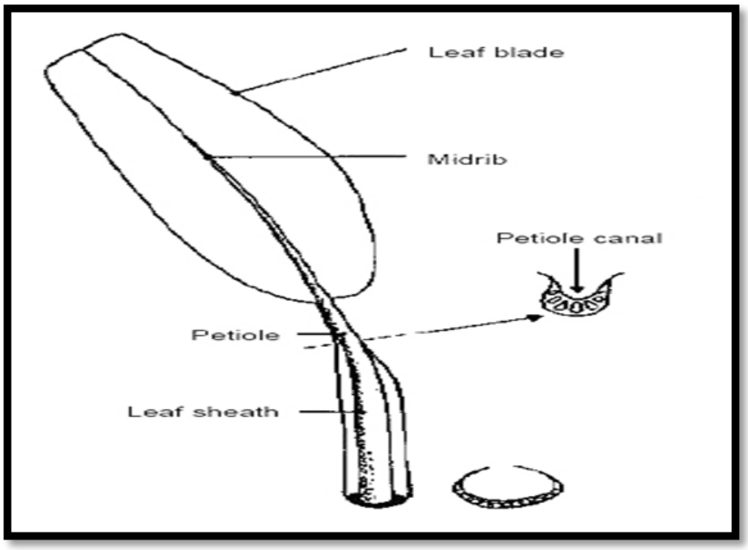

Figure 2.5 Illustration of banana leaves (Sumardi and Wulandri, 2010)

2.4.1.2 Anatomy of Banana Leaf

The blade in other names Lamina consisted of epidermis layer, vascular bundles and parenchyma cells. The shape of epidermis cells was rectangular. Adaxial epidermis is the upper side of banana leaves and abaxial epidermis is the lower side. The size of adaxial epidermis was bigger than that of abaxial epidermis. The abaxial epidermis of banana leaf was covered with cuticle, which is a protecting film consists of lipid and hydrocarbon polymers impregnated with wax (Sylvester et al., 2001).

Vascular tissues distributed in mesophyll, consisted of small and big. The big vascular bundle compossed of vessel, tracheid, fiber, parenchyma cells and phloem (Stevenson, 1984). The vascular bundle is compossed of xylem and phloem elements and surrounded by the parenchymatic or sclerenchymatic cells, called bundle sheath. The small bundles were not protected by bundle sheath. The anatomy character of leaf blade can be seen Figure 2.6. Stomata were found on both surface of epidermis layer. The type of stomata was predominantly paractic because the potition of guard cell in line with epidermis layer. This result was supposed by Tomlinson's research (1969). The shape of guard cell was kidney-like and each stoma was surrounded by 4-6 cells.

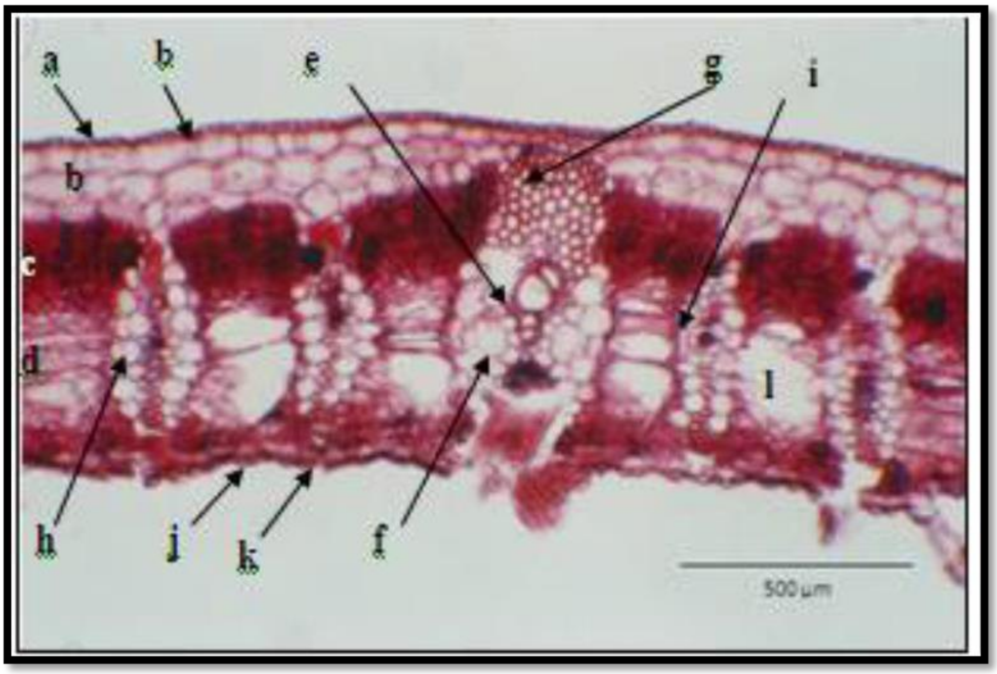

Figure 2.6 Leaf cross section a. adaxial epidermis; b. cuticle; c. pallisade tissues; d. spongy tissue; e. xylem; f. phloem; g. schlerenchyma; h. bundle sheath; i. laticifer; j. abaxial epidermis; k. stomata; l. air space. (Sumardi and Wulandri, 2010)

2.4.2 Chemical Composition of Banana Leaf

Banana leaves generally can be described as lignocellulosic which are complex in structure and consist of cellulose microfibril in amorphous matrix of lignin and hemicellulose. The functional properties of chosen raw material are important for wrapping material properties.

As report by Olievera et al (2010) the chemical composition of banana leaves include around 37% of cellulose, 37% α-cellulose as shown in Table 2.2.

Table 2.2 Chemical composition of banana leaf

Components	Percentage
Cellulose	37.3
Hemicellulose	12.4
Lignin	13.3
Starch	8.4

The present of hemicellulose in banana leaves fiber which about 12.4% also might help in the formation of hydrogen bonding due to the present of carboxylic acid group (Preechawong et al., 2005). Since hemicellulose (Figure 2.7) is a non crystalic polymer with hydrophilic properties, thus it may also contribute towards the swelling ability of the fiber and will improve the flexibility of the wrapping material.

The present of lignin (Figure 2.8) in a plant material strengthening agent in the composite wood structure and as a middle lamella, the intercellular material which react as cement to bind the fiber together (Smook, 1992). High content of lignin in fiber will make the fiber become tougher and will reduce the flexibility of the fiber thus may interfere the hydrogen bonding between the fiber. Addition of glycerol in banana fiber film making will increase the lignin solubility thus will enhance the flexibility of the fiber film produced (Carlos et al., 2013).

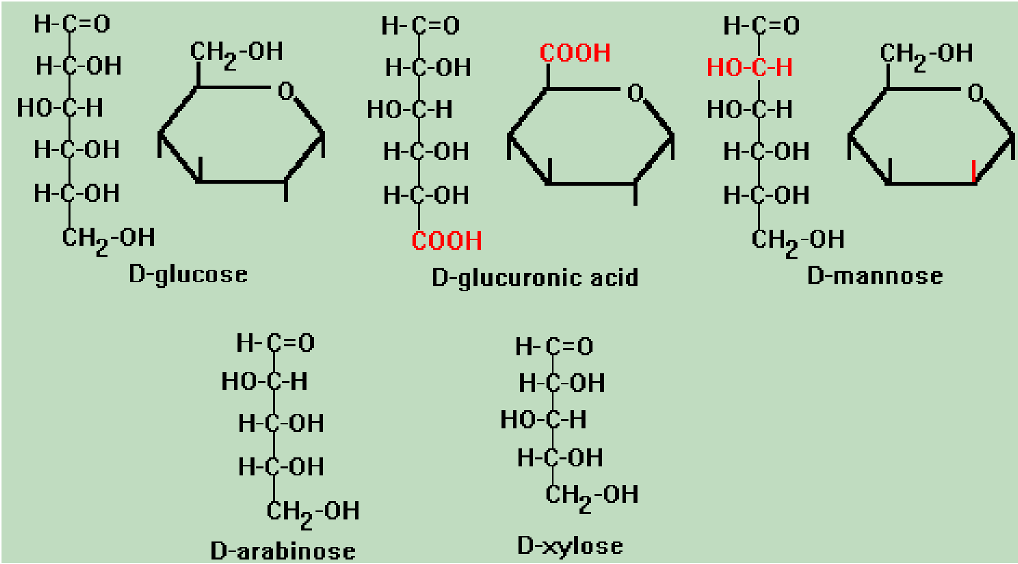

Figure 2.7 Molecular structure of hemicellulose

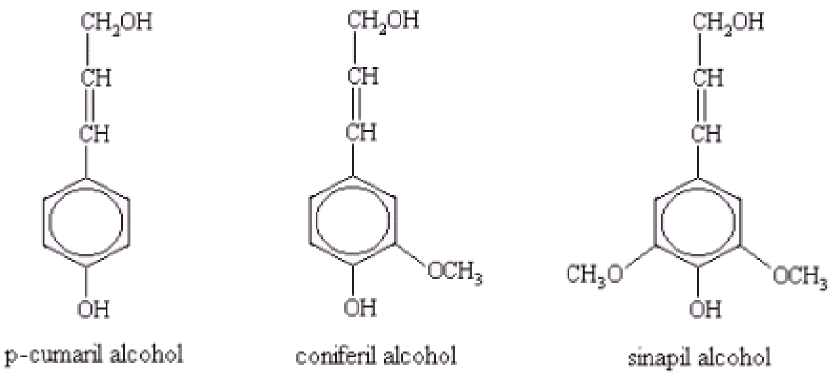

Figure 2.8 Chemical structure of the main component of lignin

2.5 Glycerol

2.5.1 Glycerol Overview

Glycerol (1.2.3-propanetriol) in Figure 2.9 is a colorless, odorless, viscous liquid with a sweet taste, derived from both natural and petrochemical feedstocks. The name glycerol is derived from the Greek word for ‘‘sweet,’’ *glykys*, and the terms glycerin, glycerine, and glycerol tend to be used interchangeably in the literature. On the other hand, the expressions glycerin generally refers to a commercial solution of glycerol in water of which the principal component is glycerol. Crude glycerol is 70–80% pure and is often concentrated and purified prior to commercial sale to 95.5–99% purity. Glycerol is virtually nontoxic in the digestive system and non-irritating to the skin and sensitive membranes, except in very high concentrations when a dehydrating effect is noted (Goshman, 1985).

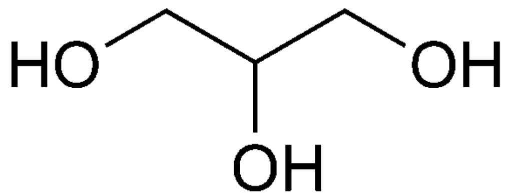

Figure 2.9 Chemical structure of Glycerol

Glycerol is one of the most versatile and valuable chemical substances known to man. It is completely soluble in water and alcohols, is slightly soluble in many common solvents such as ether and dioxane, but is insoluble in hydrocarbons (Gontard et al., 1993). In its pure anhydrous condition, glycerol has a specific gravity of 1.261gmL^{-1}, a melting point of 18.2°C and a boiling point of 290°C under normal atmospheric pressure, accompanied by decomposition. At low temperatures, glycerol may form crystals which melt at 17.9°C.

Glycerol contains three hydrophilic alcoholic hydroxyl groups, which are responsible for its solubility in water and its hygroscopic nature. It is a highly flexible molecule forming both intra- and intermolecular hydrogen bonds. Overall, it possesses a unique combination of physical and chemical properties as shown in Table 2.3, which are utilized in many ways of commercial products.(Parra et al., 2004) Indeed, glycerol has over 1500 known end uses, including applications as an ingredient or processing aid in cosmetics, toiletries, personal care products, pharmaceutical formulations and foodstuffs (Jouki et al., 2013).

Table 2.3 Physical and chemical properties of glycerol

Chemical formula	$C_3H_5(OH)_3$
Molecular mass	92.09382 g mol^{-1}
Density	1.261 g cm^{-3}
Melting point	18.2 °C
Boiling point	290 °C

Glycerol is highly stable under normal storage conditions, compatible with many other chemical materials, virtually non-irritating in its various uses, and has no known negative environmental effects. There are 126 possible conformers of glycerol, all of which have been characterized in a recent study using density functional theory (DFT) methods (Callam et al., 2001). In the aqueous phase, glycerol is stabilized by a combination of intramolecular hydrogen bonds and intermolecular solvation of the hydroxyl groups. This is due to the fact that in aqueous solution conformation, glycerol have higher relative energy, because all three hydroxyl groups are involved in intramolecular hydrogen bonding and are therefore unavailable to interact with the solvent. Many structures that possess intramolecular hydrogen bonding arrays still provide low energy conformations in aqueous solution, even when compared to structures without intramolecular hydrogen bonding (Segur and Oberstar, 1951).

In condensed phases, glycerol is characterized by a high degree of association because of hydrogen bonding. A first molecular dynamics simulation suggests that on average 95% of molecules in the liquid are connected (Chelli et al., 1999). This network is very stable and very rarely, especially at high temperature, releases a few short living (less than 0.5 ps) monomers. In the glassy state, a single hydrogen-bonded network is observed, involving 100% of the molecules present. A highly branched network of molecules connected by hydrogen bonds exists in all phases and at all temperatures. Crystallization of glycerol, which occurs at 18°C, cannot be directly achieved from the liquid state but requires special procedures. Due to the existence of such an extended hydrogen bonded network, the viscosity and the boiling point of glycerol are unusually high. Glycerol readily forms a supercooled liquid which, by lowering the temperature undergoes at about -89°C transition to a glassy state.

The intramolecular energy is the prevailing factor in determining the average molecular structure in the condensed phases. The intermolecular hydrogen bonds, however, do not significantly stabilize energetically gas phase structures. The activation energy for a conformational transition is much higher at room temperature