Preparation and Properties of Polyurethane Foams from Toluene Diisocyanate and Mixtures of Castor Oil and Polyol

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ABSTRACT

Castor oil is obtained by extracting the crushed seeds in a soxhlet extractor. The oil is characterized and used wholly in the preparation of polyurethane foam. Additionally, some polyurethane foams are prepared from mixtures of castor oil and polyol (hydroxy-terminated polyether). The mechanical properties of the foams are comparable to that in which 100% polyol is used. The use of 100% castor oil in foam synthesis produces a semi-rigid material that can be used in various applications.

Key Words: castor oil, polyol, toluene diisocyanate, polyurethane foam, mechanical properties

INTRODUCTION

Castor oil is obtained from the seed of a plant with the botanical name Ricinus Communis of the family Euphorbiaceae.

The oil contains mainly esters of 12-hydroxy-9-octadecanoic acid [1,2]; thus the presence of hydroxyl groups makes the oil suitable for use in urethane type reactions. Also, the hydrogen bonding of its hydroxyl group confers a high viscosity on the oil [2,3].

Although the oil is not edible, it is widely used as a starting material for many industrial products. Castor oil has been used in isocyanate reactions to make polyurethane elastomers [4], millable [5], castable [6,7], applicable as adhesives and coatings [8,9], and as polyurethane foams [10].

Also, the pyrolysis of castor oil at 700 °C under reduced pressure has been used to obtain heptaldehyde and undecylenic acid [11] while various treatments of the oil can be used to obtain sebacic acid and ω-aminoundecanoic acid [12].

In this paper we report the preparation and mechanical properties of some polyurethane foams from toluene diisocyanate and a mixture of castor oil and polyol. In addition, polyurethane foams are prepared each from 100% polyol and 100% castor oil to enable comparison to be made.

EXPERIMENTAL

Materials

Castor oil was obtained by extracting the crushed nuts with light petroleum ether at a temperature of 60 to 80 °C in a soxhlet extractor. The oil was then tested for colour, refractive index, specific gravity, iodine value, acid value, hydroxyl value, saponification value, water content and solubility in ethanol. The various test methods are described in the literature [3,13].

The following materials viz: toluene diisocyanate, TDI (80:20 of 2,4 and 2,6 isomers respectively), polyol, stannous octoate, dimethylaminoethanol, trichlorofluoromethane (TCFM) and silicone oil were kindly supplied by Vitafoam Nigeria Plc, Ikeja.

Synthesis of Polyurethane Foams

Polyol/castor oil, small amount of water, silicone oil (a foaming agent), stannous octoate, dimethylaminoethanol were mixed together. Afterwards, toluene diisocyanate was added to the mixture. The mixture was stirred with an electric stirrer to ensure good dispersion of reagents and a foam of desirable cell structure. Stirring continued until foaming commenced when the mixture was poured into a mould. The foam samples produced were left to stand for 24 hours before they were tested to ensure complete curing.

Mechanical Properties

Polyurethane samples were tested for tensile strength and elongation-at-break using a tensometer at room temperature, following the procedures of ASTM D 3489-81. The densities of samples were obtained by cutting out a known volume and obtaining the mass, and thereby calculating the density as mass per unit volume.

The colour of each sample was observed by visual examination while naked flame was also applied to each sample to observe burning characteristics. Compression set measurements were obtained according to the procedures of ASTM D 3574.

RESULTS AND DISCUSSION

General

The properties of the castor oil used are shown in Table 1. These properties do not deviate greatly from values available in the literature [1,3].

Table 1. Properties of castor oil.

Property	Value
Specific gravity (25 °C)	0.959
Appearance	clear
Refractive index (25 °C)	1.4764
Colour	yellow
Acid value	2
Hydroxyl value	164
Solubility in alcohol	complete
Iodine value	85
Water content (%)	0.3
Saponification value	178

Also the various polyurethane formulations and their respective properties are shown in Table 2. Formulation 1 constitutes a conventional polyurethane composition and it contains 100% polyol. The product of this formulation has a good texture and it is taken as the control formulation. Formulation 4 contains 100% castor oil as a substitute for polyol while formulations 2 and 3 contain 20% and 50% castor oil respectively.

It was observed that in all the products obtained, the intensity of the yellow colour increased with increase in the quantity of castor oil. This is directly attributable to the yellow colour of natural castor oil itself. However, in a separate experiment where bleached castor oil was used, the foam produced was colourless to white.

Effect of Material Variation on Foam Properties

The results (Table 2) show that with increasing quantity of castor oil in foam formulation, the tensile strength also increases except in the case of product from formulation 2.

The introduction of castor oil in formulations 2–4 lead to a dramatic increase in compression set. This could probably be due to the cleavage of rigid crosslinks formed between castor oil and toluene diisocyanate which prevents substantial elastic recovery. It then implies that foam formulations containing castor oil are not suitable for cushioning purposes since recovery from elastic deformation

Table 2. Polyurethane foam compositions and properties.

	php[a]			
	1	2	3	4
Foam composition				
Polyol	100	80	50	–
Castor oil	–	20	50	100
Hydroxyl value	48	71.2	106	164
TDI(TDI index=108)	46.2	50.6	56.4	66
Water	3.7	3.7	3.7	3.7
Amine (DMAE)	0.25	0.25	0.25	0.25
Silicone oil	1.0	1.0	1.0	1.0
Stannous octoate	0.25	0.25	0.25	0.25
TCFM	0.5	0.5	0.5	0.5
Property				
Density (kg/m^3)	24.68	23.03	31.98	61.02
Tensile strength (kN/m^2)	83.33	67.13	107.70	138.89
Compression set (%)	5.20	28.57	33.87	49.25
Elongation-at-break (%)	216.67	128.44	107.80	101.11
Colour (without pigment)	white	light yellow	yellow	dark yellow

[a] Parts per hundred parts of polyol, by weight.

will generally be poor. Among the four formulations, it is perhaps the properties of formulation 2 that is reasonably close to the control formulation. In other words, not more than 20% castor oil can be used as polyol substitute in foam applicable for cushioning.

Also, the results show a gradual decrease of the elongation-at-break with increase in the quantity of castor oil. This result is likewise due to the rigid crosslinks produced between toluene diisocyanate and castor oil. It is however unlikely that the foams will be subjected to an elongation greater than 100% in any practical application. The densities of the foams show an increase with increase in the quantity of castor oil.

It is to be noted that the properties of foam from formulation 4, where castor oil has been used wholly, compare reasonably well with properties of semi-rigid foams [14]. Thus, this type of foam can be used in thermal insulation, refrigeration packaging and transportation.

All the foam samples continued to burn when naked flame was applied and they can be classified as flammable.

Chemistry of the Synthesis Reaction

Isocyanates are extremely reactive and they react with materials containing active hydrogen.

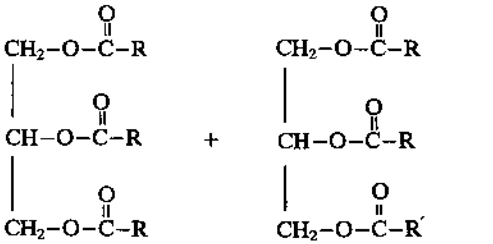
The reaction between a polyhydroxy compound (polyol) and a diisocyanate is the main reaction in foam synthesis and proceeds according to the general equation below:

$$(n+1)[OCN-R_1-NCO] + nHO-R_2-OH \longrightarrow$$

$$OCN[-R_1-NH\cdot \underset{\overset{\|}{O}}{C}O-R_2-O-\underset{\overset{\|}{O}}{C}\cdot NH-]R_1NCO$$

Castor oil, whose structure is shown according to Scheme 1 [4] to be a triol, can also react in the same way as shown above. Indeed, the reaction can proceed in three directions, leading to a large molecule that is rigidly held into a 3-dimensional structure.

Water, which is present in the formulations reacts with diisocyanate to liberate carbon dioxide and gives the foam a cellular structure. Also the activators are used to speed up the reaction.



where:

$R = -(CH_2)_7-CH=CH-CH(OH)-(CH_2)_5-CH_3$

$R' =$ other fatty acids.

Scheme 1

When trifunctional castor oil is reacted with toluene diisocyanate, a rigid structure is formed. Thus, with increasing castor oil in the formulations, there is increasing rigidity of the foam produced and consequently, the trend of mechanical properties described previously.

CONCLUSION

The investigations carried out so far indicate that foams synthesized from 100% castor oil and mixtures of castor oil and polyol do not compare with the foam produced using 100% polyol especially in compression set measurements. However, the investigations show that foams synthesized from 100% castor oil compare favourably with semi-rigid foams synthesized using polyol. The chemistry of polymerization is followed by the usual polyurethane chemistry. More important, castor oil can be used to substitute polyol in certain polyurethane foam manufacture.

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